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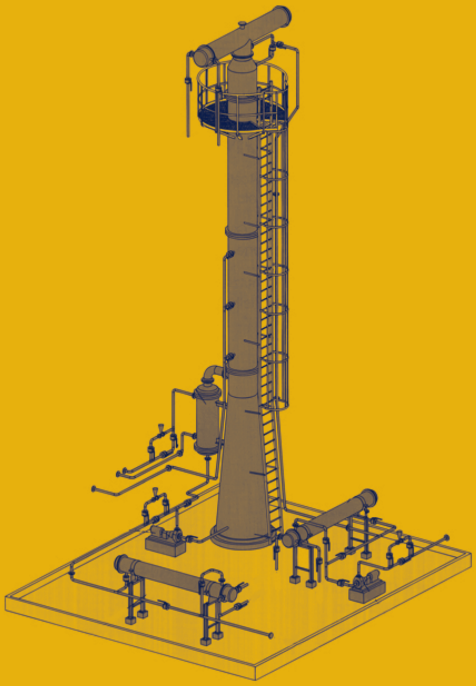

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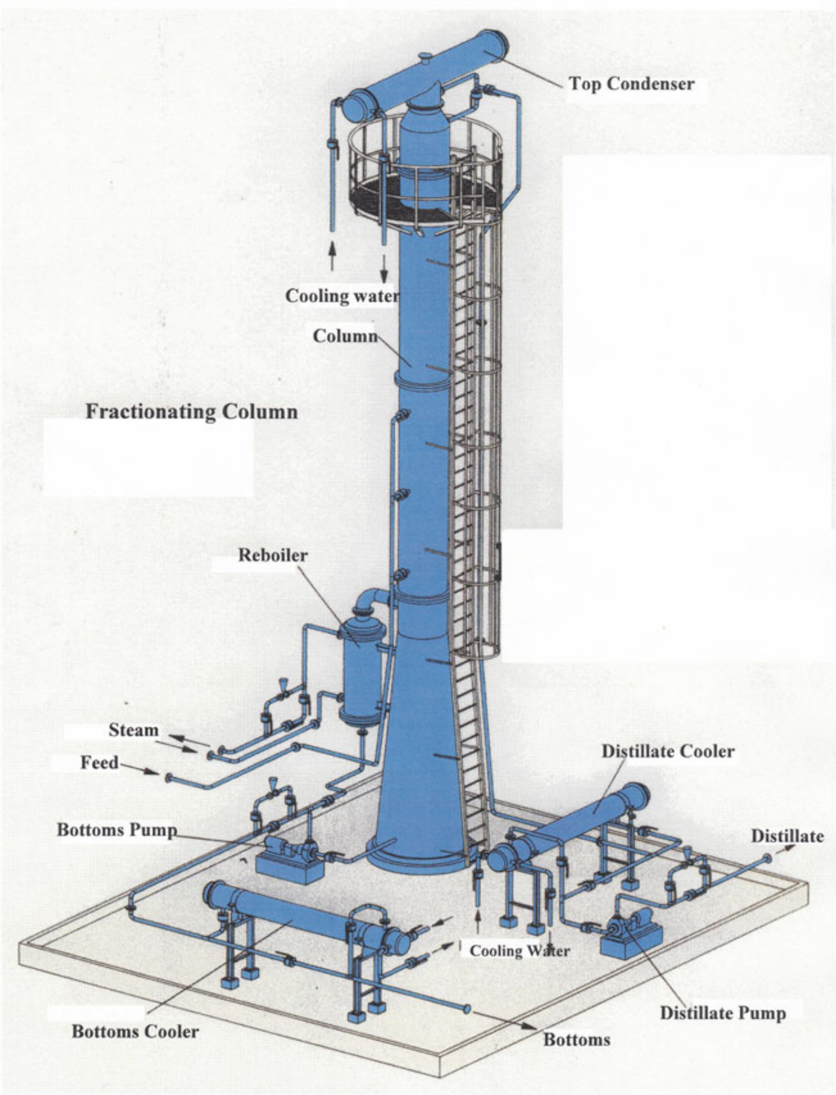

Fractionating Column

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Practical Column Design Guide

Springer

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Preface

Dear reader,

In this book the reader is shown the design aspects which must be considered when designing distillation columns in practice. The influencing parameters are presented, well explained and the equations governing them given. Several numerical examples are given. This book is written with a focus on both experienced designers as well as those who are new to the subject.

In spite of the multitude of available literature on distillation, a void still exists. Most of the existing works are academic. Hence there is a need for a book which covers the comprehensive information necessary to practically design distillation columns in a compact, clear and concise way. This book is written to fill this gap.

Today, computer programmes are used for column design. However, before the 1960s, in the pre-computer era, diverse distillation processes were also designed and operated including azeotropic distillation.

In those days the required number of trays and the reflux ratio were graphically determined with the McCabe–Thiele diagram or with Fenske–Underwood–Gilliland short cut methods.

While working with the McCabe–Thiele diagram on graph paper one appreciates the difficulty of separation.

Nowadays, you get computer output with all the data. The calculation results are generated very quickly. If the user does not have a thorough understanding of what the computer is asked to do, the user can easily misinterpret the output as an accurate design even if this is not the case. Some process simulators facilitate the trace of the calculation steps performed by the computer to a desired level. It is therefore possible to generate a very large output containing all the calculation steps. If desired, the user can then check each step by written calculation. However, this is very impractical due to the enormous effort involved. Following the guide given in this book, the designer will be able to develop the required skills needed for practical column design and will therefore be in a position to make a better judgement of the calculation results presented by the computer.

A very good understanding of the principles involved is inevitable. Starting with the selection of the appropriate equilibrium correlation, there is a great number of measured equilibrium data for the same material system. For instance, there are more than 100 for ethanol/water. Besides, different computer models also exist for the calculation of equilibrium. If another method for the calculation of the equilibrium is chosen, for instance, direct input of vapor pressure data or if different models are used for the equilibrium calculation, such as NRTL, Wilson, Uniquac or UNIFAC, the resulting required number of trays and reflux ratios will be different. Further inaccuracies occur in the determination of the efficiency of cross-flow trays or the HTU and HETP values in random and structure packed columns.

In Chap. 1 it is shown right from the start how small inaccuracies in equilibrium and in tray efficiency influence the calculated results. Often, an additional pilot plant distillation is required for the design, for instance if an odour or colour specification has to be met or if a potassium permanganate test has to be performed for methanol or if the water content specification is required in ppm.

A pilot plant distillation is recommended for extractive and azeotropic distillation in order to avoid product impurities by entrained or washing agents. A good fractionation can only be achieved at a uniform hydraulic loading. With pulsating reflux, an intermittent evaporation or a fluctuating vacuum in the column good fractionation is not achievable. In addition, proper functioning of the evaporator and the condenser without a pulsating stream is the prerequisite for a properly functioning distillation plant. An adequate process control system is very important for the given separation task, for instance the control of the pressure, the heating, the loading and the levels. With potentially explosive materials expolosions can occur (own experience) if the maximum allowable temperature is exceeded for a long period of time. All these important aspects of distillation column practical design, along with many more, are covered in this book.

Hamburg, Germany
2016

M. Nitsche
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Contents

Recommendation for Further Reading: Literature

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Chapter 1
Planning of Distillation and Absorption Columns

1.1 Planning Information

The basis for each plan of a distillation or absorption plant is the determination of the required number of trays and the required reflux ratio for fractionating, the required absorption fluid flow rate for absorption or the stripping gas flow rate.

These calculations are mostly performed with computers. However, care must be taken in the unchecked acceptance of a computer generated result.

There are several measured physical properties and measured vapour–liquid equilibrium data showing comparably deviating results. Small inaccuracies in vapour pressure or different equilibrium data or the choice of the calculation model for the equilibrium can result in substantial deviations in the design.

Figure 1.1 shows how the required number of trays and the reflux ratio change if the equilibrium is better or worse, by the order of 0.2%, than that assumed. Since the number of trays in an existing plant cannot be increased distillation has to be achieved with a higher reflux ratio, for instance, with $R = 20$ instead of $R = 15$, if the vapour–liquid equilibrium is worse.

Figure 1.2 shows the influence of tray efficiency on the required reflux ratio.

If the tray efficiency is poor the reflux ratio has to be increased, for instance from $R = 16$ to $R = 18.5$ for 60 trays, if the tray efficiency is only 75% rather than 80%.

The additional vapour and liquid loadings at a higher reflux ratio, due to poorer vapour–liquid equilibrium or poorer tray efficiency, must be considered while designing column internals. Sufficient reserve capacities must be available in the column.

Reboilers and condensers must be dimensioned for higher heat loads at higher reflux ratios.

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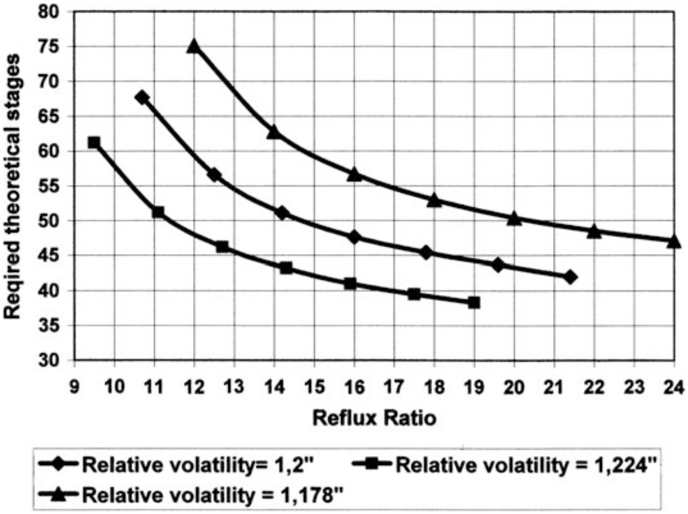
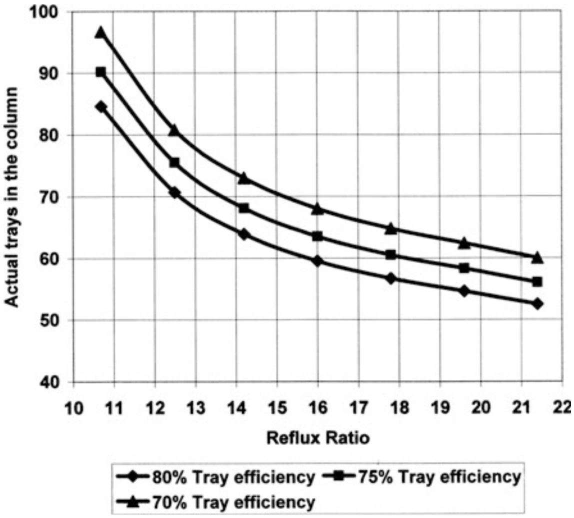


Fig. 1.1 Required theoretical trays as a function of the reflux ratio for different relative volatilities

Fig. 1.2 Actual trays required for different tray efficiencies



Rules for a trouble-free operation

The flow chart in Fig. 1.3 shows the required accessories for a distillation plant. Each individual piece of equipment, each pump, each control valve, each vessel and each component of piping must be accurately designed and its control system must function properly:

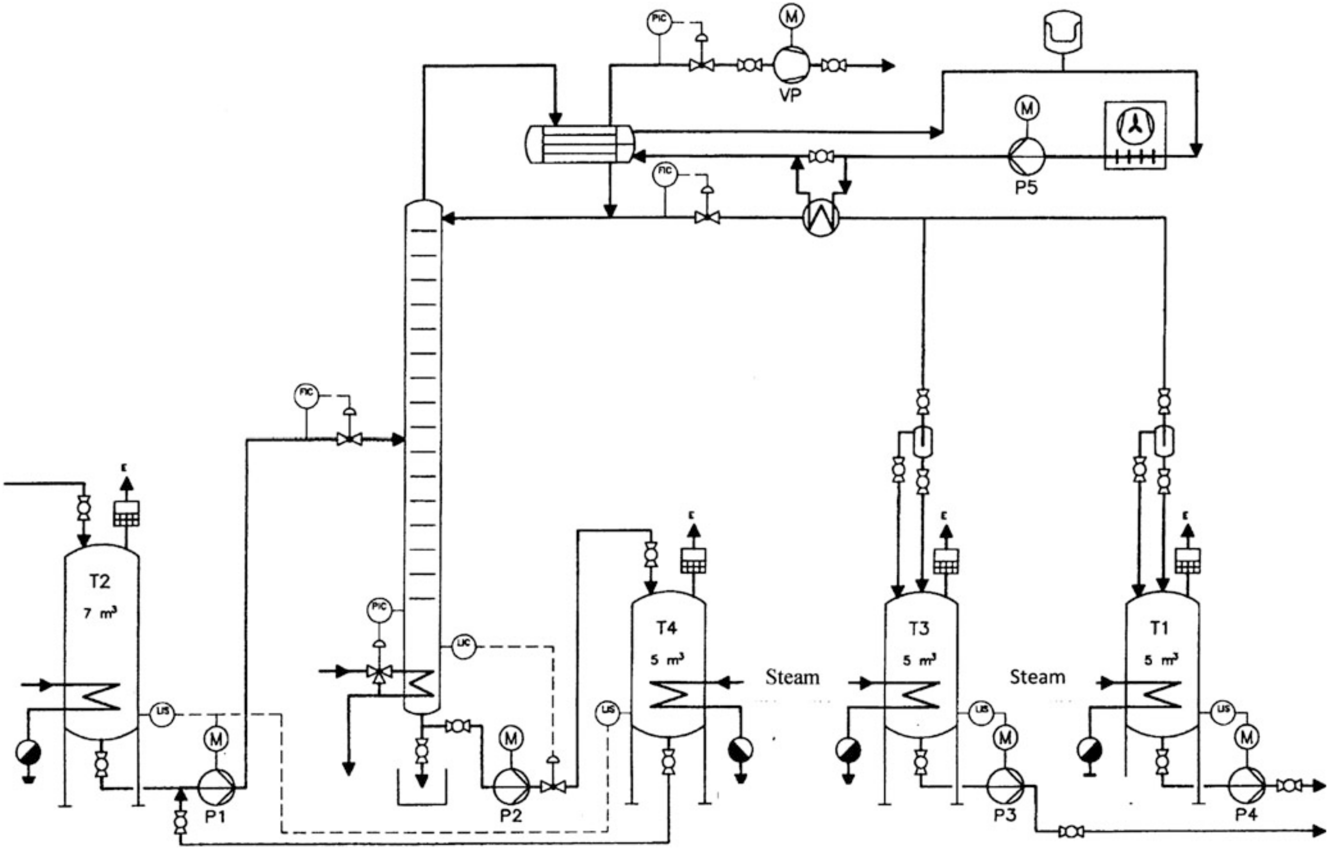


Fig. 1.3 Fractionation column with feed and product vessels

- A sufficient feed height must be present for top condensers in order to avoid reflux variations [2].
- Where there is condensation in tubes, for instance in air coolers, the maximal vapour flow capacity of the condenser must be determined with an adiabatic flow factor [1, 2].
- The outlet pipe from the condenser to the accumulator should be self-venting [1].
- Vibrations in the U-tube formed by the column and thermosiphon reboiler can be a problem. The frequency of the vibrations depend on the tube length. These vibrations can be removed by applying a greater pressure drop, for instance by using a larger circulation, or an orifice plate, in the downcomer.
- When drawing boiling liquids as side streams from the column, a sufficient liquid height over the nozzle must be provided in order to avoid flash evaporation in the withdrawal pipe [1].
- Measurement nozzles for temperature, pressure and level must be provided.
- The piping with flow meters and control valves must be accessible in the steel framework for maintenance purposes.
- Depending on the mass and energy balance and the available utilities, for instance 12-bar of steam and cooling water at 25 °C, the reboilers, condensers and heat exchangers used for heating the feed and cooling the distillate and bottoms streams must be appropriately dimensioned [2].
- When using the pumps the required Net Positive Suction Head (NPSH) value must be kept in order to avoid cavitation [1].
- In practice the columns are installed on 3-m foundations in order to provide sufficient liquid height.
- If the boiling point is higher than the temperature of the given heating medium the vacuum distillation has to be adopted.
- In order to decide on the dimensions of the vacuum pump the required suction pressure and the required suction capacity is needed [3]. There should be a minimum pressure drop in the vacuum piping.
- The choice of the column internals should be determined using the allowable pressure loss and the available construction height, for instance in a production hall.
- Demisters should be used in order to minimize the loss of valuable materials and to protect the vacuum pumps and compressors.
- When deciding upon the dimensions of the piping for the product and utility streams, high-pressure losses or cavitation on bottlenecks should be avoided [1].
- The control valves must be designed for a functional working pressure drop [1].
- If sharp reduction occurs in valves which are designed too large, choked flow with cavitation may occur in the valve.

Construction notes

- The columns must be calculated based on the pressure or vacuum and wind loads. The columns should not sway at high wind velocities.
- In construction, consideration must be given to how internals can be installed into the column (manways) and what type of support is necessary in the column.

- The support rings must have tight tolerances in order to allow an even installation of the trays or liquid distributors.
- The nozzles for the evaporator, condenser, feed and side streams or side strippers must be properly arranged.
- Sufficient flexibility must be provided for thermal expansion of hot piping in order to avoid large thermal stresses and protect the equipment and pump nozzles. Leakages must be avoided especially in the vacuum columns.
- In order to avoid heat loss, and to provide surface protection, hot surfaces are appropriately insulated, mostly with mineral wool mats [3].

What basic data are required for the design?

- Flow rates with physical properties and equilibrium data, compositions, temperatures and pressures.
- Heating and cooling medium along with temperatures and pressures: steam, organic heat transfer media, cooling water, cold water, and cooling brine.
- Required materials: steel, stainless steel, monel, plastic, and graphite.

1.2 Mass Balance for the Separation Task

The starting point for every separation calculation is a mass balance with the required component distributions.

Example 1.2.1: Mass balance for a four-component mixture

Component	Feed				Distillate			Bottoms		
	M	kg/h	kMol/h	x_E	kg/h	kMol/h	x_D	kg/h	kMol/h	x_B
Light comp.	78	1952	25	0.25	1952	25	0.48	0.0	0.0	0.0
LK	92.1	2303	25	0.25	2081	22.6	0.44	219	2.4	0.05
HK	106.1	2652	25	0.25	228	2.15	0.04	2425	22.85	0.48
Heavy comp.	104.1	2602	25	0.25	239	2.3	0.04	2580	24.77	0.47
		9508	100		4500	52.05		5008	47.95	

Conversions:

$$\text{kmol/h} = \frac{\text{kg/h}}{M}$$

M = mole weight
Average mole weight $M_m = \sum x_i * M_i$
Feed: $M_m = 95.075$
Distillate: $M_m = 86.37$
Bottoms: $M_m = 104.46$
LK = light key component

HK = heavy key component
x_E = feed compositions (molfraction)
x_D = distillate compositions (molfraction)
x_B = bottoms compositions(molfraction)

Conversion of weight, volume, and mole percentages

$$\text{Weight}\%A = \frac{\text{Vol}\%A * \rho_A}{\text{Vol}\%A * \rho_A + \text{Vol}\%B * \rho_B} \qquad \text{Vol}\%A = \frac{\text{Weight}\%A/\rho_A}{\text{Weight}\%A/\rho_A + \text{Weight}\%B/\rho_B}$$

$$\text{Weight}\%A = \frac{\text{Mol}\%A * M_A}{\text{Mol}\%A * M_A + \text{Mol}\%B * M_B} \qquad \text{Mol}\%A = \frac{\text{Weight}\%A/M_A}{\text{Weight}\%A/M_A + \text{Weight}\%B/M_B}$$

$$\text{Molfraction } A = \frac{\text{Mol}\%}{100} \qquad \text{Weightfraction } A = \frac{\text{Weight}\%}{100}$$

1.3 Separation Conditions

First, the pressure and temperature in the column have to be fixed for the given problem definition.

- With a steam heated reboiler the boiling temperature in the bottom should be at least 20 °C below the dew point temperature of the available heating steam. A remedial measure for lowering the boiling temperature is vacuum distillation.
- Often the bottom temperature must not exceed a certain value in order to avoid thermal cracking of the product. One supporting measure for lowering the boiling temperature is vacuum distillation.
- A high pressure drop in the column, for instance from bubble cap trays with large slot seals, increases the bottom pressure and therefore increases the boiling temperature. One remedial measure is to have column internals demonstrating low pressure losses, for instance random or structured packing.
- With low top temperatures, for instance those under 30 °C, chilled water must be used to cause condensation. Alternatively, a higher pressure would also increase the dew point.

The decision becomes difficult if in the bottom a high boiling material can only be evaporated under vacuum and the separated low-boiling component on the top can only be condensed under pressure (e.g., stripping of gasoline from gasoil in order to improve its flash point). One remedial measure is steam-stripping distillation.

1.4 Vapour-Liquid Equilibrium [4]

The appropriate equilibrium- and physical property models must be chosen for the given mixture.

1.4.1 The Ideal Equilibrium According to Raoult–Dalton

1.4.2 Equations of State

The equation of states being: Benedict–Webb–Rubin for KWST C_1 to C_7 (BWR); Soave–Redlich–Kwong (SRK) for hydrocarbons; Redlich-Kwong (RK); and Peng–Robinson (PR) for small non-polar molecules

1.4.3 Equilibrium Models for Non-polar Materials Considering the Non-ideal Behaviour in the Liquid Phase Based on Pure Component Data

The models include: Chao–Seader (CS) for hydrocarbons from −20 to 260 °C and Grayson–Streed (GS) | CS with corrected data for higher temperatures and pressures, which is better suited to mixtures containing hydrogen.

1.4.4 Equilibrium Models for Polar Components with High Non-ideal Behaviour in the Liquid Phase

Here is a list of models with interaction parameters from measured vapour–liquid equilibria data for mixtures: Margules; van Laar; Wilson; NRTL; Uniquac; and UNIFAC (which is a group contribution method for structural groups).

1.5 Energy and Mass Balance in the Column

These balances are required for the fluid dynamic design of stages or packings and for the dimensioning of reboilers and condensers.

1.5.1 Mass Balance (Fig. 1.4)

In the rectification section—the section of the column above the feed stage—results from the vapour and liquid loading from the distillate flow rate and the reflux ratio. The loadings in kg/h or kMol/h are constant if the molar latent heat does not change and if no side draws exist. If the reflux feedback to the column is subcooled the vapour and liquid loadings increase. In the stripping section—the section of the column under the feed stage—the heat loss of the column must be additionally considered as must the thermal condition of the feed which is characterized by the q-value.

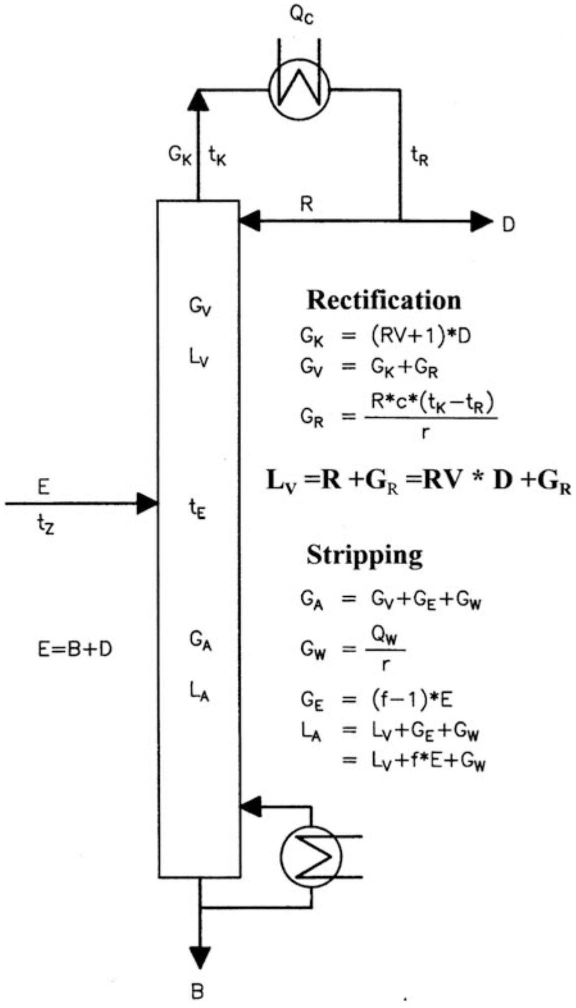


Fig. 1.4 Mass balance of a fractionation column

Due to the fact that the feed rate is mostly fed into the column in a subcooled condition the vapour and liquid flow rates in the stripping section increase accordingly.

It has to be considered that, over the length of the column, the physical properties change as a function of pressure, temperature, and composition. In particular, in **vacuum distillation columns**, the vapour volume changes greatly as pressure changes due to the pressure loss at the stages.

Example 1.5.1

Here is a calculation of the vapour loading for 2500 kg/h vapour at different pressures.

At column top	10 stages below
P = 6.65 mbar	P = 26.6 mbar
T = 185 °C	T= 220 °C
ϱ_D = 0.0473 kg/m^3	ϱ_D = 0.178 kg/m^3
V = 52,854 m^3/h	V = 14,045 m^3/h

where T = temperature; P = pressure; V = vapour volume (m^3/h); and ϱ_D = vapour density (kg/m).

At the top of the column the vapour loading is greater than 10 stages below by a factor of 3.7.

In a 3.5 m diameter column the vapour flow velocity at the top of the column is 1.52 m/s and 10 stages below it is only 0.4 m/s.

Checks must be completed to identify if the separation is hindered by droplet entrainment at high vapour flow velocities or by weeping at low gas flow velocities.

Explanations for the mass and energy balances in Figs. 1.4 and 1.5

Rectification section:

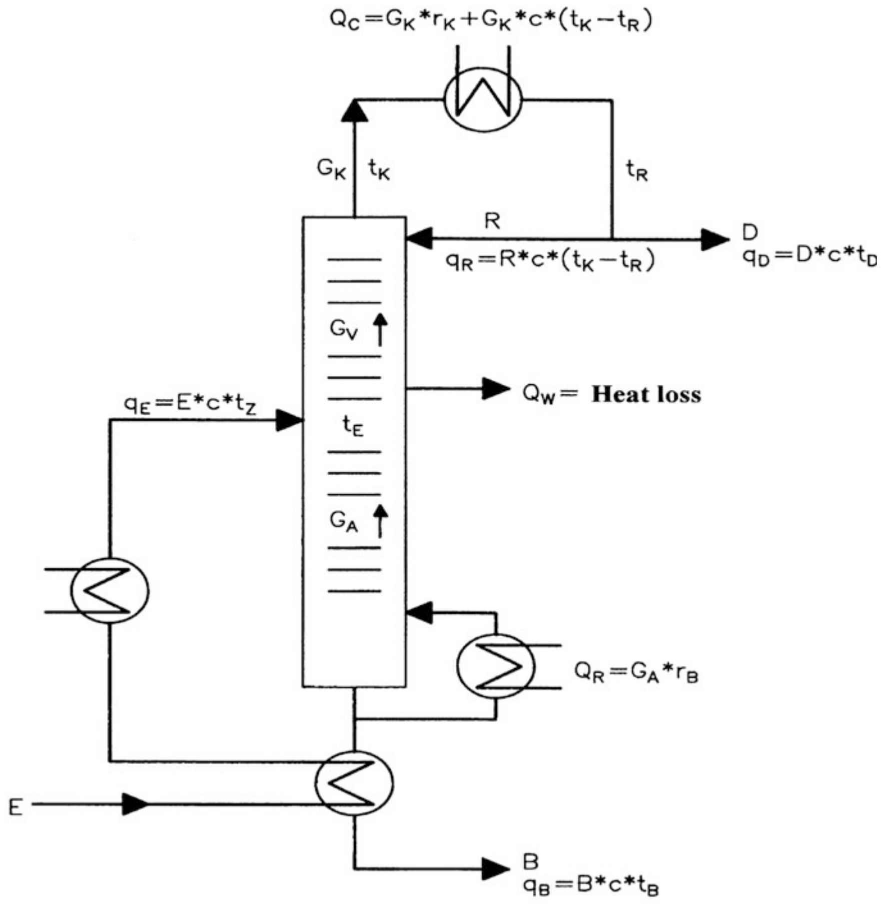
D = distillate flow rate (kg/h)
E = feed flow rate (kg/h)
G_K = vapour flow rate to the condenser = (RV + 1) * D (kg/h)
RV = reflux ratio
G_V = vapour flow rate in the stripping section = G_K + G_R (kg/h)
G_R = vapour flow rate for heating the reflux to top temperatures

$$G_R = \frac{R * c * (t_K - t_R)}{r} \text{ (kg/h)}$$

R = reflux flow rate (kg/h)
c = specific heat capacity (Wh/kg K)
t_K = column top temperature (°C)
t_R = reflux temperature (°C)
L_V = liquid flow rate in the stripping section = R + G_R = RV * D + G_R (kg/h).

Stripping section:

B = bottom draw flow rate (kg/h)
G_A = vapour flow rate in the stripping section = G_V + G_E + G_W (kg/h)
G_E = vapour flow rate for heating the feed (E) from the feed temperature (t_Z) to the column temperature (t_E) on the feed stage
E = feed flow rate (kg/h)



$$\begin{aligned} Q_R - Q_C &= q_D + q_B - q_E + q_V \\ Q_R + q_E &= Q_C + q_D + q_B + q_V \\ Q_R &= Q_C + q_D + q_B + q_V - q_E \\ Q_C &= Q_R + q_E - q_D - q_B - q_V \end{aligned}$$

Fig. 1.5 Energy balance for a fractionation column

G_W = vapour flow rate for balancing the heat losses (kg/h)
r = latent heat (Wh/kg)
L_A = liquid flow rate in the stripping section (kg/h).

Energy:

Q_C = condensation duty = $G_K * (r + c * (t_K - t_R))$ (W)
r = latent heat (Wh/kg)
c = specific heat capacity (Wh/kgK)
t_K = top temperature (°C)

t_R = reflux temperature (°C)
q_R = heating load for the reflux (R)
$q_R = R * c * (t_K - t_R)$ (W)
q_D = heat content of the distillate (D)
$q_D = D * c * t_D$ (W)
D = distillate flow rate (kg/h)
t_D = distillate temperature (°C)
q_E = heat content of the feed
$q_E = E * c * t_Z$ (W)
t_Z = feed temperature (°C)
t_B = bottom draw temperature (°C)
q_B = heat content of the bottom draw (B)
$q_B = B * c * t_B$ (W)
Q_R = reboiler duty = $G_A * r$ (W) = $Q_C + q_D + q_B + q_V - q_E$ (W)
G_A = vapour flow rate in the stripping section (kg/h)
$q_V = Q_W$ = heat loss of the column (W).

When determining the flow loadings in the rectification and stripping sections the thermal condition q of the feed mixture must be considered. This q value also has an influence on the required number of theoretical stages. The calculation of the q value is covered in Chap. 3.

q = 1 for the liquid feed at bubble point temperature.
q = 0 for the vapour feed at dew point temperature.
q = 0.75 for a two-phase mixture with 75% liquid.
q < 0 for superheated vapour.
q > 1 for the liquid feed below the bubble point temperature.

Calculation formula for the loading in the column:

$$\begin{aligned} G_V &= (RV + 1) * D = G_A + (1 - q) * E \text{ (kg/h)} \\ L_V &= RV * D \text{ (kg/h)} \\ G_A &= G_V - (1 - q) * E = L_A - B \text{ (kg/h)} \\ L_A &= L_V + q * E \text{ (kg/h)} \\ G_V - G_A &= (1 - q) * E \text{ (kg/h)} \\ L_A - L_V &= (1 - q) * E \text{ (kg/h)}. \end{aligned}$$

1.5.2 Energy Balance (Fig. 1.5)

The required heating energy is supplied by the reboiler with the necessary cooling energy by the condenser. Within the column the heating energy is transported with the vapour and the cooling energy with the liquid. For a subcooled reflux or a cold feed more vapour is needed to heat the liquid. The condensed vapour for heating increases the exiting liquid flow rate. The calculation equations listed in Figs. 1.4

and 1.5 are used whilst preparing the energy and mass balances. The use of these equations is shown in the following examples.

Example 1.5.2.: Flow and energy balance of a distillation column

Calculation data:

Feed flow rate, E = 2467 kg/h
Distillate flow rate, D = 740 kg/h
Bottom draw flow rate, B = 1727 kg/h
Feed temperature, t_Z = 174 °C or 90 °C
Temperature at the feed stage, t_E = 174 °C
Top temperature, t_K = 160 °C
Bottom temperature, t_B = 210 °C
Latent heat, r = 100 Wh/kg
Specific heat capacity, c = 0.4 Wh/kgK
Reflux ratio, RV = 12.5
Reflux temperature, t_R = 160 °C or 153 °C.

Example 1.5.2.1: Mass and energy balance for liquid feed with a bubble point temperature (q = 1) Without heat loss

$$t_R = t_K = 160\,^\circ\mathrm{C} \quad t_Z = t_E = 174\,^\circ\mathrm{C} \quad q = 1 \quad \mathrm{RV} = 12.5 \quad q_V = Q_W = 0\,\mathrm{W}$$

Mass balance in the rectification section:

Vapour flow rate in the rectification section, G_V = (RV + 1) * D = (12.5 + 1) * 740 = 9990 kg/h
Liquid flow rate in the rectification section, L_V = RV * D = 12.5 * 740 = 9250 kg/h

Mass balance in the stripping section:

Vapour flow rate, $G_A = G_V - (1 - q) * E$ = 9990 − (1 − 1) * 2467 = 9990 kg/h
Liquid flow rate, $L_A = L_V + q * E$ = 9250 + 1 * 2,467 = 11,717 kg/h
Bottom draw flow rate $B = L_A - G_A$ = 11,717–9990 = 1727 kg/h
Distillate flow rate $D = E - B$ = 2467 − 1727 = 740 kg/h

Energy balance:

$$\text{Condenser duty, } Q_C = G_K * r = 9990 * 100 = 999{,}000\,\mathrm{W}$$

$$\text{Reboiler duty } Q_R = Q_C + q_D + q_B + q_V - q_E$$

Distillate heat $q_D = D * c * t_D$ = 740 * 0.4 * 160 = 47,369 W
Bottom draw heat $q_B = B * c * t_B$ = 1727 * 0.4 * 210 = 145,068 W
Feed heat $q_E = E * c * t_E$ = 2467 * 0.4 * 174 = −171,703 W

$$Q_R = 999{,}000 + 47{,}369 + 145{,}068 + 0 - 171{,}703 = 1{,}019{,}734\,\mathrm{W}$$

Cross-check:

$$G_A = \frac{1019734}{100} = 10197\ \mathrm{kg/h}\ >\ 9990\ \mathrm{kg/h}$$

$$L_A = G_A + B = 10{,}197 + 1727 = 11{,}924\,\mathrm{kg/h} > 11{,}717\,\mathrm{kg/h}$$

For energy balances, insignificant higher vapour and liquid loadings result in the stripping section at q = 1.

Example 1.5.2.2: Mass and energy balance for vapour feed at dew point temperature (*q* = 0) without heat losses

$$t_R = t_K = 160\,^\circ\mathrm{C} \quad t_Z = t_E = 174\,^\circ\mathrm{C} \quad q = 0 \quad \mathrm{RV} = 12.5 \quad q_V = Q_W = 0\,\mathrm{W}$$

Mass balance in the rectification section:

Vapour flow rate, $G_V = (\mathrm{RV} + 1) * D + (1 - q) * E$
Vapour flow rate $G_V = (12.5 + 1) * 740 + (1 - 0) * 2467 = 12{,}457$ kg/h
Liquid flow rate, $L_V = G_V - \mathrm{D} = 12{,}457 - 740 = 11{,}717$ kg/h
Distillate flow rate, $D = G_V - L_V = 12{,}457 - 11{,}717 = 740$ kg/h

Mass balance in the stripping section:

Vapour flow rate, $G_A = G_V - (1 - q) * E = 9990 - 0(1 - 0) * 2467 = 12{,}457 - 2467 = 9990$ kg/h
Liquid flow rate, $L_A = L_V + q * E = 11{,}717 + 0 * 2467 = 11{,}717$ kg/h
Bottom draw flow rate, $B = L_A - G_A = 11{,}717–9990 = 1727$ kg/h

Energy balance:

$$\text{Condenser duty, } Q_C = G_K * r = 12{,}457 * 100 = 1{,}245{,}700\,\mathrm{W}$$

$$\text{Reboiler duty, } Q_R = Q_C + q_D + q_B + q_V - q_E$$

Distillate heat $q_D = D * c * t_D = 740 * 0.4 * 160 = 47{,}360$ W
Bottom draw heat $q_B = B * c * t_B = 1727 * 0.4 * 210 = 145{,}068$ W
Feed heat $q_E = E * (c * t_E + r) = 2467 * (0.4 * 174 + 100) = 418{,}403$ W

$$Q_R = 1{,}245{,}700 + 47{,}360 + 145{,}068 + 0 - 418{,}403 = 1{,}019{,}725\,\mathrm{W}$$

Cross-check:

$$G_A = \frac{1{,}019{,}725}{100} = 10{,}197\ \text{kg/h} > 9990\ \text{kg/h}$$

$$L_\text{A} = G_\text{A} + B = 10{,}197 + 1727 = 11{,}924\,\text{kg/h} > 11{,}717\,\text{kg/h}$$

With the energy balance, insignificant higher vapour and liquid loadings result in the stripping section.

Example 1.5.2.3: Mass and energy balance for q = 0.75 (25% vapour) and Q_W = 0

$$t_\text{R} = t_\text{K} = 160\ ^\circ\text{C}\ t_\text{Z} = t_\text{E} = 174\,^\circ\text{C}\ q = 0.75 \quad \text{RV} = 12.5 \quad q_\text{V} = Q_\text{W} = 0\,\text{W}$$

Mass balance in the rectification section:

Vapour flow rate, G_V = (RV + 1) * D + (1 − q) * E = (12.5 + 1) * 740 + (1 − 0.75) * 2467 = 10,607 kg/h
Liquid flow rate, L_V = G_V − D = 10,607 − 740 = 9867 kg/h
Distillate flow rate, D = G_V − L_V = 10,607 − 9867 = 740 kg/h

Mass balance in the stripping section:

G_A = G_V − (1 − q) * E = 10,607 − (1 − 0.75) * 2467 = 10,607 − 617 = 9990 kg/h vapour
L_A = L_V + q * E = 9867 + 0.75 * 2467 = 11,717 kg/h liquid in the striping section
Bottom draw, B = L_A − G_A = 11,717–9990 = 1727 kg/h bottom draw flow rate

Energy balance:

$$\text{Condenser duty},\ Q_\text{C} = G_\text{K} * r = 10{,}607 * 100 = 1{,}060{,}700\,\text{W}$$

$$\text{Reboiler duty},\ Q_\text{R} = Q_\text{C} + q_\text{D} + q_\text{B} + q_\text{V} - q_\text{E}$$

Distillate heat q_D = D * c * t_D = 740 * 0.4 * 160 = 47,360 W
Bottom draw heat q_B = B * c * t_B = 1727 * 0.4 * 210 = 145,068 W
Feed heat q_E = E * (c * t_E + (1 − q) * r) = 2467 * (0.4 * 174 + 25) = 233,378 W

$$Q_\text{R} = 1{,}060{,}700 + 47{,}360 + 145{,}068 + 0 - 233{,}378 = 1{,}019{,}750\,\text{W}$$

Cross-check:

$$G_A = \frac{1019750}{100} = 10197\ \text{kg/h}\ >\ 9990\ \text{kg/h}$$

$$L_A = G_A + B = 10{,}197 + 1727 = 11{,}924\ \text{kg/h} > 11{,}717\ \text{kg/h}$$

With the energy balance, insignificant higher vapour and liquid loadings result in the stripping section.

Example 1.5.2.4: Mass and energy balance for q = 1 considering a heat loss of Q_W = 60 kW in the column

$$t_R = t_K = 160\,^\circ\text{C} \quad t_Z = t_E = 174\,^\circ\text{C} \quad q = 1 \quad \text{RV} = 12.5 \quad q_V = Q_W = 60\,\text{kW}$$

Mass balance in the rectification section:

Vapour flow rate, G_V = (RV + 1) * D + (1 − q) * E = (12.5 + 1) * 740 + (1 − 1) * 2467 = 9990 kg/h
Liquid flow rate, L_V = G_V − D = 9990 − 740 = 9250 kg/h = RV * D = 12.5 * 740
Distillate flow rate, D = G_V − L_V = 9990–9250 = 740 kg/h

Mass balance in the stripping section with G_W for the heat loss Q_W = q_V = 60 kW

$$G_W = \frac{Q_W}{r} = \frac{60000}{100} = 600\ \text{kg/h}$$

Vapour flow rate, G_A = G_V − (1 − q) * E + G_W = 9990 − (1 − 1) * 2467 + 600 = 10,590 kg/h
Liquid flow rate, L_A = L_V + q * E + G_W = 9250 + 1 * 2467 + 600 = 12,317 kg/h
Bottom draw flow rate, B = L_A − G_A = 12,317 − 10,590 = 1727 kg/h

Energy balance:

$$\text{Condenser duty, } Q_C = G_K * r = 9990 * 100 = 999{,}000\,\text{W}$$

Distillate heat q_D = D * c * t_R = 740 * 0.4 * 160 = 47,360 W
Bottom draw heat q_B = B * c * t_B = 1727 * 0.4 * 210 = 145,068 W
Feed heat q_E = E * c * t_Z = 2467 * 0.4 * 174 = 171,703 W
Heat loss Q_W = q_V = 60,000 W

$$\text{Reboiler duty, } Q_R = Q_C + q_D + q_B + Q_W - q_E$$

$$Q_R = 999{,}000 + 47{,}360 + 145{,}068 + 60{,}000 - 171{,}703 = 1{,}079{,}725\,\mathrm{W}$$

Required vapour flow rate to bring the required heat from the bottom:

$$G_A = \frac{1{,}079{,}725}{100} = 10{,}797\ \mathrm{kg/h}\ >\ 10{,}590\ \mathrm{kg/h}$$

$$L_A = G_A + B = 10{,}797 + 1727 = 12{,}524\,\mathrm{kg/h} > 12{,}317\,\mathrm{kg/h}$$

With this energy balance, rather higher vapour and liquid loadings result in the stripping section due to heat losses.

Example 1.5.2.5: Mass and energy balance for real conditions with heat loss, subcooled reflux, and subcooled feed

$$t_Z = 90\,°\mathrm{C} \quad t_R = 153\,°\mathrm{C} \quad q = 1336 \quad \text{heat loss}\, Q_W = q_V = 60\,\mathrm{kW}$$

Mass balance in the rectification section considering the subcooled reflux:

$$\text{Reflux rate}\, R = \mathrm{RV} * D = 12.5 * 740 = 9250\,\mathrm{kg/h}$$

Calculation of the vapour flow rate, G_R, for heating the subcooled reflux to the top temperature:

$$G_R = \frac{R * c * (t_K - t_R)}{r} = \frac{9250 * 0.4 * (160 - 153)}{100} = 259\ \mathrm{kg/h}$$

Vapour flow rate, G_V = (RV + 1) * D + G_R = (12.5 + 1) * 740 + 259 = 10,249 kg/h
Liquid flow rate, L_V = R + G_R = 9250 + 259 = 9509 kg/h
Distillate flow rate, D = G_V − L_V = 10,249 − 9509 = 740 kg/h.

Mass balance in the stripping section considering the heat loss of the column and the subcooled feed:

$$\text{Heat loss of the column, } Q_W = q_V = 60{,}000\,\mathrm{W}$$

Required vapour flow rate, G_W, to balance the heat loss

$$G_W = \frac{Q_W}{r} = \frac{60{,}000}{100} = 600\ \mathrm{kg/h}$$

Calculation of the q value for the subcooled feed with 90 °C

$$q = 1 + \frac{0.4 * (174 - 90)}{100} = 1,336$$

Calculation of the vapour flow rate, G_E, for heating the subcooled feed to the bubble point temperature of the feed stage:

$$G_E = (q - 1) * E = (1.336 - 1) * 2.467 = 828.9\,\text{kg/h}$$

Vapour flow rate, $G_A = G_V + G_E + G_W = 10{,}249 + 828.9 + 600 = 11{,}677.9$ kg/h

Vapour flow rate, $G_A = G_V - (1 - q) * E + G_W = 10{,}249 - (1 - 1.336) * 2467 + 600 = 11{,}677.9$ kg/h

Liquid flow rate, $L_A = L_V + (q * E) + G_W = 9{,}509 + 1{,}336 * 2{,}467 + 600 = 13{,}404.9$ kg/h

Bottom draw flow rate, $B = L_A - G_A = 13{,}404.9 - 11{,}677.9 = 1727$ kg/h

Energy balance:

$$\text{Condenser duty, } Q_C = G_K * (r + c * (t_K - t_R)) = 9990 * [100 + 0.4 * (160 - 153)] = 1{,}026{,}972\,\text{W}$$

Distillate heat $q_D = D * c * t_R = 740 * 0.4 * 153 = 45{,}288$ W

Draw stage heat $q_B = B * c * t_B = 1727 * 0.4 * 210 = 145{,}068$ W

Feed heat $q_E = E * c * t_Z = 2467 * 0.4 * 90 = 88{,}812$ W

Heat loss $Q_W = q_V = 60{,}000$ W

Reboiler duty $Q_R = Q_C + q_D + q_B + Q_W - q_E$

$$Q_R = 1026{,}972 + 45{,}288 + 145{,}068 + 60{,}000 - 88{,}812 = 1{,}188{,}516\,\text{W}$$

Required vapour flow rate to bring the required heat to the bottom:

$$G_A = \frac{1{,}188{,}516}{100} = 11{,}885\ \text{kg/h} > 11{,}677.9\ \text{kg/h}$$

$$L_A = G_A + B = 11{,}885 + 1727 = 13{,}612\,\text{kg/h} > 13{,}404.9\,\text{kg/h}$$

With this energy balance, slightly higher vapour and liquid loadings result for the stripping section.

1.5.3 Required Column Diameter

The required flow cross section, A, in the column or the column diameter, D, for the vapour flow rates, G_V and G_A, in the rectification and stripping section are determined with the F factor (see Chaps. 9 and 10)

$$A = \frac{G(\text{kg/h})}{3600 * F * \sqrt{\rho_\text{V}}} = \frac{G}{3600 * w * \rho_\text{V}} (\text{m}^2) \qquad F = w * \sqrt{\rho_\text{V}}$$

$$D = \sqrt{\frac{4 * A}{\pi}} (\text{m})$$

where A = flow cross section (m^2); D = column diameter (m); w = vapour flow velocity (m/s); and ρ_D = vapour density (kg/m^3)

Example 1.5.3.1: Determination of the required column diameter

$$G_\text{V} = 5000\,\text{kg/h} \quad F = 1.2 \quad \rho_\text{V} = 1.45\,\text{kg/m}^3$$

$$w = \frac{F}{\sqrt{\rho_\text{V}}} = \frac{1.2}{\sqrt{1.45}} = 1 \text{ m/s}$$

$$A = \frac{5000/3600}{1.2 * \sqrt{1.45}} = 0.96 \text{ m}^2 = \frac{5000/3600}{1 * 1.45} = 0.96 \text{ m}^2$$

$$D = \sqrt{\frac{0.96 * 4}{\pi}} = 1.1 \text{ m}$$

1.6 Selection of Column Internals

In selecting the column internals the following points have to be considered: throughput capacity, pressure loss, number of separation stages, side draw facility, fouling dangers (for instance, by residue or tar).

The internals determine the required height of the column. For instance you may have a 13-m high column for 50 theoretical stages with gauze packing or 25-m high column for 50 theoretical stages with cross flow stages.

Design criteria

Random packed and structured packed columns:

HTU value = packing height for a transfer unit (m packing)
HETP value = packing height for a theoretical stage (m packing)
Flooding factor and pressure drop
Minimum irrigation rate
Internals: support plates, liquid distributors, liquid collectors and redistributors, and gas distributors

Design information:

Random packing: NT = 1.5–2 theoretical stages per metre of packing height
Sheet packing: NT = 2–3 theoretical stages per metre of packing height

Gauze packing: NT = 4–5 theoretical stages per metre of packing height
Ratio of column diameter/packing diameter ≈ 10: 1
Gas loading factor, $F = w * \sqrt{\rho_G} = 2-2.5$
Liquid loading ~4–80 m^3/m^2h
Pressure drop ~1–4 mbar/m
A good liquid distribution is very important for to the overall effectiveness of the process.

Tray columns:

NT = 1.6 theoretical stages per metre of column height for valve, sieve, tunnel, or bubble cap trays
Allowable vapour velocities in view of entrainment and pressure drop
Dimensioning of the downcomer area for the liquid

Design information:

Gas loading factor, $F = w * \sqrt{\rho_G} = 1.5-2.$
Gas velocity = 80% of w_{max}.
Determination of the column diameter assuming an 80% active area for the vapour and a 20% active area for the liquid downcomer.
Free hole area ~8–10% of the cross sectional area.
Weir height ~30–60 mm.
Weir overflow height ~5–40 mm.
Tray spacing ~400–600 mm.

Cross-check calculations for weeping, entrainment, and flooding for all column cross sections with different vapour and liquid loadings should be carried out. In Chaps. 9 and 10 the fluid dynamic dimensioning is covered in detail.

1.7 Condensers [2]

The selection of an adequate condenser and the calculation of dew and bubble points as well as the condensation lines and the determination of the heat transfer, and overall heat transfer, coefficients for a given problem are dealt with in numerous examples found in the "Heat Exchanger Design Guide" [2].

The different condenser construction types are shown in Fig. 1.6:

- Condensation horizontal in shells or in the tubes.
- Condensation vertical in shells or in the tubes.

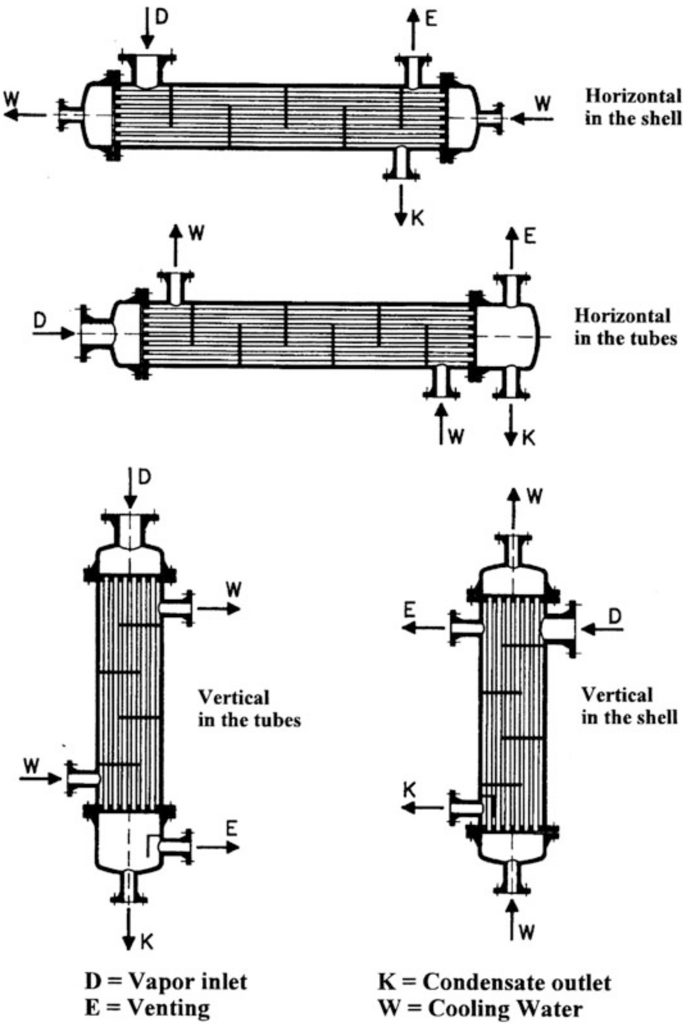


Fig. 1.6 Condenser construction types

1.8 Reboiler [2]

The different evaporator types are shown in Figs. 1.7 and 1.8. The advantages and disadvantages of the different construction types along with the designs with the calculations of the overall heat transfer coefficients are covered in the "Heat Exchanger Design Guide" [2]. Reboiler/evaporator types are:

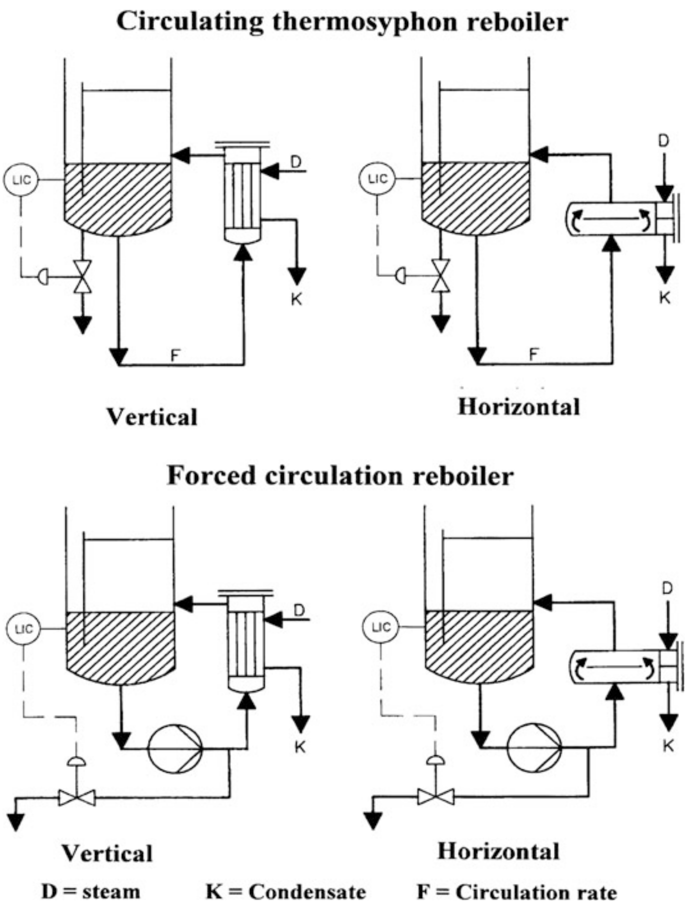


Fig. 1.7 Thermosiphon and forced circulation evaporators

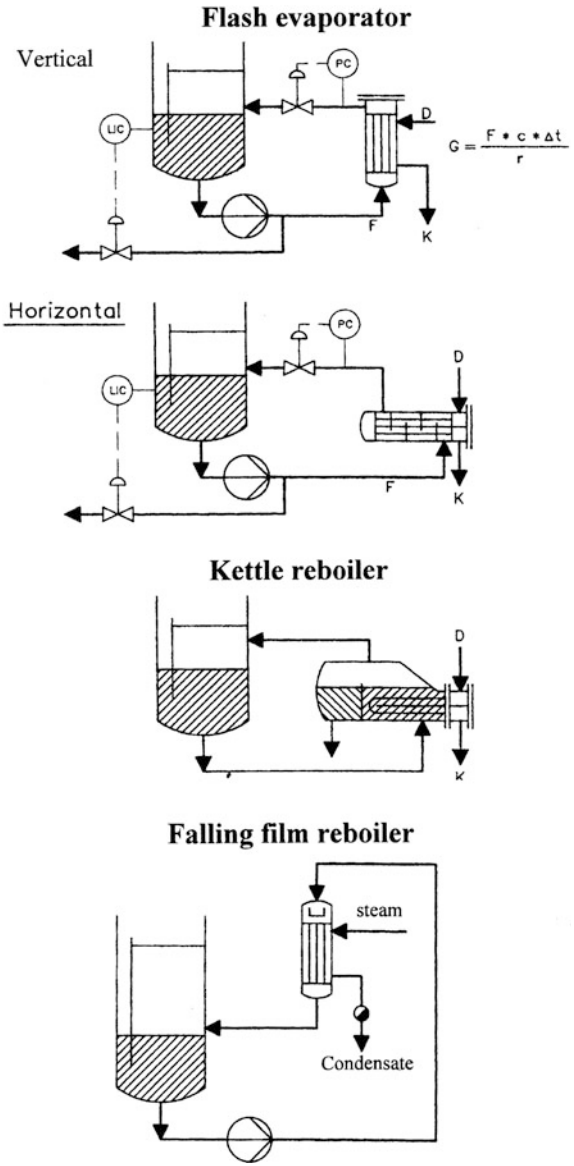
- Thermosiphon circulation reboiler, vertical or horizontal.
- Thermosiphon once-through reboiler, vertical or horizontal.
- Forced circulation and flash evaporator.
- Shell-and-tube and internal evaporators (heating coils).
- Falling film reboiler.

1.9 Vacuum Pumps [3]

First the required suction capacity is determined for a given problem and then a suitable vacuum pump, with a corresponding suction capacity at the required operating pressure, is selected.

In addition to the leak rate from leakages, non-condensable gases from reactions or degassings have also to be considered.

Fig. 1.8 Reboiler types for distillation plants



In the “Wärmetausch-Fibel II” [3] it is shown how required suction capacities for different problem definitions is determined in addition to what has to be considered in the selection of the different vacuum pumps, i.e.:

Required suction capacity for the evacuation.
Required suction capacity for inert gases and vapours.
Determination of the leak rate from the equipment.

Flow velocities and pressure drops in the vacuum lines.
Unloading of the vacuum pumps by condensation.
Optimal combination of different vacuum pumps.

Selection of vacuum pumps with advantages and disadvantages:

Oil lubricated rotary disk pumps (problem: vapor condensation).
Liquid ring pumps (problem: cavitation and suction capacity).
Dry running vacuum pumps (problem: high temperature and explosion protection).
Steam jet pumps (problem: waste water contamination).

1.10 Control Facilities [5]

The required process conditions in a column are determined by the composition of the feed mixture and the required specifications for the top and bottom product. In order to achieve the desired separation the column must operate under equilibrium conditions.

The evaporator must steadily supply the required heating energy.
The pressure in the column must be held constant.
The condensation of the vapour must be correctly controlled.
The flows must be fed and drawn steadily.

- Instruments for the following problem definitions are required:
- Feed flow control and control of product draws from the column: distillate, side streams and bottom products.
- Level control and heat supply control from steam or hot oil.
- Cooling of the condenser and the after coolers for the products.
- Column pressure control.

Often a special control has to be installed for the special separation problem. In the following text are some examples of the control facilities in distillation columns (Figs. 1.9, 1.10, 1.11, 1.12, 1.13, 1.14, 1.15, 1.16, 1.17, 1.18, 1.19, 1.20, 1.21, 1.22, 1.23, 1.24, 1.25 and 1.26).

Fig. 1.9 Conventional column control according to F.G. Shinskey (5)

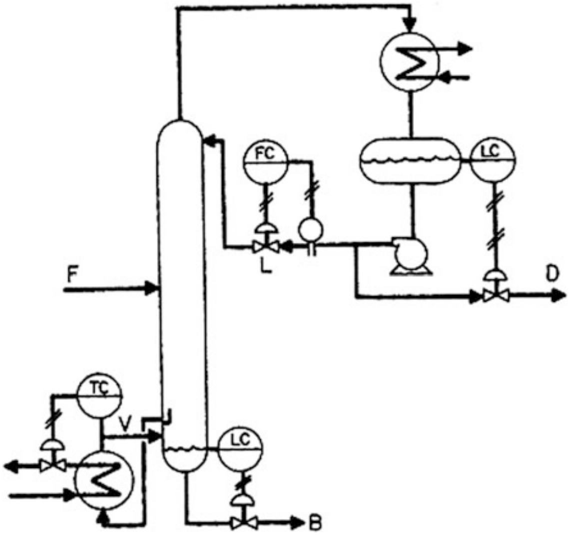
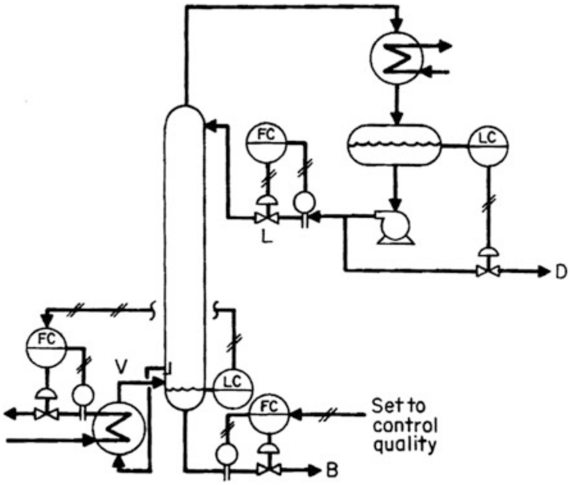


Fig. 1.10 Suitable control for small bottom rates according to F.G. Shinskey (5)



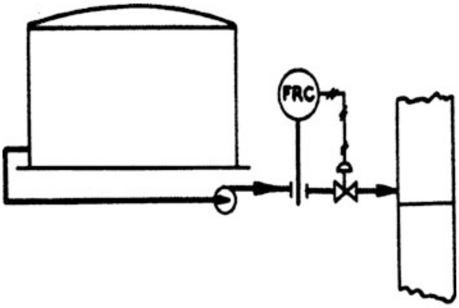


Fig. 1.11 Feed control from tank

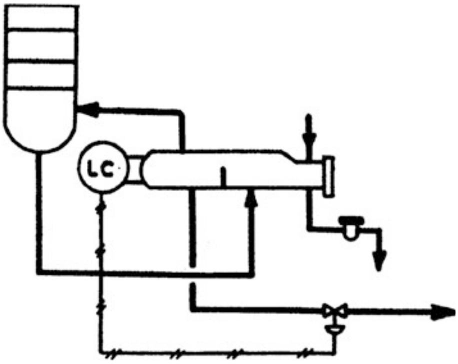


Fig. 1.12 Level control for bottom product

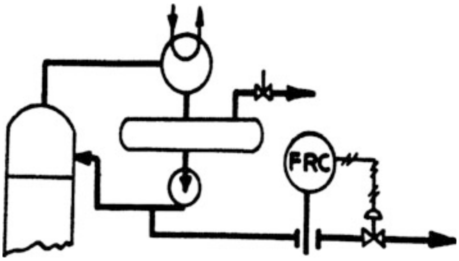


Fig. 1.13 Distillate control for constant feed

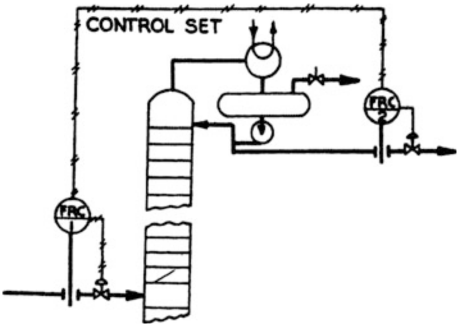


Fig. 1.14 Distillate control for variable feed

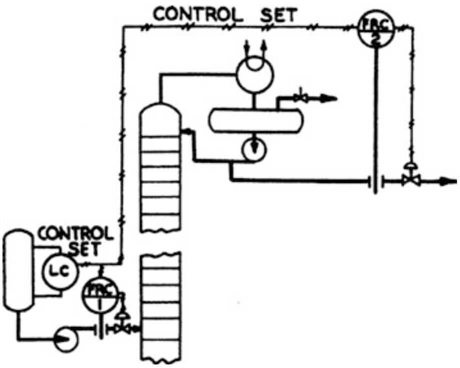


Fig. 1.15 Cascade control for feed

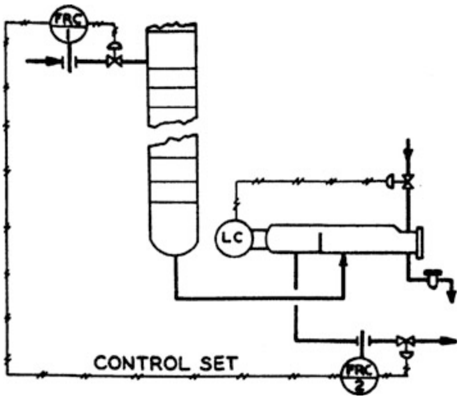


Fig. 1.16 Heat supply on level control

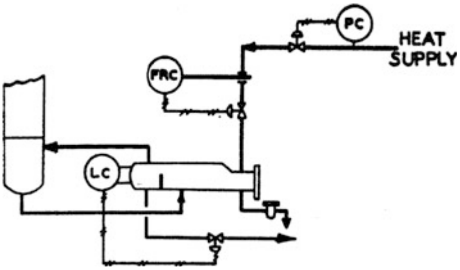


Fig. 1.17 Heat supply on flow control

Fig. 1.18 Heat supply on temperature control

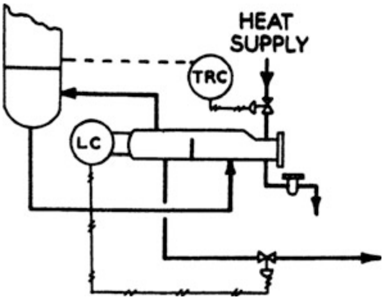


Fig. 1.19 Stable heat flow by temperature and flow control

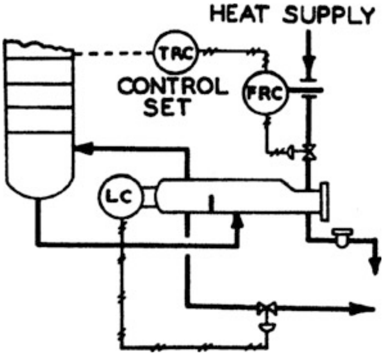


Fig. 1.20 Optimum temperature point for controlling heat supply

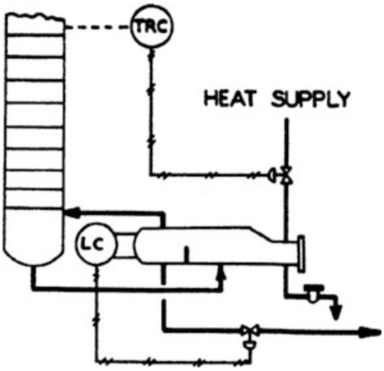


Fig. 1.21 Temperature controlled reflux

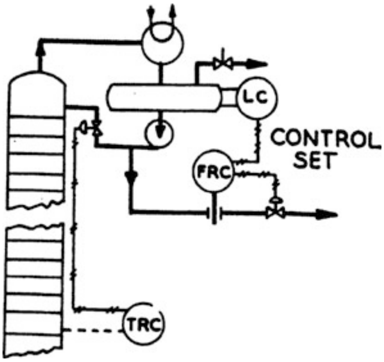


Fig. 1.22 Differential pressure control for heat supply

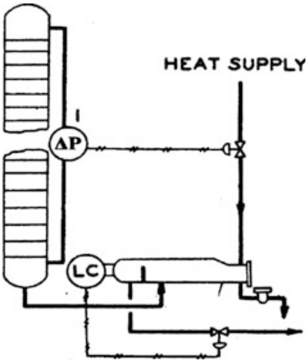


Fig. 1.23 Temperature controlled cooling water

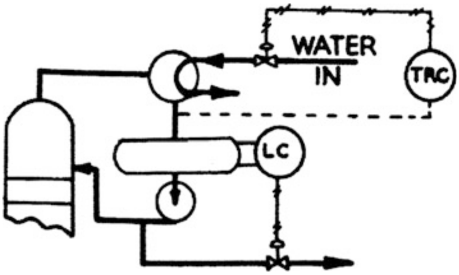
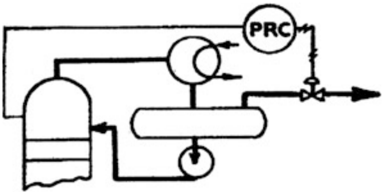


Fig. 1.24 Pressure control by venting



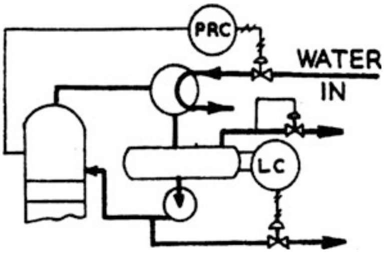


Fig. 1.25 Pressure control with cooling water

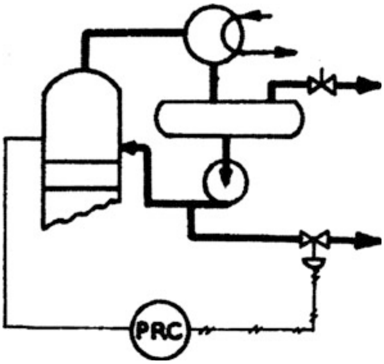


Fig. 1.26 Pressure control by flooding condenser bundle

1.11 Heating Systems with Steam or Hot Oil [3]

The most important aspects in the selection of a heating system with steam- or liquid-heating fluids are covered in [3] and what has to be considered in the design and control of the heating system is also shown.

1.11.1 Heat Transfer Coefficients

Figure 1.27 shows that the heat transfer coefficients of condensing steam and hot water are substantially better than the heat transfer coefficients of organic heat transfer fluids.

1.11.2 Steam Heating [3]

Steam heating is preferentially used because it has great advantages:

- Extensive isothermal heating over the whole heating area.
- Very good heat transfer coefficients >6000 W/m^2K.
- No large circulation rates as in heat transfer fluids.

Figure 1.28 shows the steam feed control, for fast control, whereas in Fig. 1.29 the control of the condensate drain is shown for a very wide working range [3].

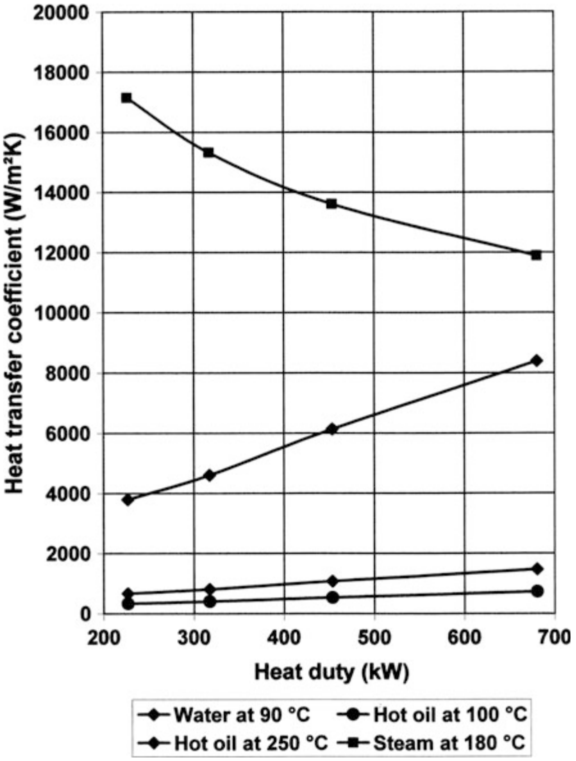


Fig. 1.27 Heat transfer coefficients of condensing steam, hot water, and hot oil

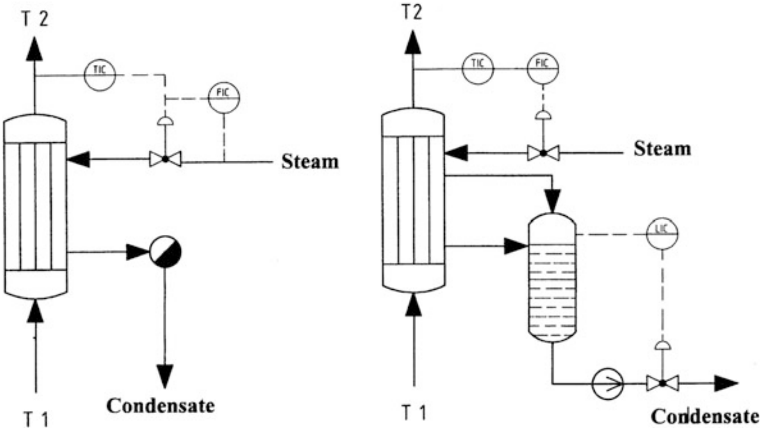


Fig. 1.28 Steam feed control for steam heated equipment

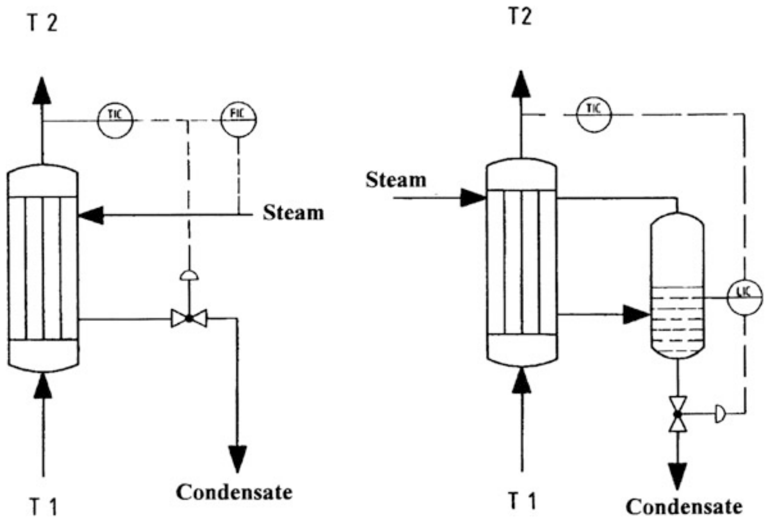
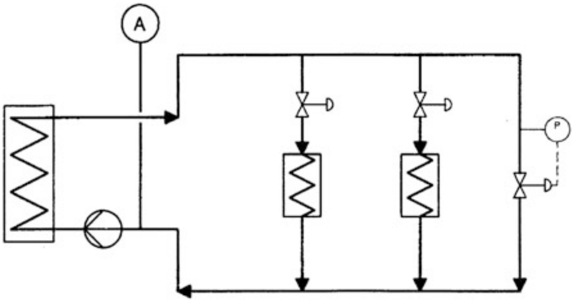
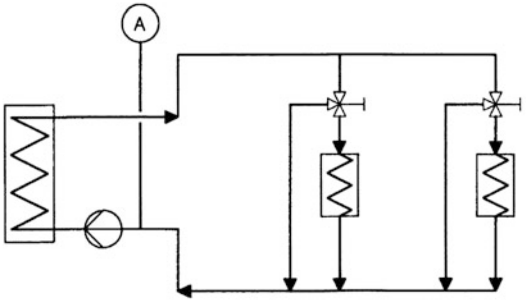


Fig. 1.29 Condensate drain control for steam heated equipment

Fig. 1.30 Primary heating circuit for hot oil



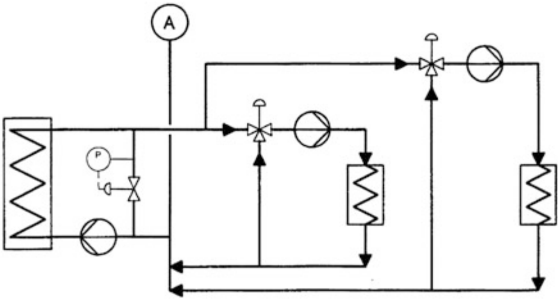
Constant high hot oil inlet temperature and relief valve



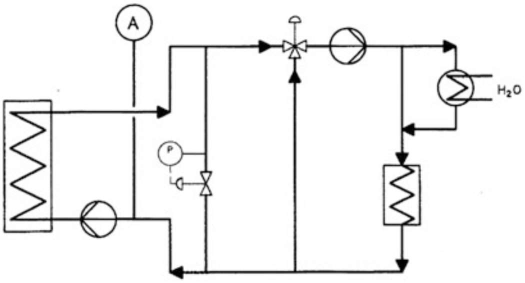
Threeport control valve for hot oil with bypass line

Disadvantage: High inlet temperature for all consumers

Fig. 1.31 Hot oil heating with secondary circulations



Secondary circuit with variable inlet temperatures



Secondary circuit for heating and cooling

Advantage: Heating with the lowest required inlet temperature

1.11.3 Heating with Hot Oil [3]

An organic heat transfer agent has the advantage that the heating system and the heated equipment only needs to be designed for low pressures even at high temperatures above 200 °C.

Disadvantages:

- Poor heat transfer coefficients in comparison to steam or hot water.
- No isothermal heating.
- Large heat exchange areas are required.
- Large heat transfer fluid rates must be moved by pumping.

The possible heating systems are shown in Figs. 1.30 and 1.31.

In the primary heating circulation, according to Fig. 1.30, all heat exchangers are fed with the highest oil temperature exiting the oil pipe still. Therefore, thermal damage of the product can occur.

The heating loads are influenced by the heating demands of other consumers and by the variations in the heater. By throttling the hot oil rate the flow velocity is reduced and hence so is the overall heat transfer coefficient.

Heating with secondary circulations is shown in Fig. 1.31 and is considered much better.

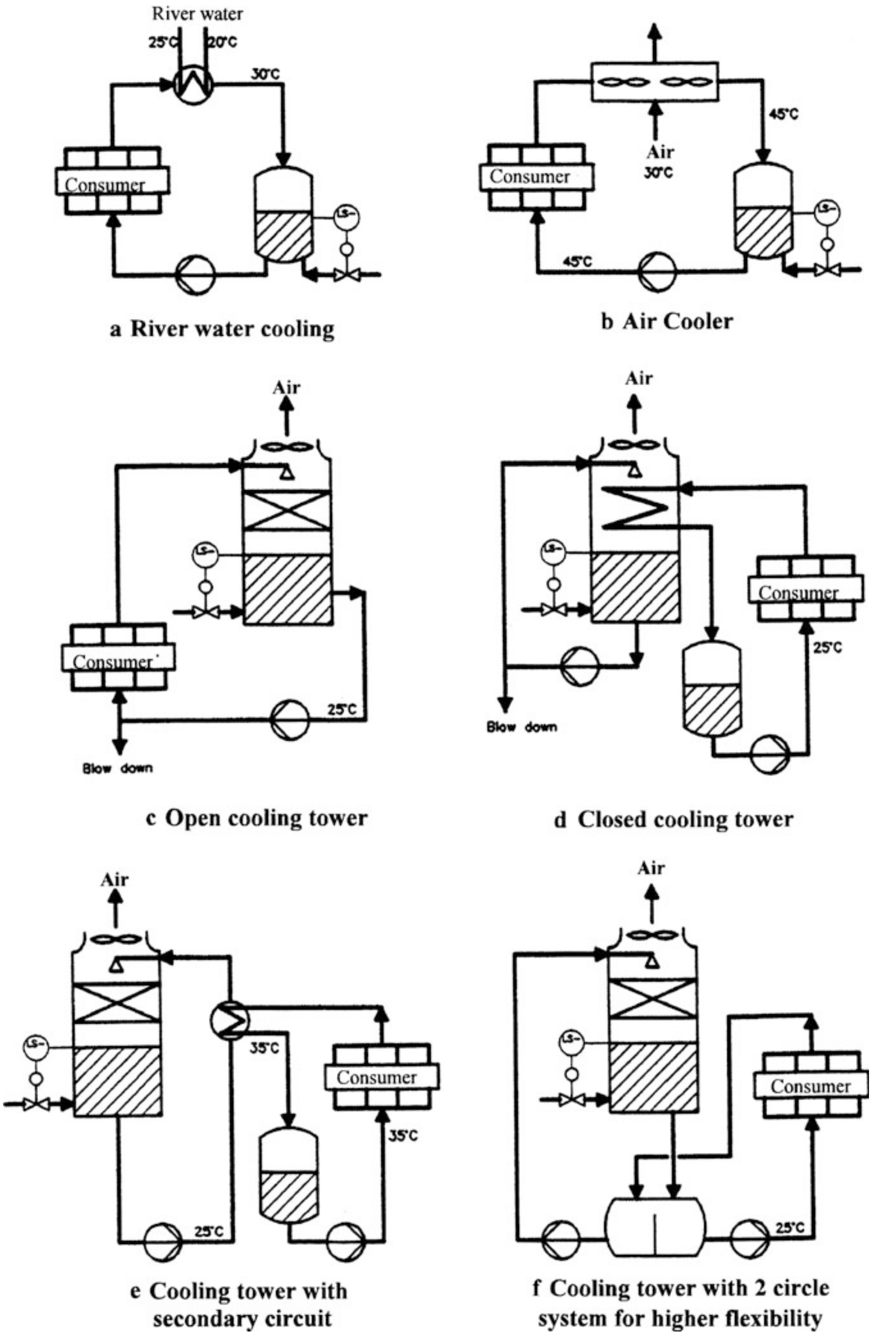


Fig. 1.32 Cooling water systems

1.12 Cooling Systems [3]

1.12.1 Cooling Water Circulation Systems

Figure 1.32 shows the different possible systems for cooling the water: river water cooling, air cooling, as well as open and closed cooling towers.

1.12.2 Comparison Between a Cooling Tower and an Air Cooler

Advantages of the cooling tower

- Lower cooling water temperatures than with air coolers because the wet-bulb temperature and not the dry-air temperature determines the possible cooling.
- Due to the constant wet-bulb temperature there are only low variations in the cooling water flow temperature.
- Lower investment costs.

Disadvantages of the cooling tower

- Treatment and fresh water costs leading to higher operating costs.
- Enrichment of salts and of air in the cooling water leading to corrosion and precipitation.
- Salt precipitation makes this method unsuitable for higher temperatures >50 °C.
- Fog and ice formation at cold temperatures.

Advantages of the air cooler

- No problem with corrosion, salt precipitation, biological fouling, and freezing.
- No additional water and water treatment needed – inhibiting costs.
- No problems with product contamination.

Disadvantages of air coolers

- Strong dependence on the air temperature leading to high water exit temperatures in the summer.
- Overdimensioned design for hot days in summer leading to overcooling in the winter.
- Maldistribution by wind and fouling.

The main problem with air coolers is their dependency on the ambient temperature which can be in the range 35–40 °C for summer daytime. This can be resolved by spraying water which leads to evaporation and thus a reduction in the air temperature. For example, 35 °C hot air with a 40% relative humidity can be cooled to 27 °C using this technique.

The following points must be considered thereby

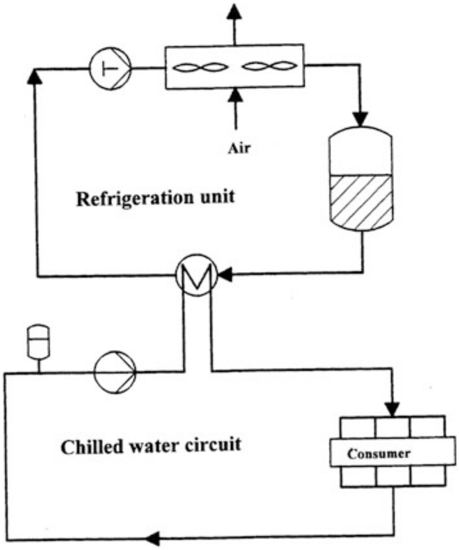
- The danger of salt or calcium precipitation from salty water exists. It is recommended to use condensate during the hottest summer days.
- The indosed water droplets must vaporize before the heat exchanger in order to affect air cooling. The residence time must therefore be sufficient.
- Salty droplets must not hit and evaporate on the finned tubes of the heat exchanger.

1.12.3 *Cooling Water by Evaporating a Refrigerant or Adiabatic Evaporation*

If very low water temperatures are required a refrigeration unit must be used. The flow chart in Fig. 1.33 illustrates this mode of operation [3].

Another method is adiabatic water evaporation in the vacuum. In Fig. 1.34 the cooling time at different suction capacities of the vacuum pump is shown.

Fig. 1.33 Chilled water circulation cooled by a refrigeration unit



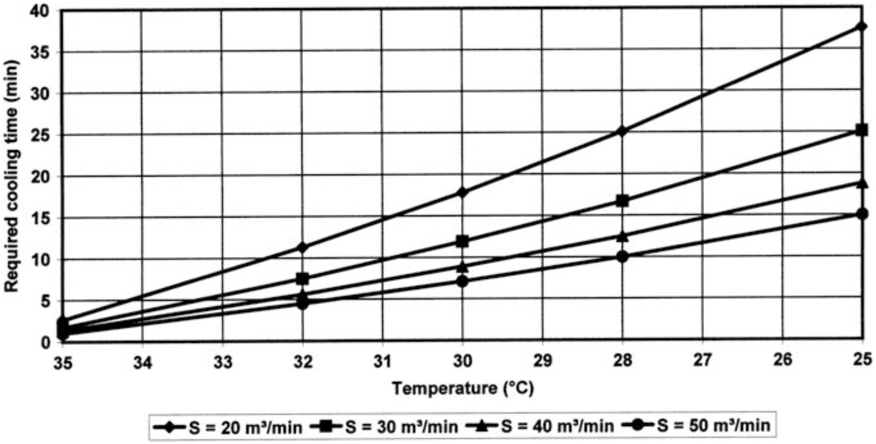
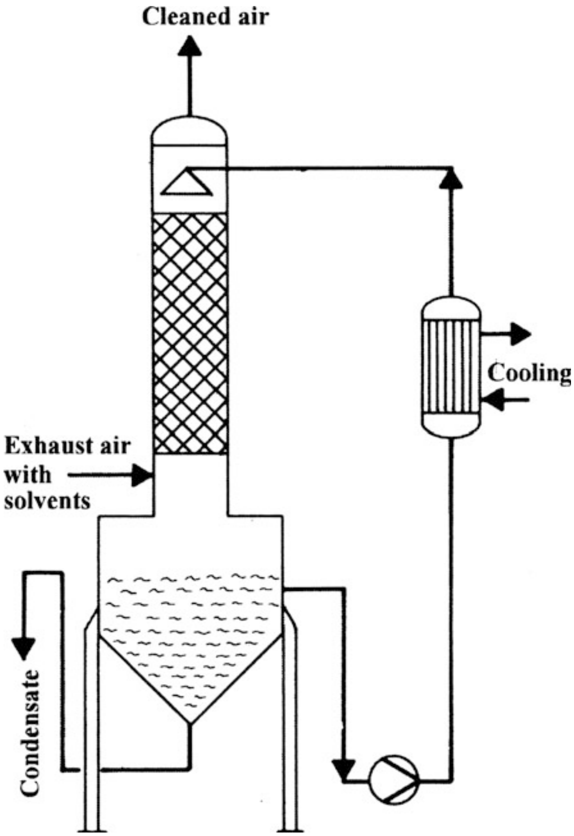


Fig. 1.34 Cooling times for 1 tonne of water at different suction capacities, S

Fig. 1.35 Cold wash for solvent-rich exhaust air



1.12.4 Direct Condensation in Columns [6]

If the vapour to be condensed contains a high melting point product, for instance Naphthalene with a melting point of 80 °C, these products crystallize out in a water-cooled condenser and create a blockage. In such cases it makes more sense to bring the vapour into direct contact with a suitable lean oil, for instance tar oil, in a packed column for direct condensation.

Another example is the direct condensation of solvents from exhaust air. The heat transfer coefficient in the condensing solvent vapour, containing inert gas, is poor and the undesired fog formation results in heavy cooling.

In such cases a cold wash is adopted. The exhaust air stream is washed with a cold solvent. For instance exhaust air containing methanol is washed with −20 °C cold liquid methanol or on the other hand exhaust air containing gasoline with −30 °C cold liquid gasoline.

The flow sheet of a "cold wash with its own juice" is shown in Fig. 1.35.

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Chapter 2
Equilibria, Bubble Points, Dewpoints, Flash Calculations, and Activity Coefficients

2.1 Vapour Pressure Calculations

The basis for all phase equilibrium calculations are the vapour pressures of the components. The vapour pressure is derived using the Antoine Equation and Antoine Constants A, B, and C.

$$\text{Antoine Equation}: \lg\ p_0 = \frac{A - B}{C + t(^\circ\text{C})}$$

Example 1.1: Calculation of the vapour pressures of benzene and toluene (Fig. 2.1).

Benzene	Toluene
$A = 7.00481$	$A = 7.07581$
$B = 1196.76$	$B = 1342.31$
$C = 219.161$	$C = 219.187$

Temperature	Benzene vapour pressure	Toluene vapour pressure
50 °C	$p_{0\text{B}} = 362\,\text{mbar}$	$p_{0\text{T}} = 123\,\text{mbar}$
98 °C	$p_{0\text{B}} = 1704\,\text{mbar}$	$p_{0\text{T}} = 698\,\text{mbar}$
103 °C	$p_{0\text{B}} = 1950\,\text{mbar}$	$p_{0\text{T}} = 812\,\text{mbar}$

2.2 Phase Equilibrium of Ideal Binary Mixtures

The equilibrium between the liquid and the vapour phase is calculated according to the laws of Dalton and Raoult.

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_2

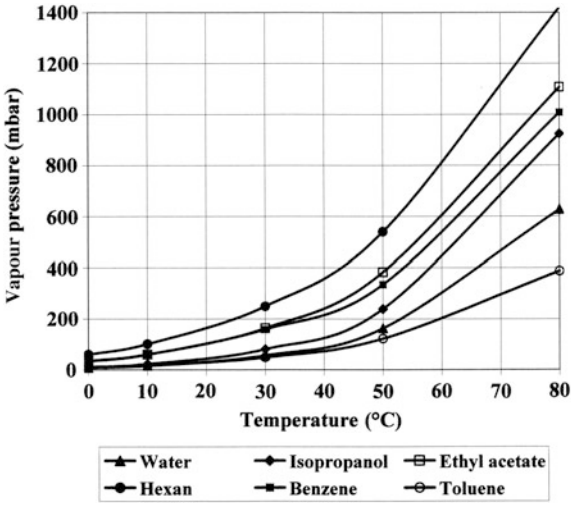


Fig. 2.1 Vapour pressure of different components as a function of temperature

Dalton:

$$p_1 = y_1 * P_{\text{tot}} \qquad P_{\text{tot}} = p_1 + p_2 + p_3 + \ldots p_i$$

Raoult (Fig. 2.2):

$$p_1 = x_1 * p_{01} \qquad p_2 = x_2 * p_{02}$$
$$P_{\text{tot}} = x_1 * p_{01} + x_2 * p_{02} + x_3 * p_{03} + \ldots . x_i * p_{0\text{i}}$$

Equilibrium equation: $y_i * P_{\text{tot}} = p_i = x_i * p_{0\text{i}}$

$$y_i = \frac{x_i * p_{0\text{i}}}{P_{\text{tot}}} = \frac{p_i}{P_{\text{tot}}}$$

y_i = concentration of the component i in the vapour phase (mole fraction)
x_i = concentration of the component i in the liquid phase (mole fraction)
P_{tot} = total pressure (mbar)
$p_{0\text{i}}$ = vapour pressure of the component i (mbar)
p_i = partial pressure of the component i (mbar)

Example 2.2.1: Calculation of the partial pressures and the vapour compositions for an ideal binary mixture.

$$x_1 = 0.6 \quad p_{01} = 800\,\text{mbar}$$
$$x_2 = 0.4 \quad p_{02} = 1300\,\text{mbar}$$

Calculation of the partial pressures according to Raoult:

$$p_1 = x_1 * p_{01} = 0.6 * 800 = 480\,\text{mbar}$$
$$p_2 = x_2 * p_{02} = 0.4 * 1300 = 520\,\text{mbar}$$
$$P_{\text{tot}} = 1000\,\text{mbar}$$

Calculation of the vapour concentration according to Dalton:

$$y_1 = \frac{p_1}{P_{\text{tot}}} = \frac{480}{1000} = 0.48 \text{ molfr.} = 48 \text{ mol\%}$$

$$y_2 = \frac{p_2}{P_{\text{tot}}} = \frac{520}{1000} = 0.52 \text{ molfr.} = 52 \text{ mol\%}$$

In order to simplify the calculation of phase equilibria a separation factor α is introduced, often also called the relative volatility α, defined as the ratio of the vapour pressures of the two components, or the ratio of the equilibrium constants, K, of the components of the ideal mixture.

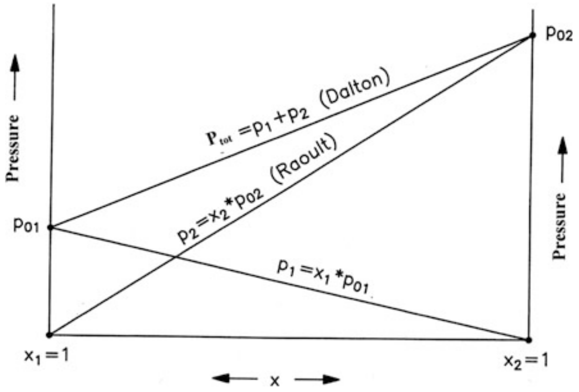
$$\alpha_{1/2} = \frac{P_{01}}{P_{02}} = \frac{K_1}{K_2}$$

Calculation with the relative volatility α assumes that both vapour pressure curves are fairly parallel in the logarithmic representation (see Fig. 2.3).

In Fig. 2.4 it can be seen that the relative volatility becomes smaller with rising temperatures. The separation becomes more difficult with increasing temperatures.

Due to the fact that the relative volatility in the rectification section, and in the stripping section, is different, a geometrical average is formed from the separation factor α_V in the rectification section and the separation factor α_A in the stripping section.

Fig. 2.2 Graphical representation of the laws of Dalton and Raoult for an ideal mixture



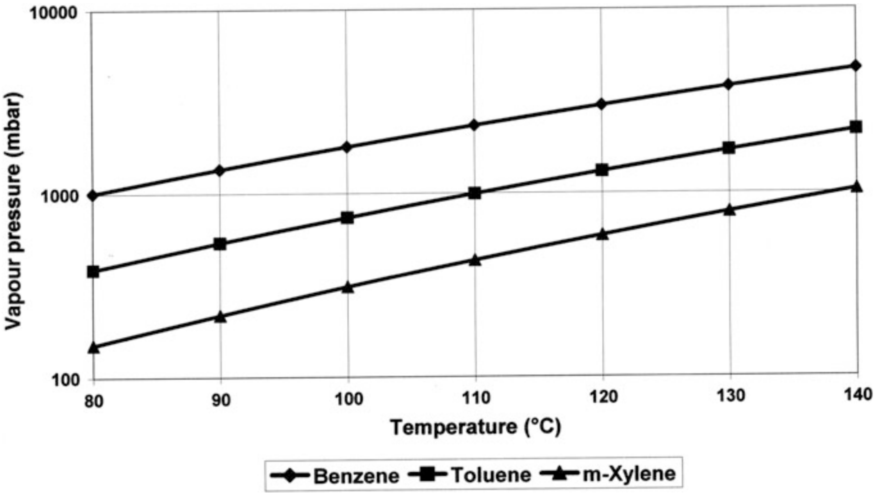


Fig. 2.3 Vapour pressure *curves* of benzene, toluene, and xylene

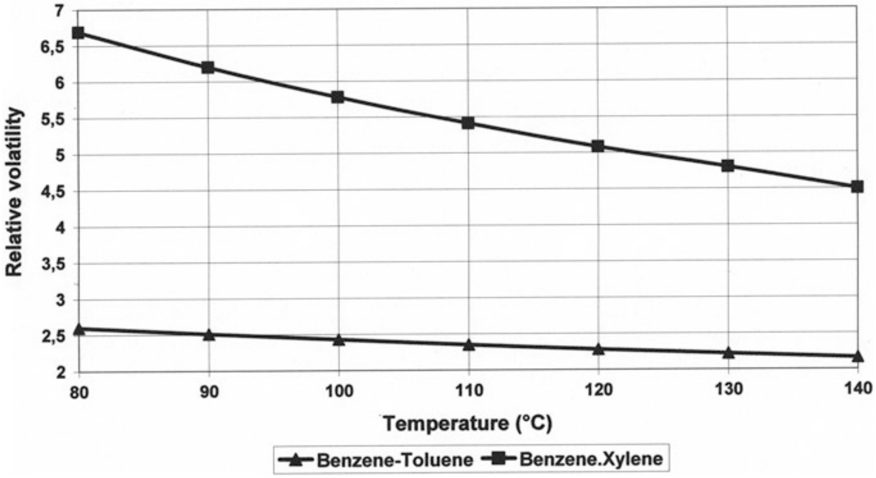


Fig. 2.4 Relative volatilities for the separation of benzene/toluene and benzene/xylene as a function of temperature

$$\alpha_{\mathrm{av}} = \sqrt{\alpha_V * \alpha_A}$$

Using the relative volatility α one gets a very simple equation for the calculation of the phase equilibrium between the composition in the vapour and the composition in the liquid.

$$y = \frac{\alpha * x}{1 + (\alpha - 1) * x} \text{ (molfraction)} \qquad x = \frac{y}{\alpha - (\alpha - 1) * y} \text{ (molfraction)}$$

Example 2.2.2: Calculation of the vapour composition y_1 for a liquid composition of x_1 = 0.2. p_{01} = 400 mbar p_{02} = 200 mbar x_1 = 0.2 x_2 = 0.8

$$\alpha = \frac{400}{200} = 2$$

$$y_1 = \frac{\alpha * x_1}{1 + (\alpha - 1) * x_1} = \frac{2 * 0.2}{1 + (2 - 1) * 0.2} = 0.33 \text{ molfr.}$$

$$P_{\text{tot}} = x_1 * p_{01} + x_2 * p_{02} = 0.2 * 400 + 0.8 * 200 = 240 \text{ mbar}$$

$$y_1 = \frac{x_1 * p_{01}}{P_{\text{tot}}} = \frac{0.2 * 400}{240} = 0.33 \text{ molfr.}$$

Cross-check calculation for x:

$$x_1 = \frac{y_1}{\alpha - (\alpha - 1) * y_1} = \frac{0.33}{2 - (2 - 1) * 0.33} = 0.2 \text{ molfr.}$$

$$x_1 = \frac{y_1 * P_{\text{tot}}}{p_{01}} = \frac{0.33 * 240}{400} = 0.2 \text{ molfr.}$$

In American literature the equilibrium constant K, which is defined as the ratio of the compositions in vapour and liquid, is often used instead of the relative volatility α.

$$K = \frac{y_i}{x_i} = \frac{p_{0i}}{P_{\text{ges}}}$$

$$y_1 = K_1 * x_1 = K_1 * \frac{1 - K_2}{K_1 - K_2}$$

$$x_1 = \frac{y_1}{K_1} = \frac{1 - K_2}{K_1 - K_2}$$

Example 2.2.3: Equilibrium calculation with the equilibrium constant K.

$x_1 = 0.6 \quad p_{01} = 800\,\text{mbar} \quad p_1 = 0.6 * 800 = 480\,\text{mbar}$

$x_2 = 0.4 \quad p_{02} = 1300\,\text{mbar} \quad p_2 = 0.4 * 1300 = 520\,\text{mbar} \quad P_{\text{tot}} = 1000\,\text{mbar}$

Calculation of the equilibrium factor K:

$$K_1 = \frac{y_1}{x_1} = \frac{p_{01}}{P_{\text{tot}}} = \frac{800}{1000} = 0.8$$

$$K_2 = \frac{y_2}{x_2} = \frac{p_{02}}{P_{\text{tot}}} = \frac{1300}{1000} = 1.3$$

Calculation of the vapour composition y:

$$y_1 = K_1 * x_1 = 0.8 * 0.6 = 0.48 \text{ molfr.}$$

$$y_1 = K_1 * \frac{1 - K_2}{K_1 - K_2} = 0.8 * \frac{1 - 1.3}{0.8 - 1.3} = 0.48 \text{ molfr.}$$

Cross-check calculation of x_1:

$$x_1 = \frac{y_1}{K_1} = \frac{0.48}{0.8} = 0.6 \text{ molfr.}$$

$$x_1 = \frac{1 - K_2}{K_1 - K_2} = \frac{1 - 1.3}{0.8 - 1.3} = 0.6 \text{ molfr.}$$

2.3 Bubble Point Calculation

The bubble point of a mixture is defined as follows:

$$\Sigma y_i = \Sigma K_i * x_i = 1$$

The bubble pressure P_{boil} can be calculated directly.

$$P_{\text{boil}} = x_1 * p_{01} + x_2 * p_{02}$$

A simple method for calculating the bubble temperature of a mixture is the calculation of the bubble pressure from the sum of the partial pressures.

At the bubble temperature the bubble point pressure must be equal to the system pressure P_{tot}. The following example shows the procedure.

Example 3.1: Iterative bubble point calculation for a benzene-toluene mixture

30 mol% benzene in the liquid phase ($x = 0.3$)
70 mol% toluene in the liquid phase ($x = 0.7$)
$P_{\text{tot}} = 1000$ mbar p_{0B} = vapor pressure of benzene
p_{0T} = vapor pressure of toluene

$$\text{First choice}: \quad t = 95\,^\circ\text{C} \qquad p_{0B} = 1573\,\text{mbar} \qquad p_{0T} = 634.4\,\text{mbar}$$

$$P_{\text{boil}} = 0.3 * 1573 + 0.7 * 634.4 = 916\,\text{mbar} \qquad P_{\text{boil}}\,\text{is too low!}$$

$$\text{Second choice}: \quad t = 100\,^\circ\text{C} \qquad p_{0B} = 1807\,\text{mbar} \qquad p_{0T} = 740\,\text{mbar}$$

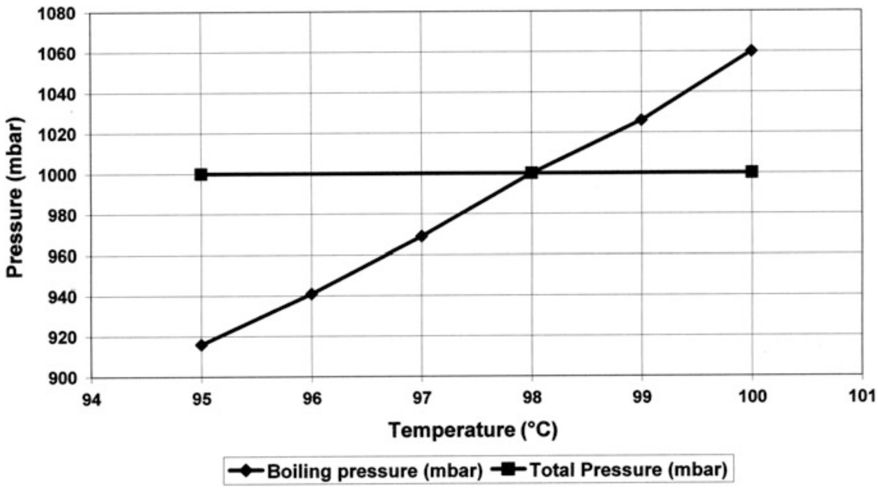


Fig. 2.5 Bubble point determination by graphical interpolation

$$P_{\mathrm{boil}} = 0.3 * 1807 + 0.7 * 740 = 1060\,\mathrm{mbar} \qquad P_{\mathrm{boil}} \text{ is too high!}$$

$$\text{Third choice :} \quad t = 98\,^{\circ}\mathrm{C} \quad p_{0\mathrm{B}} = 1710\,\mathrm{mbar} \quad p_{0\mathrm{T}} = 696\,\mathrm{mbar}$$

$$P_{\mathrm{boil}} = 0.3 * 1710 + 0.7 * 696 = 1000\,\mathrm{mbar} \qquad P_{\mathrm{boil}} = 1000\,\mathrm{mbar} = \text{correct!}$$

Figure 2.5 shows how the bubble point determination can be simplified by graphical interpolation. The sum of the two partial pressures must be equal to the system pressure.

Cross-check calculation of the bubble point at 98 °C:
Vapour pressure of benzene $p_{0\mathrm{B}}$ = 1710 mbar
Vapour pressure of toluene $p_{0\mathrm{T}}$ = 696 mbar

$$K_1 = \frac{p_{0\mathrm{B}}}{P_{\mathrm{tot}}} = \frac{1710}{1000} = 1.71$$

$$K_2 = \frac{p_{0\mathrm{T}}}{P_{\mathrm{tot}}} = \frac{696}{1000} = 0.696$$

$$\sum K_i = K_1 * x_1 + K_2 * x_2 = 1.71 * 0.3 + 0.696 * 0.7 = 1$$

The bubble point specification is therefore fulfilled.

2.4 Dew Point Calculation

The dew point of a mixture is defined as follows:

$$\Sigma x_i = \sum y_i/K_i = 1$$

The dew point pressure P_{dew} can be calculated directly.

$$\frac{1}{P_{\text{dew}}} = \frac{y_1}{p_{01}} + \frac{y_2}{p_{02}} \qquad P_{\text{dew}} = \left[\sum \frac{y_i}{p_{0\text{i}}}\right]^{-1}$$

The dew point temperature for a specific pressure is calculated iteratively until the sum of the quotients $y_i/p_{0\text{i}}$ is equal to the reciprocal value of the system pressure P_{tot}. The following example shows the procedure.

Example 2.4.1: Iterative dew point calculation for a benzene-toluene mixture.
30 mol% benzene in the vapour phase (y = 0.3)
70 mol% toluene in the vapour phase (y = 0.7)
P_{tot} = 1000 mbar

$$\text{First choice}: \quad t = 100\,^\circ\text{C} \qquad p_{0\text{B}} = 1807\,\text{mbar} \qquad p_{0\text{T}} = 740\,\text{mbar}$$

$$\frac{1}{P_{\text{dew}}} = \frac{y_1}{p_{01}} + \frac{y_2}{p_{02}} = \frac{0.3}{1807} + \frac{0.7}{740} = 0.0011 \quad P_{\text{dew}} = 899\,\text{mbar is too low!}$$

$$\text{Second choice}: \quad t = 104\,^\circ\text{C} \qquad p_{0\text{B}} = 2013\,\text{mbar} \qquad p_{0\text{T}} = 834.4\,\text{mbar}$$

$$\frac{1}{P_{\text{dew}}} = \frac{y_1}{p_{01}} + \frac{y_2}{p_{02}} = \frac{0.3}{2013} + \frac{0.7}{834.4} = 0.00099 \quad P_{\text{dew}} = 1012\,\text{mbar is too high!}$$

$$\text{Third choice}: \quad t = 103.8\,^\circ\text{C} \qquad p_{0\text{T}} = 2002\,\text{mbar} \qquad p_{0\text{T}} = 829\,\text{mbar}$$

$$\frac{1}{P_{\text{dew}}} = \frac{y_1}{p_{01}} + \frac{y_2}{p_{02}} = \frac{0.3}{2002} + \frac{0.7}{829} = 0.001 \quad P_{\text{ges}} = 1000\,\text{mbar is correct!}$$

Cross-check calculation for the dew point at 103.8 °C:

$$K_1 = \frac{2002}{1006} = 1.99 \quad K_2 = \frac{829}{1006} = 0.824$$

$$\sum \frac{y_i}{K_i} = \frac{0.3}{1.99} + \frac{0.7}{0.824} = 1$$

The condition for the dew point is fulfilled.

Figure 2.6 shows how the dew point can be determined by graphical interpolation.

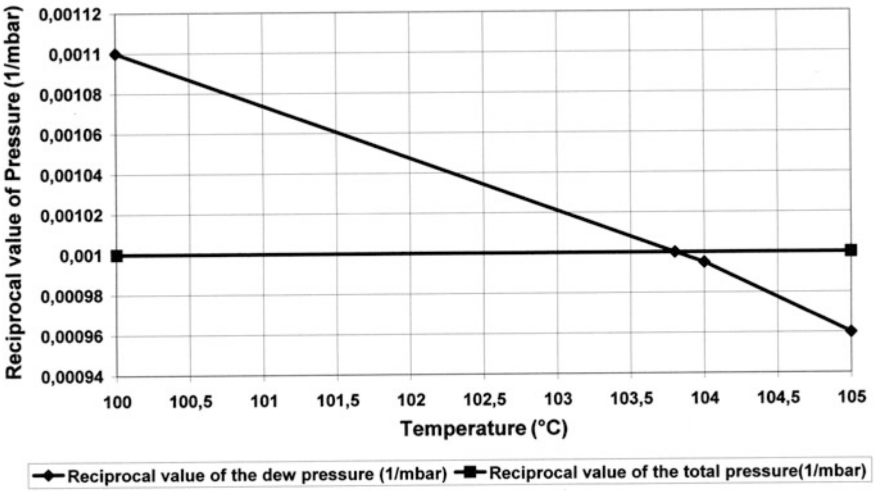


Fig. 2.6 Dew point determination by graphical interpolation

2.5 Dew Point Calculation of Vapour Containing Inert Gases

The dew point of a vapour mixture containing inert gas is reached if the sum of the partial pressures of the vapours ($\sum y_i * P_{\text{ges}}$) reaches the vapour pressure of the liquid phase by cooling.

$$\sum y_i * P_D = \sum z_i * P_{\text{tot}} = \sum x_i * p_{0\text{i}}$$

$$P_D = P_{\text{tot}} - P_{\text{IN}}$$

P_D = sum of the vapours partial pressures (mbar)
P_{IN} = inert gas partial pressure (mbar)
P_{tot} = total pressure in the system with inert gas (mbar)
y_i = vapour composition based on the vapour partial pressure P_D
z_i = vapour composition based on the total pressure P_{tot} with inert gas

Calculation of the dew point pressure without inert gas:

$$P_{\text{dew}} = \left(\sum \frac{y_i}{P_{0\text{i}}}\right)^{-1} \qquad \sum \frac{y_i}{K_i} = 1 \qquad K_i = \frac{p_{0\text{i}}}{P_D}$$

Calculation of the dew point pressure with inert gas:

$$P_{\text{dew}} = \left(\sum \frac{z_i}{P_{0\text{i}}}\right)^{-1} \qquad \sum \frac{z_i}{K_i} = 1 \qquad K_i = \frac{p_{0\text{i}}}{P_{\text{tot}}}$$

Example 2.5.1: Dew point pressure calculation without inert gas.

$$\begin{aligned} y_1 &= 0.413 \quad P_{01} = 3009.3\,\text{mbar at } 102\,^\circ\text{C} \\ y_2 &= 0.587 \quad P_{02} = 830.8\,\text{mbar} \end{aligned}$$

$$P_{\text{dew}} = \left[\sum \frac{y_i}{P_{0\text{i}}}\right]^{-1} = \left[\frac{0.413}{3009.3} + \frac{0.587}{830.8}\right]^{-1} = 1185\ \text{mbar}$$

$$K_1 = \frac{3009.3}{1185} = 2.54 \qquad K_2 = \frac{830.8}{1185} = 0.7$$

$$\sum x_i = \frac{0.413}{2.54} + \frac{0.587}{0.7} = 1$$

Example 2.5.2: Dew point pressure calculation with inert gas.

$$\begin{aligned} &40\,\text{Vol\% vapour} + 60\,\text{Vol\% inert gas} \\ &y_1 = 0.413\,\text{molfr.} \qquad P_{01} = 3009.3\,\text{mbar at } 102\,^\circ\text{C} \\ &y_2 = 0.587\,\text{molfr.} \qquad P_{02} = 830.8\,\text{mbar} \end{aligned}$$

$$\begin{aligned} &z_1 = 0.4 * y_1 = 0.4 * 0.413 = 0.165\,\text{molfr.} \\ &z_2 = 0.4 * y_2 = 0.4 * 0.587 = 0.235\,\text{molfr.} \\ &\text{Vapour fraction}: \quad \sum z_1 + z_2 = 0.4 \\ &\text{Inert gas fraction}: \quad z_{\text{IN}} = 0.6 \end{aligned}$$

$$P_{\text{dew}} = \left[\sum \frac{z_i}{p_{0\text{i}}}\right]^{-1} = \left[\frac{0.165}{3009.3} + \frac{0.235}{830.8}\right]^{-1} = 2961.3\ \text{mbar}$$

$$K_1 = \frac{3009.3}{2961.3} = 1.016 \qquad K_2 = \frac{830.8}{2961.3} = 0.28$$

$$\sum x_i = \frac{0.165}{1.016} + \frac{0.235}{0.28} = 1$$

With inert gas the dew point pressure is much higher and the dew point temperature lies lower than it would without inert gas. In addition, with inert gas in the vapour a much deeper cooling must take place in order to condense the vapour.

2.6 Dew and Bubble Point Lines of Ideal Binary Mixtures

The bubble point of a liquid mixture is defined such that the sum of the partial pressures of the mixture reaches the system pressure with the first droplet being evaporated. Due to the preferred evaporation of light-boiling components, high-boiling components increase in concentration and the bubble point rises. The curve of the boiling temperature as a function of the composition of the light-boiling components in the mixture is known as the boiling line.

Equation for the boiling point line:

$$x_1 = f(t) = \frac{P_{\mathrm{tot}} - p_{02}}{p_{01} - p_{02}} \text{ (molfraction light boilers in the liquid)}$$

The boiling point temperature increases with decreasing composition of light-boiling components.

The dew point of a vapour mixture is the temperature at which the first droplet is condensed. Due to the preferred condensing of high-boiling components the vapour mixture is enriched with light-boiling components and the dew point temperature drops.

The representation of the dew point temperature as function of the vapour composition is referred to as the dew point line.

Equation for the dew point line:

$$y_1 = f(t) = \frac{p_{01}}{P_{\mathrm{tot}}} * \frac{P_{\mathrm{tot}} - p_{02}}{p_{01} - p_{02}} \text{ (molfraction light boilers in the vapor)}$$

A diagram with bubble and dew point lines is called a phase diagram or temperature–composition diagram.

Example 2.6.1: Construction of the temperature–composition diagram for benzene [1]-toluene [2] at 1013 mbar

Procedure:

1. Calculation of the two boiling points with the Antoine Equation.
   The **two boiling points are the end points** in the temperature–composition diagram.
   Bubble point of benzene: 80.1 °C
   Bubble point of toluene: 110.6 °C
2. Calculation of vapour pressures at different temperatures with the Antoine equation.
3. Determination of the liquid composition x and the vapour composition y at the different temperatures using the equations for the bubble and dew pointo lines.

Calculation results:

Temperature (°C)	p_{01} (mbar)	p_{02} (mbar)	x_1 (molfr.)	y_1 (molfr.)
80.1	1013	390	1.000	1.000
83	1107	430	0.861	0.941
86	1211	476	0.731	0.874
89	1322	525	0.612	0.799
92	1442	578	0.504	0.717
95	1569	636	0.404	0.626
98	1705	698	0.313	0.527
101	1850	765	0.229	0.418
104	2004	836	0.151	0.300
107	2168	913	0.080	0.170
110.6	2378	1013	0.0	0.0

Bubble point line : $x_1 = f(\textbf{temperature})$ **Dew point line** : $y_1 = f(\textbf{temperature})$

p_{01} = vapour pressure of benzene p_{02} = vapour pressure of toluene
x_1 = liquid composition of the lighter boiling component of benzene (molfraction)
y_1 = vapour composition of the lighter boiling component benzene (molfraction)

Figure 2.7 depicts the temperature–composition diagram of the benzene–toluene mixture.

The dew point of a vapour mixture with 30 mol% benzene and 70 mol% toluene lies at 104 °C. The bubble point of the mixture lies at 98 °C. The first liquid droplet

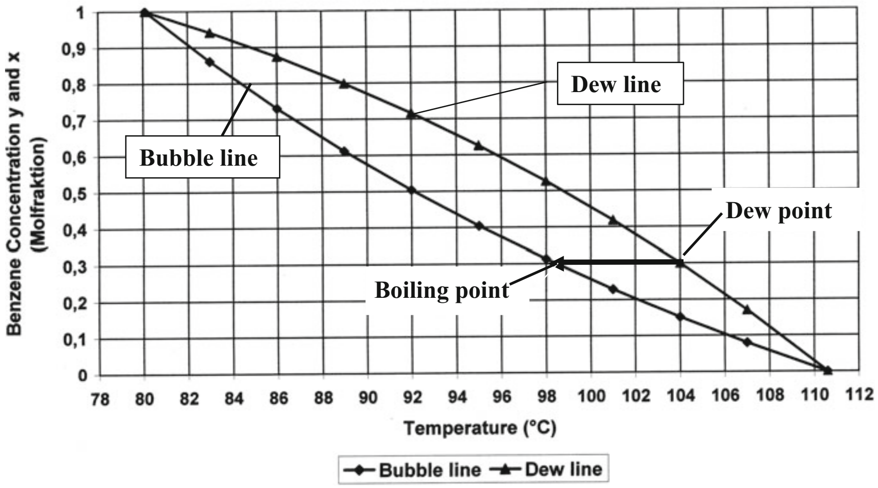


Fig. 2.7 Temperature–composition diagram for the benzene–toluene mixture

condenses at a 104 °C dew point. At the bubble point of 98 °C the total mixture is liquid. In order to condense the total mixture the mixture has to be cooled down from 104 to 98 °C. When evaporating, the mixture must on the contrary be heated from the bubble point to the dew point.

2.7 The Bubble Point and Dew Point of Immiscible Mixtures

One example of common mixtures of this type is the mixture of hydrocarbons and water. In an immiscible mixture both liquid phases exert temperature dependent vapour pressures.

Bubble point:

The bubble point pressure P_{boil} results from the sum of the hydrocarbon vapour pressures P_{org} and the water vapour pressures P_{W}.

$$P_{\mathrm{boil}} = P_{\mathrm{org}} + P_{\mathrm{W}}$$

This equation is the foundation for steam stripping.

By introducing water or steam the bubble point of hydrocarbons is reduced.

Example 2.7.1: Bubble point of a toluene–water mixture at 1010 mbar.

Temperature: 84 °C.

Toluene vapour pressure at 84 °C = 444 mbar.

Water vapour pressure at 84 °C = 566 mbar.

P_{boil} = 444 + 666 = 1010 mbar.

The bubble point for the toluene–water mixture is 84 °C at 1010 mbar.

Dew point:

In the dew point calculation the composition of the vapour is used as opposed to the bubble point calculation. The dew point is defined as the point at which the partial pressure equals the vapour pressure of the respective component. In a vapour mixture the component that first condenses out is the component whose partial pressure reaches the vapour pressure of the component. The higher the vapour composition the higher the partial pressure and the earlier condensing out of the component occurs.

$$P_{\mathrm{org}} = y_{\mathrm{org}} * P_{\mathrm{tot}} \qquad P_{\mathrm{W}} = y_{\mathrm{W}} * P_{\mathrm{tot}}$$

The dew point is reached when the vapour pressure of the component falls below the partial pressure of the component.

$P_{0\mathrm{org}} < P_{\mathrm{org}}$	The vapour pressure of the organic component is lower than the partial pressure, leading to the dew point of the organic component.
$P_{0\mathrm{W}} < P_{\mathrm{W}}$	The vapour pressure of water is lower than the partial pressure, leading to the dew point of water.

Example 2.7.2: Determination of the dew point of a toluene–water mixture.

(a) **Water condenses first**:
Water vapour composition in the vapour $y_\mathrm{W} = 0.63$; $P_\mathrm{tot} = 1$ bar.
Water vapour partial pressure $P_\mathrm{W} = 0.63 * 1000 = 630$ mbar.
Water has a vapour pressure of $P_{0\mathrm{W}} = 630$ mbar at 87.2 °C.
The dew point is 87.2 °C.
Water condenses first.

(b) **Toluene condenses first**:
Toluene composition in the vapour $y_\mathrm{org} = 0.578$; $P_\mathrm{tot} = 1$ bar.
Toluene partial pressure $P_\mathrm{org} = 0.578 * 1000 = 578$ mbar.
Toluene has a vapour pressure of $P_{0\mathrm{org}} = 578$ mbar at 92 °C.
The dew point is 92 °C.
Toluene condenses first.

2.8 Flash Calculations for Ideal Binary Mixtures [1]

At the bubble point the total mixture is liquid.

At the dew point the total mixture is vapour.

The vapour and liquid rates change between bubble point and dew point.

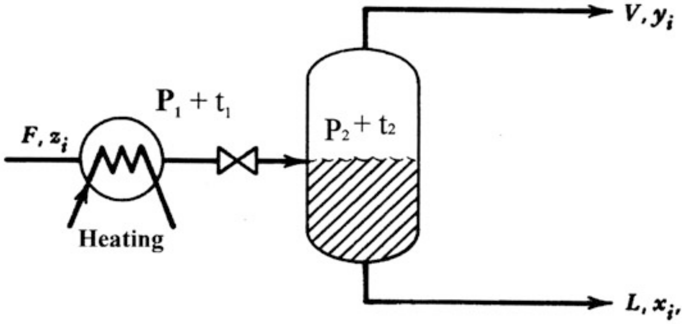
When heated to t_1 and vaporized at pressure P_2 a part of the liquid will be vaporized (Fig. 2.8).

When cooling the vapour mixture to the temperature t_2 a part of the vapour condenses (Fig. 2.8).

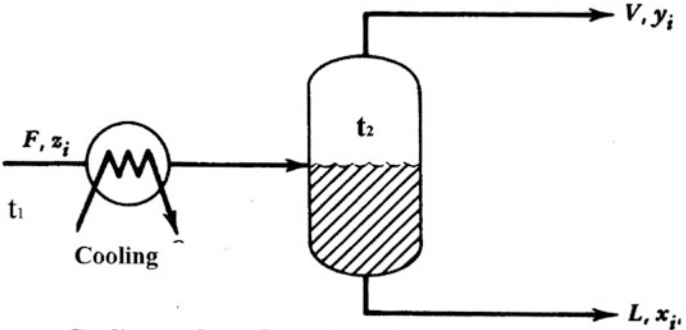
Using the flash calculation the vapour composition of the mixture at temperatures between bubble point and dew point is calculated. The compositions in the vapour and liquid phase when cooling or heating are also determined with the equilibrium factors.

How much of the mixture is vapour at temperatures between bubble point and dew point?

The calculation of the vapour fraction V of the feed F is accomplished with the use of the equilibrium constants K_1 and K_2 for the vapour composition of the light-boiling component z_1 as follows:



Heating and evaporation of liquids



Cooling and condensation of vapours

Fig. 2.8 Flash separation after heating liquid mixtures or cooling vapour mixtures

$$\frac{V}{F} = \frac{z_1 * \frac{K_1 - K_2}{1 - K_2} - 1}{K_1 - 1}$$

What is the composition of the liquid and vapour fractions of the mixture?

$$x_1 = \frac{1 - K_2}{K_1 - K_2}$$

$$y_1 = K_1 * x_1$$

V = vapour rate (kmol/h).
F = feed rate (kmol/h).
K_1 = equilibrium constant of the lighter component 1.
K_2 = equilibrium constant of the heavier component 2.
z_1 = composition of the lighter component 1 in the feed (molfraction).
x_1 = composition of the lighter component in the liquid phase (molfraction).
y_1 = composition of the lighter component in the vapour (molfraction).

Example 2.8.1: Flash calculations for a benzene–toluene mixture with $z_1 = 0.3 = 30$ mol% benzene in the vapour.

At the bubble point (98 °C) all is liquid.
At the dew point (104 °C) all is vapor.
Feed composition: 30 mol% benzene ($z = 0.3$ molfr.).

The vapour fraction at 100 °C has to be calculated:

$t = 100$ °C.
$P_{tot} = 1000$ mbar.
Vapour pressure of benzene $p_{0B} = 1807$ mbar.
Vapour pressure of toluene $p_{0T} = 740$ mbar.
$P_{tot} = 1000$ m:

$$\text{Benzene } K_1 = \frac{p_{0B}}{P_{tot}} = \frac{1807}{1000} = 1.807$$

$$\text{Toluene } K_2 = \frac{p_{oT}}{P_{tot}} = \frac{740}{1000} = 0.74$$

$$\frac{V}{F} = \frac{0.3 * \frac{1.807-0.74}{1-0.74} - 1}{1.807 - 1} = 0.2864$$

Therefore, 28.64 mol% from the feed is vapour at 100 °C!

Calculation of the compositions in liquid and vapour at $t = 100$ °C:

$$x_1 = \frac{1 - 0.74}{1.807 - 0.74} = 0.2437$$

➔ 24.37 mol% benzene in the liquid.
$y_1 = 1.807 * 0.2437 = 0.44$
➔ 44 mol% benzene in the vapour phase.

For the design of condensers and reboilers for mixtures the condensation curve or the flash curve is required.

In these curves the vapour fraction V/F of the mixture based on the feed rate F is plotted over the temperature of the mixture.

Example 2.8.2: Calculation of the condensation curve for the mixture benzene–o–xylene.

Inlet composition: $z = 0.576 = 57.6$ mol% benzene with vapour mixture.

T (°C)	K_1	K_2	V/F	x_1	y_1
96	1.57	0.22	0	0.576	0.906
98.9	1.74	0.25	0.2	0.502	0.874
104	2	0.3	0.4	0.41	0.82
110.2	2.34	0.37	0.6	0.318	0.748
116.2	2.72	0.448	0.8	0.242	0.66
121	3.07	0.52	1	0.188	0.576

Calculation at *T* = 96 °C:

$$\frac{V}{F} = \frac{z_1 * \frac{K_1 - K_2}{1 - K_2} - 1}{K_1 - 1} = \frac{0.576 * \frac{1.57 - 0.22}{1 - 0.22}}{1.57 - 1} = 0$$

$$x_1 = \frac{1 - K_2}{K_1 - K_2} = \frac{1 - 0.22}{1.57 - 0.22} = 0.576 \qquad y_1 = K_1 * x_1 = 1.57 * 0.576 = 0.906$$

Calculation at *T* = 98.9 °C:

$$\frac{V}{F} = \frac{0.576 * \frac{1.74 - 0.25}{1 - 0.25} - 1}{1.74 - 1} = 0.2$$

$$x_1 = \frac{1 - 0.25}{1.74 - 0.25} = 0.502 \qquad y_1 = 1.74 * 0.502 = 0.874$$

Calculation at *T* = 116.2 °C:

$$\frac{V}{F} = \frac{0.576 * \frac{2.72 - 0.448}{1 - 0.448} - 1}{2.72 - 1} = 0.8$$

$$x_1 = \frac{1 - 0.448}{2.72 - 0.448} = 0.242 \qquad y_1 = 2.72 * 0.242 = 0.66$$

Calculation at *T* = 121 °C:

$$\frac{V}{F} = \frac{0.576 * \frac{3.07 - 0.52}{1 - 0.52} - 1}{3.07 - 1} = 1$$

$$x_1 = \frac{1 - 0.52}{3.07 - 0.52} = 0.188 \qquad y_1 = 3.07 * 0.188 = 0.576$$

The condensation curve for the benzene–o–xylene mixture is depicted in Fig. 2.9. The molar vapour fraction *V*/*F* drops from *V*/*F* = 1 at dew point at 121 °C to *V*/*F* = 0 at bubble point 96 °C. The concentration of the light components of benzene in the vapour and liquid phase against temperature are plotted in Fig. 2.10.

The required heat loads for the condensation of the benzene–o–xylene mixture result from the enthalpies for the cooling of the vapour mixture along with the condensing and the cooling of the condensate. Figure 2.11 gives the calculated heat loads for condensing a mixture of 1000 kg/h benzene and 1000 kg/h o–xylene as function of temperature. In condensing and cooling from the dew point (121 °C) to the bubble point (96 °C) of the mixture the required heat load increases from 0 to 230 kW.

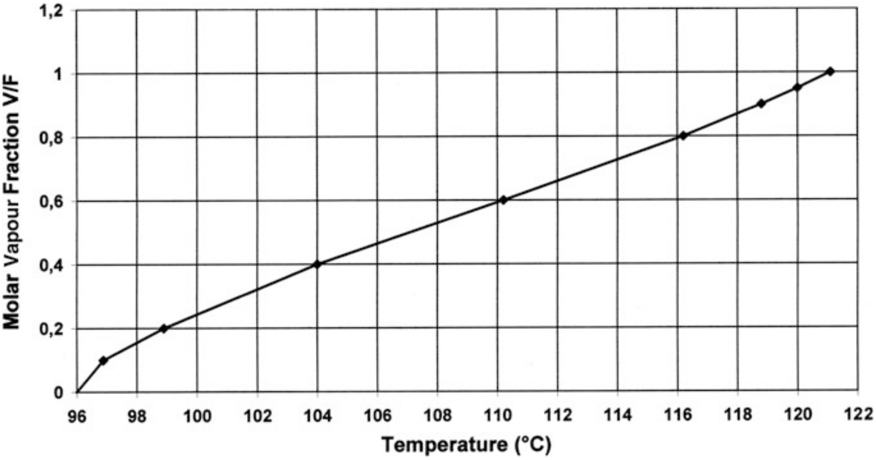


Fig. 2.9 Condensation *curve* for the benzene–o–xylene mixture given in Example 2.8.2

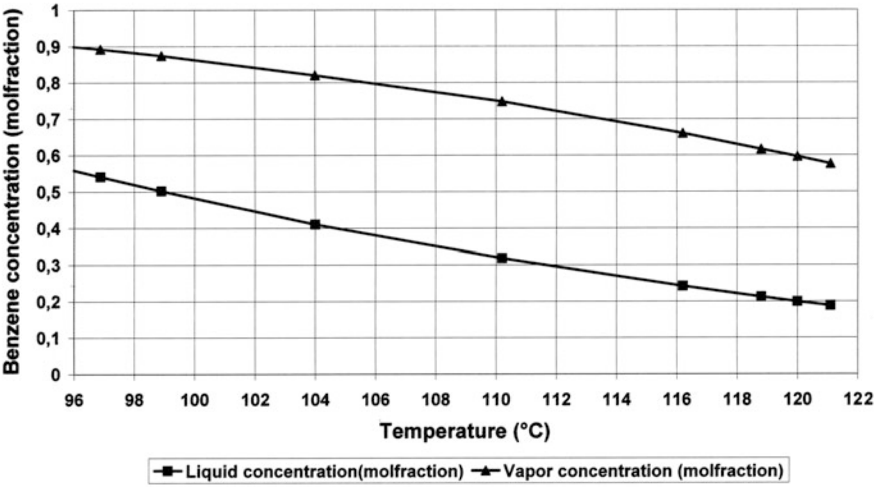


Fig. 2.10 Benzene compositions in the vapour and liquid phase as function of temperature

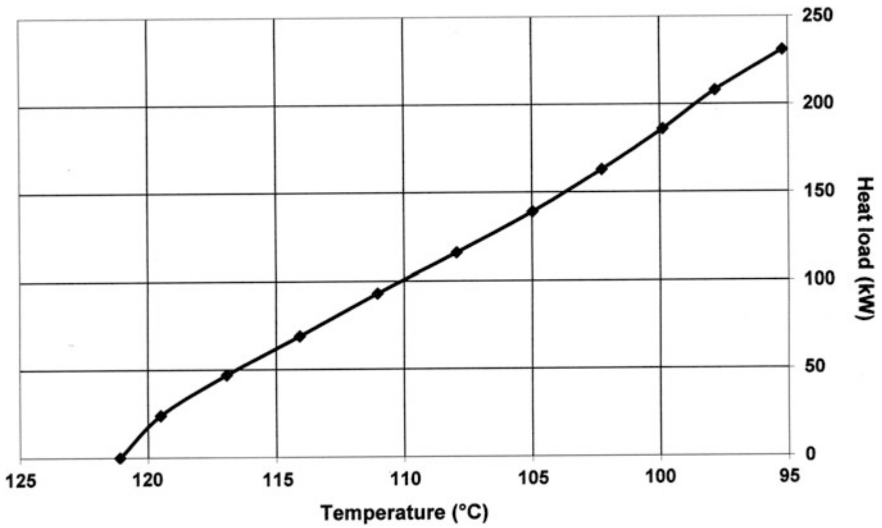


Fig. 2.11 Heat load *curve* for the condensation of 2 tonnes/h of the benzene–o–xylene mixture as a function of temperature

Example 2.8.3: Flash calculations for a mixture of 30 mol% butane and 70 mol% pentane.

Pressure (bar)	Boiling point temperature (°C)	Dew point temperature (°C)
	$x_{\mathrm{But}} = 0.3$ $x_{\mathrm{Pen}} = 0.7$	$y_{\mathrm{But}} = 0.3$ $y_{\mathrm{Pen}} = 0.7$
1	19.5	28.9
2	41	50
3	55.3	64
4	66.3	74.7

Flash calculation at 4 bar:

Temperature (°C)	Molar ratio *V*/*F*
66	0.0
67	0.061
68	0.149
69	0.242
70	0.341
71	0.448
72	0.567
73	0.703
74	0.861
75	1.0

V = vapour rate (kmol/h); F = feed rate (kmol/h)

Figure 2.12 depicts the bubble points and dew points of the mixture as a function of pressure.

The flash curve of the mixture of 30 mol% butane and 70 mol% pentane at a pressure of 4 bar is shown in Fig. 2.13.

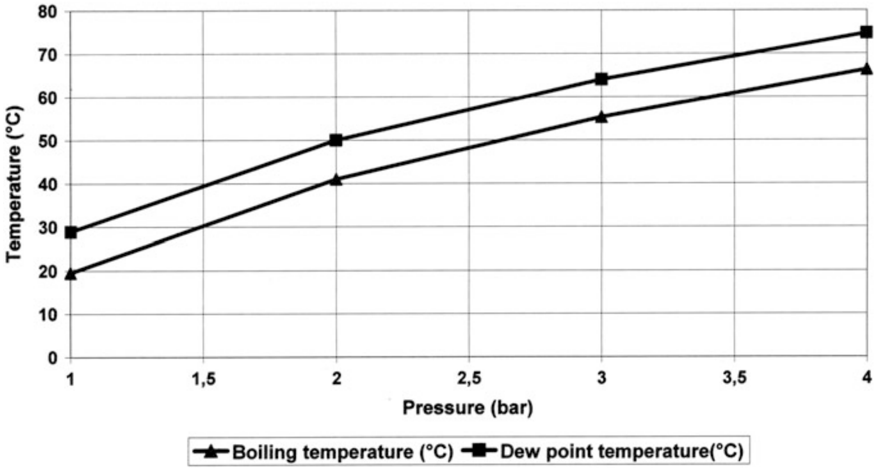


Fig. 2.12 Bubble points and dew points of the butane–pentane mixture as function of pressure

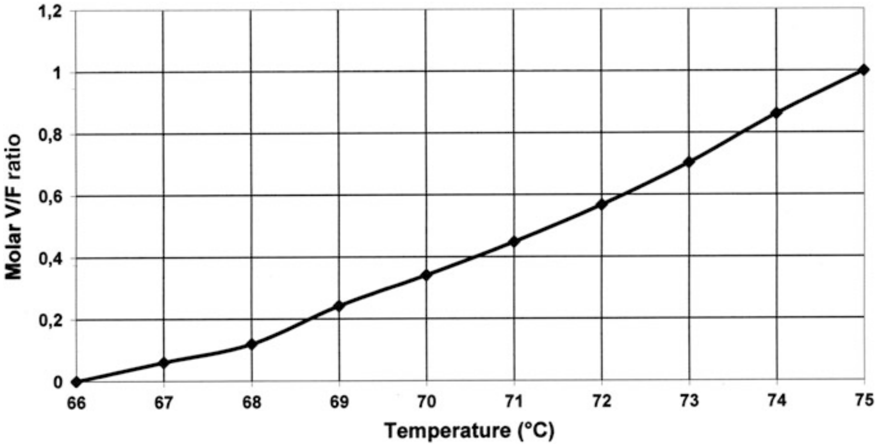


Fig. 2.13 Flash *curve* for the V/F ratio of the butane–pentane mixture at 4 bar as a function of temperature

2.9 Calculation of the Equilibrium and the Bubble and Dew Point Temperatures of Ideal Multi-component Mixtures

In principle the same laws and equations hold as in the calculations for binary component mixtures.

$$P_{\text{tot}} = x_1 * p_{01} + x_2 * p_{02} + x_3 * p_{03} + x_i * p_{0\text{i}}$$

$$y_i = K_i * x_i = x_i * \frac{p_{0\text{i}}}{P_{\text{tot}}} \qquad x_i = y_i * \frac{P_{\text{tot}}}{p_{0\text{i}}} = \frac{y_i}{K_i}$$

With the relative volatility α based on the vapour pressure $p_{0\text{h}}$ of the heaviest component

$$\alpha_1 = \frac{p_{01}}{p_{0\text{h}}} \qquad \alpha_2 = \frac{p_{02}}{p_{0\text{h}}} \qquad \alpha_3 = \frac{p_{03}}{p_{0\text{h}}}$$

$$y_1 = \frac{\alpha_1 * x_1}{\sum(\alpha_1 * x_1 + \alpha_2 * x_2 + \alpha_3 * x_3)} = \frac{\alpha * x}{\sum \alpha_i * x_i}$$

$$x_1 = \frac{y_1/\alpha_1}{\sum(y_1/\alpha_1 + y_2/\alpha_2 + y_3/\alpha_3)} = \frac{y/\alpha}{\sum y_i/\alpha_i}$$

Example 2.9.1: Calculation of the vapour phase composition for a benzene–toluene–xylene mixture.

Benzene : 30 mol%	$x_1 = 0.3$	$p_{01} = 1795$ mbar at 100 °C
Toluene : 60 mol%	$x_2 = 0.6$	$p_{02} = 732$ mbar at 100 °C
Xylene : 10 mol%	$x_3 = 0.1$	$p_{03} = p_{0\text{S}} = 306$ mbar at 100 °C

Calculation of the bubble pressure:

$$P_{\text{boil}} = 0.3 * 1795 + 0.6 * 732 + 0.1 * 306 = 1008\,\text{mbar}$$

The bubble point lies at 100 °C and 1008 mbar total pressure.
What is the composition of the vapour?

$$\text{Benzene } y_1 = x_1 * \frac{p_{01}}{P_{\text{tot}}} = 0.3 * \frac{1795}{1008} = 0.534 \text{ molfr.}$$

$$\text{Toluene } y_2 = 0.6 * \frac{732}{1008} = 0.435 \text{ molfr.}$$

$$\text{Xylene } y_3 = 0.1 * \frac{306}{1008} = 0.031 \text{ molfr.}$$

Cross-check calculation for the liquid composition x_1 of benzene:

$$x_1 = \frac{y_1 * P_{\text{tot}}}{P_{01}} = \frac{0.534 * 1008}{1795} = 0.3 \text{ molfr.}$$

Alternative calculation of the vapour composition using the relative volatility α based on the vapour pressure of the heaviest component xylene with P_{0h} = 306 mbar:

$$\alpha_1 = \frac{1795}{306} = 5.87 \qquad \alpha_2 = \frac{732}{306} = 2.39 \qquad \alpha_3 = \frac{306}{306} = 1$$

$$y_1 = \frac{0.3 * 5.87}{0.3 * 5.87 + 0.6 * 2.39 + 0.1 * 1} = 0.534 \text{ molfr.}$$

$$y_2 = \frac{0.6 * 2.39}{0.3 * 5.87 + 0.6 * 2.39 + 0.1 * 1} = 0.435 \text{ molfr.}$$

$$y_3 = \frac{0.1 * 1}{0.3 * 5.87 + 0.6 * 2.39 + 0.1 * 1} = 0.031 \text{ molfr.}$$

Cross-check calculation for x_1:

$$x_1 = \frac{y_1/\alpha_1}{\sum y/\alpha} = \frac{0.534/5.87}{0.534/5.87 + 0.435/2.39 + 0.031/1} = 0.3 \text{ molfr.}$$

The calculation of the bubble and dew points follows using the equations from Sects. 2.3 **and** 2.4.

The **bubble point** of a mixture is defined as follows: $\Sigma y_i = \Sigma K_i * x_i = 1$
The **bubble pressure** can be calculated directly: $P_{\text{boil}} = x_1 * p_{01} + x_2 * p_{02} + x_3 * p_{03}$
The **dew point** of a mixture is defined as follows: $\Sigma x_i = \Sigma y_{i/} K_i = 1$
The **dew pressure** for the vapour composition z can be calculated directly:

$$\frac{1}{P_{\text{dew}}} = \frac{z_1}{p_{01}} + \frac{z_2}{p_{02}} + \frac{z_3}{p_{03}} + \frac{z_4}{p_{04}} \qquad P_{\text{dew}} = \left[\sum \frac{z_i}{p_{0i}}\right]^{-1}$$

Example 2.9.2: Calculation of the bubble point for a four-component mixture C_{14}–C_{17} at a pressure of 100 mbar.

$$x_1 = 0.315 \quad x_2 = 0.276 \quad x_3 = 0.227 \quad x_4 = 0.182$$

The vapour pressures of the individual components are calculated.
The sum of the partial pressures $\sum P_i$ is plotted against temperature.

Temperature (°C)	Vapour pressure (mbar)				$\sum x_i * p_{0i} = \sum P_i$
	C_{14}	C_{15}	C_{16}	C_{17}	
175	116.4	68.7	40.7	24.5	69.3 mbar
180	137.2	82.3	49.5	29.9	82.6 mbar
184	156.1	94.6	57.5	34.9	94.7 mbar
186	166.3	101.4	62	37.6	101.3 mbar

A bubble point temperature of 185.5 °C at 100 mbar is achieved by interpolation (Fig. 2.14).

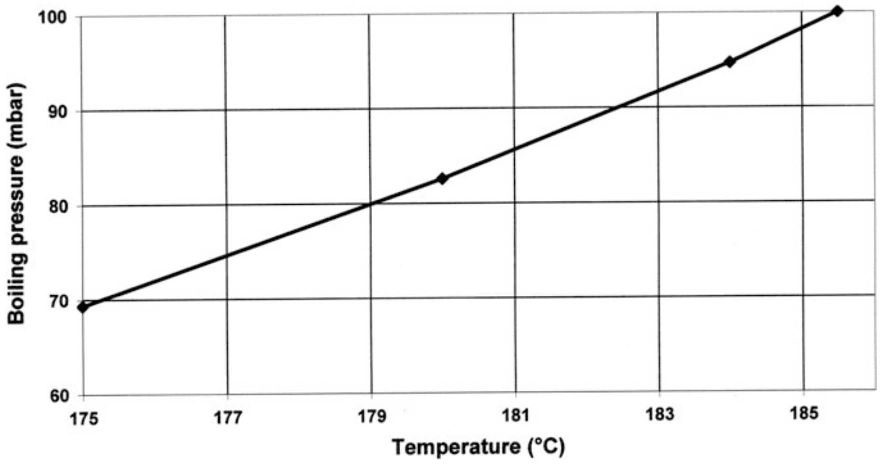


Fig. 2.14 Bubble point determination for the C_{14}–C_{17} mixture

Example 2.9.3: Calculation of the dew point for a four-component C_{14}–C_{17} mixture at 100 mbar.

$$\text{Vapor composition}: z_1 = 0.315 \qquad z_2 = 0.276 \qquad z_3 = 0.227 \qquad z_4 = 0.182$$

The vapour pressures are calculated using the Antoine Constants.

The quotient $\sum z_i/p_{0i}$ is calculated for different temperatures.

At total pressure $P = 100$ mbar the dew point lies at the quotient $\sum z_i/p_{0i} = 1/100 = 0.01$.

Temperature (°C)	Vapor pressure (mbar)				$\sum z_i/p_{0i}$
	C_{14}	C_{15}	C_{16}	C_{17}	
200	255.0	160.2	101.3	62.7	0.0081
198	240.3	150.4	94.7	58.4	0.00866
196	226.4	141.1	88.4	54.4	0.00925
194	213.0	132.3	82.5	50.6	0.00985
192	200.5	123.9	76.9	47.1	0.0106

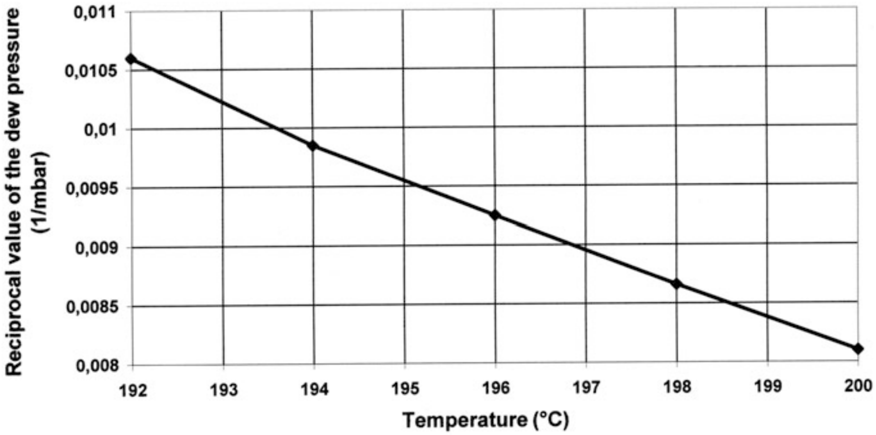


Fig. 2.15 Determination of the dew point temperature for a C_{14}–C_{17} mixture

A dew point temperature of 193.6 °C at 100 mbar is achieved by interpolation (Fig. 2.15).

2.10 Flash Calculations for Ideal Multi-component Mixtures [2]

For mixtures with more than two components the calculation must be performed iteratively. The individual V/F values of the different components are calculated with an estimate of V/F. The sum of the V/F values of the component must equal the V/F estimate.

$$\frac{V}{F} = \sum \frac{z_i}{1 + \frac{L}{V * K_i}} \qquad \frac{L}{V} = \frac{F}{V} - 1 = \frac{1}{V/L}$$

$$y_i = \frac{F}{V} * \left(\frac{z_i}{1 + \frac{L}{V * K_i}} \right) \qquad x_i = \frac{F}{V} * \left(\frac{z_i}{K_i + \frac{L}{V}} \right)$$

The following is required for the calculation: the vapour composition z_i of the individual components as mole fractions and the equilibrium constants $K_i = p_{0i}/P_{\text{tot}}$. The calculation is carried out iteratively with an estimate of V/F value.

$$\frac{L}{V} = \frac{F}{V} - 1$$

V/*F* = molar ratio of the vapour rate *V* to the feed rate *F*.
F/*V* = molar ratio of the feed rate *F* to the vapour rate *V*.
L/*V* = molar ratio of the liquid rate *L* to the vapour rate *V*.

Example 2.10.1: Calculation of the *L*/*V* ratio.
V/*F* = 0.5 which means that 50% of the feed in kmol/h is vapour.

$$\frac{L}{V} = \frac{F}{V} - 1 = \frac{1}{0.5} - 1 = 1$$

Example 2.10.2: Flash calculation for a four-component C_{14}–C_{17} mixture.
Pressure: 100 mbar
Temperature: 188 °C

First estimate: *V*/*F* = 0.3; *L*/*F* = 2.33

Component	z_i (molfr.)	P_{0i} (mbar)	K_i	$\frac{z_i}{1+2.33*\frac{1}{K_i}}$
C14	0.315	177	1.77	0.1359
C15	0.276	109	1.09	0.0879
C16	0.227	67	0.67	0.0507
C17	0.182	41	0.41	0.0272
				0.3017 = V/F_i

$\sum V/F_i = 0.3017 > V/F_{\text{chosen}}$ → choose the higher value for *V*/*F* → *V*/*F* = 0.32 → *L*/*V* = 2.125

Component	z_i (molfr.)	$\frac{z_i}{1+2.125*\frac{1}{K_i}}$
C14	0.315	0.14315
C15	0.276	0.09357
C16	0.227	0.05442
C17	0.182	0.02944
		0.32058 = V/F_i

$\sum V/F_i > V/F_{\text{chosen}}$ → choose the higher value for *V*/*F* → *V*/*F* = 0.33 → ***L*/*V* = 2.03**

Component	z_i (molfr.)	$\frac{z_i}{1+2.03*\frac{1}{K_i}}$
C14	0.315	0.14671
C15	0.276	0.09641
C16	0.227	0.05632
C17	0.182	0.03058
		0.33002 = V/F_i

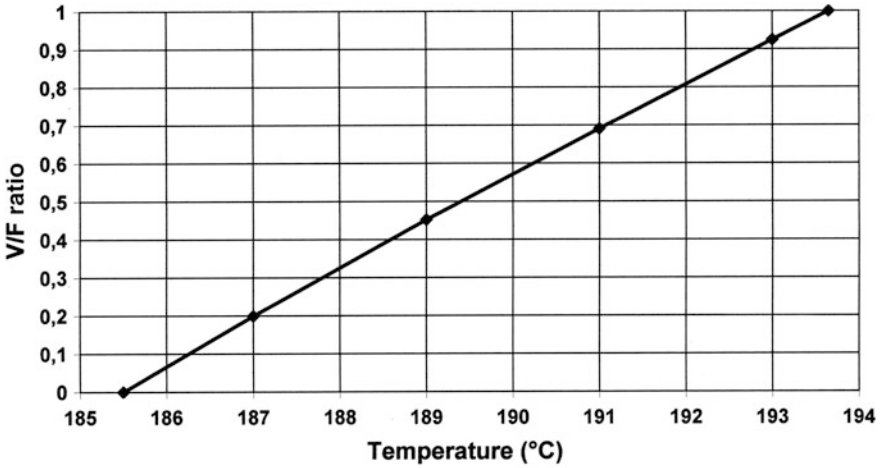


Fig. 2.16 Flash *curve* for the C_{14}–C_{17} mixture with a molar V/F ratio as a function of temperature

If the ratio $\sum V_i/F_i < V/F \rightarrow$ choose the lower value of *V/F*!
If the ratio $\sum V_i/F_i > V/F \rightarrow$ choose the higher value for *V/F*!
A deviation of 0.0005 is sufficiently accurate!
The flash curve for the C_{14}–C_{17} mixture is depicted in Fig. 2.16.

2.11 Phase Equilibrium of Non-ideal Binary Mixtures

With non-ideal mixtures the laws of Raoult and Dalton are invalid. The partial pressure lines are non-linear. Instead they curve upward or downward. Figure 2.17 shows the real partial pressures of methanol and water at 60 °C, considering the activity coefficient and also the total pressure resulting from the partial pressures as functions of the methanol composition.

With the ideal calculation the curves are linear according to the laws of Raoult and Dalton. This is shown in Fig. 2.2. With the real calculation, considering the activity factor γ for the non-ideal behavior, the curves of partial pressure and total pressure curve upward. A higher total pressure and a lower bubble point temperature results for the mixture.

With azeotropic mixtures vapour pressure maxima and vapour pressure minima can occur. This is shown in Figs. 2.18 and 2.19 for a mixture from *A* and *B*. The calculation must be performed with a correction factor for the interaction of the partial pressures. This correction factor is termed the activity coefficient γ. The activity coefficient is dependent on the composition in the liquid phase and the temperature.

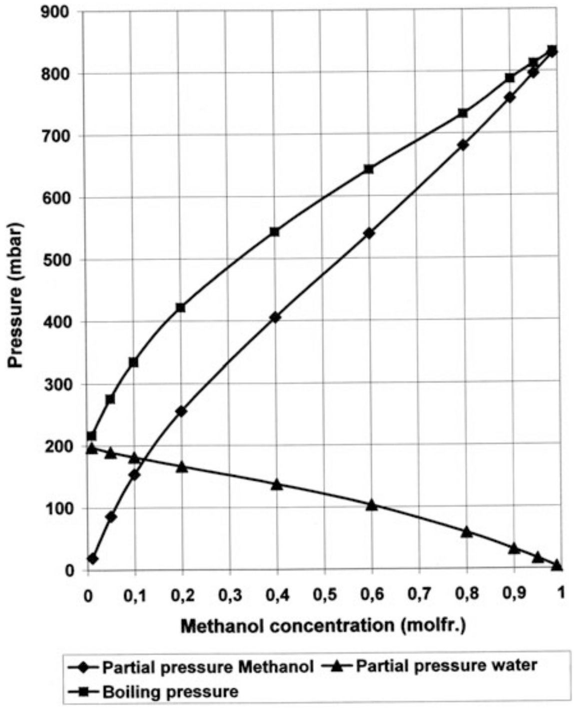


Fig. 2.17 Partial pressure and total pressure for the non-ideal methanol–water mixture at 60 °C as function of methanol composition in the liquid

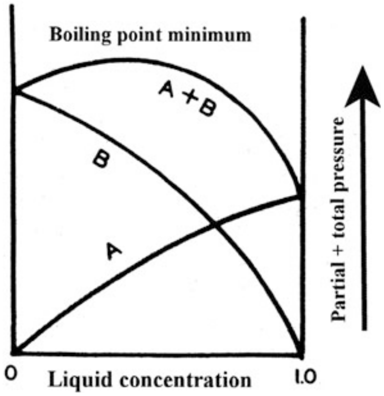


Fig. 2.18 Partial pressures for *A* and *B* and total pressure *A* + *B* for an azeotropic mixture with a bubble point minimum

In the calculation of the equilibria for two-component and multi-component mixtures the interactions of the partial pressures are considered using the **activity coefficients**. Section 2.12 shows how the activity coefficient is calculated using different models. The following table of activity coefficients for methanol and water at 60 °C illuminates the influence of the composition on the activity coefficient.

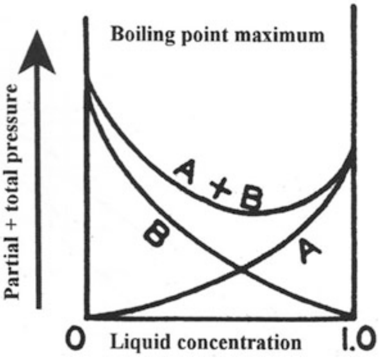


Fig. 2.19 Partial pressures for *A* and *B* and total pressure *A* + *B* for an azeotropic mixture with a bubble point maximum

Methanol composition (molfraction)	Activity coefficient of methanol	Activity coefficient of water
0.01	2.3069	1.002
0.05	2.0657	1.0035
0.1	1.8356	1.0131
0.2	1.5263	1.0462
0.4	1.2113	1.152
0.6	1.0737	1.2967
0.8	1.0153	1.4737
0.9	1.0035	1.5737
0.99	1.000	1.67

The correction of the partial pressures of the components of a mixture using the activity coefficient γ influences the vapour–liquid equilibrium as follow:

$$P_{\text{tot}} = \gamma_1 * x_1 * p_{01} + \gamma_2 * x_2 * p_{02} (\text{mbar})$$

$$y_1 * P_{\text{tot}} = \gamma_1 * x_1 * p_{01}$$

Vapor composition:

$$y_1 = \frac{x_1 * p_{01} * \gamma_1}{P_{\text{tot}}} \text{ (molfr.)} \qquad y_2 = \frac{x_2 * p_{01} * \gamma_2}{P_{\text{tot}}} \text{ (molfr.)}$$

Equilibrium constant:

$$K_1 = \frac{p_{01} * \gamma_1}{P_{\text{tot}}} \qquad K_2 = \frac{p_{02} * \gamma_2}{P_{\text{tot}}}$$

Separation factor = Relative volatility α:

$$\alpha = \frac{K_1}{K_2} = \frac{\gamma_1 * P_{01}}{\gamma_2 * P_{02}}$$

K_1 = equilibrium factor for component 1
K_2 = equilibrium factor for component 2
P_{tot} = total pressure in the system (mbar)
p_{01} = vapour pressure of component 1 (mbar)
p_{02} = vapour pressure of component 2 (mbar)
x_1 = liquid composition of component 1
y_1 = vapour composition of component 1
x_2 = liquid composition of component 2
y_2 = vapour composition of component 2
γ_1 = activity coefficient of component 1
γ_2 = activity coefficient of component 2

The activity coefficient γ is strongly dependent on composition and can be calculated using different models: Wilson, NRTL, Uniquac, and Unifac.

Example 2.11.1: Non-ideal equilibrium for **methanol–water**
Below is the equilibrium calculation for a methanol [1]–water [2] mixture at 92.1 °C and P_{tot} = 1000 mbar.

Required data for calculation:

$$\begin{array}{ll} \mathrm{x}_1 = 0.0535 & \mathrm{x}_2 = 0.9465 \\ \gamma_1 = 1.848 & \gamma_2 = 1.004 \\ \mathrm{p}_{01} = 2.817\ \mathrm{mbar} & \mathrm{p}_{02} = 756.4\ \mathrm{mbar} \end{array}$$

$$y_1 = \frac{1.848 * 0.0535 * 2817}{1000} = 0.279$$

$$y_2 = \frac{1.004 * 0.9465 * 756.4}{1000} = 0.721$$

$$K_1 = \frac{1.848 * 2817}{1000} = 5.218 \quad K_2 = \frac{1.004 * 756.4}{1000} = 0.761$$

$$\alpha = \frac{K_1}{K_2} = \frac{5.218}{0.761} = 6.853$$

For comparison purposes **the ideal relative volatility,** without considering the activity coefficient, is calculated below:

$$\alpha_{\text{ideal}} = \frac{p_{01}}{p_{02}} = \frac{2.817}{756.4} = 3.724$$

Conclusion: The influence of γ is substantial! Due to the activity coefficient the separation factor is nearly doubled. The activity coefficient γ depends on the temperature and very strongly on the composition in the liquid phase.

Example 2.11.2: Activity coefficient at different compositions.
Influence of the composition on the activity coefficient of methanol [1] in water [2] at 30 °C.

x_1 = methanol composition in the liquid γ_1 = activity coefficient of methanol

x_1	0.001	0.01	0.1	0.15	0.2
γ_1	2.596	2.521	1.968	1.765	1.609

The dependency on the *temperature* is shown in the following table for $x = 0.1$.

Temperature	30 °C	60 °C	85 °C
γ according to Wilson	1.968	1.836	1.744

Remark At an azeotropic composition $y = x$ and $\alpha = 1$. Thus it follows that $\Rightarrow p_{01}/p_{02} = \gamma_2/\gamma_1$

An azeotropic point is reached if the activity coefficient in the diluted phase is greater than the vapour pressure ratio. In the following Figs. 2.20, 2.21, 2.22 and 2.23 some vapour–liquid equilibria of non-ideal mixtures are depicted. To illuminate the pressure dependency of the phase equilibrium the equilibria at different pressures are shown.

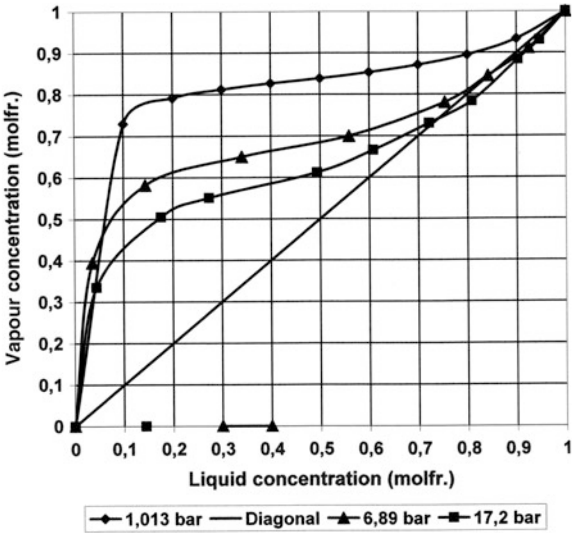


Fig. 2.20 Vapour–liquid equilibrium of acetone–water at different pressures

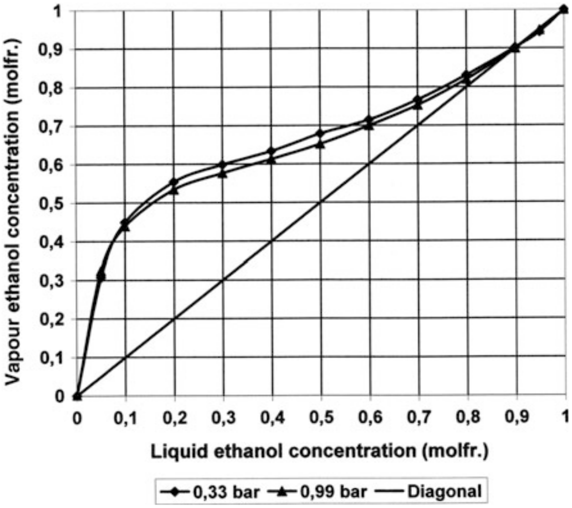


Fig. 2.21 Equilibrium of the azeotropic ethanol–water mixture at different pressures

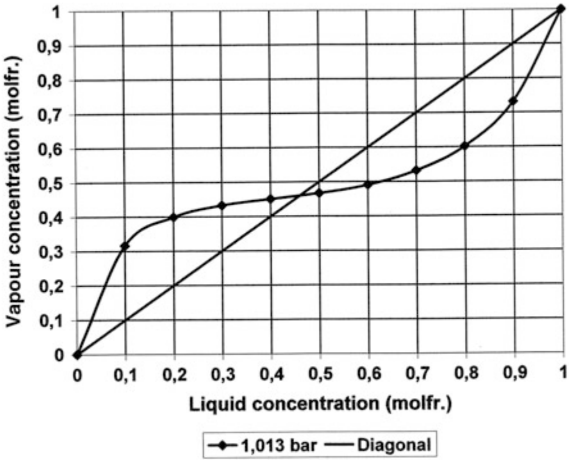


Fig. 2.22 Equilibrium of the azeotropic ethanol–benzene mixture with a minimum bubble point

Other examples for azeotropes with minimum bubble points are:
Ethylacetate–ethanol
Isopropanol–water
Methanol–benzene
Water–butanol
Methanol–trichlorethylene
Sulphur carbon–acetone

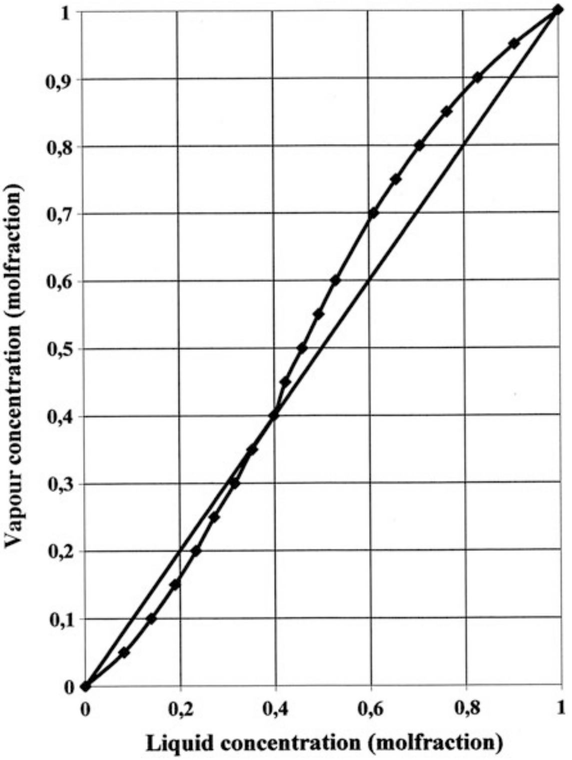


Fig. 2.23 Equilibrium of the azeotropic acetone–chloroform mixture at 1013 bar with a maximum bubble point

Other examples of azeotropes with maximum bubble points are:
Saltpetre acid–water
Water–formic acid

2.12 Calculation of the Activity Coefficients

The calculation of the activity coefficients using different models is described in the Refs. [3–6]. The required data for the calculations are given in [7]. In the following text the calculation of the activity coefficients using 3 models is shown. A fourth method is the **Unifac Model**, a group contribution method which does not require measured equilibrium data.

2.12.1 Calculation According to Wilson for Miscible Components [8]

$$\Lambda_{1,2} = \frac{V_2}{V_1} * \exp\left(\frac{\lambda_{12}}{R * T}\right)$$

$$\Lambda_{2,1} = \frac{V_1}{V_2} * \exp\left(\frac{\lambda_{12}}{R * T}\right)$$

$$\ln \gamma_1 = -\ln\left(X_1 + X_2 * \Lambda_{1,2}\right) + X_2 * \left[\frac{\Lambda_{1,2}}{X_1 + X_2 * \Lambda_{1,2}} - \frac{\Lambda_{2,1}}{X_2 + X_1 * \Lambda_{2,1}}\right]$$

$$\ln \gamma_1^{\infty} = 1 - \ln \Lambda_{1,2} - \Lambda_{2,1}$$

Required data:

λ_{12} and λ_{21} = interaction parameter.
v_1 and v_2 = molar volume of the liquid.

Example 2.12.1: Methanol [1]**–water** [2] **at 30 °C and x_1 = 0.1**.

$$\lambda_{12} = -107.389 \quad v_1 = 40.73$$
$$\lambda_{21} = 469.578 \quad v_2 = 18.07$$

$$\Lambda_{1,2} = \frac{18.07}{40.73} * \exp\left(-\frac{-107.389}{1.987 * 303}\right) = 0.371$$

$$\Lambda_{2,1} = \frac{40.73}{18.07} * \exp\left(-\frac{469.578}{1.987 * 303}\right) = 1.033$$

$$\ln \gamma_1 = -\ln(0.1 + 0.371 * 0.9) + 0.9 * \left[\frac{0.371}{0.1 + 0.371 * 0.9} - \frac{1.033}{1.033 * 0.1 + 0.9}\right]$$

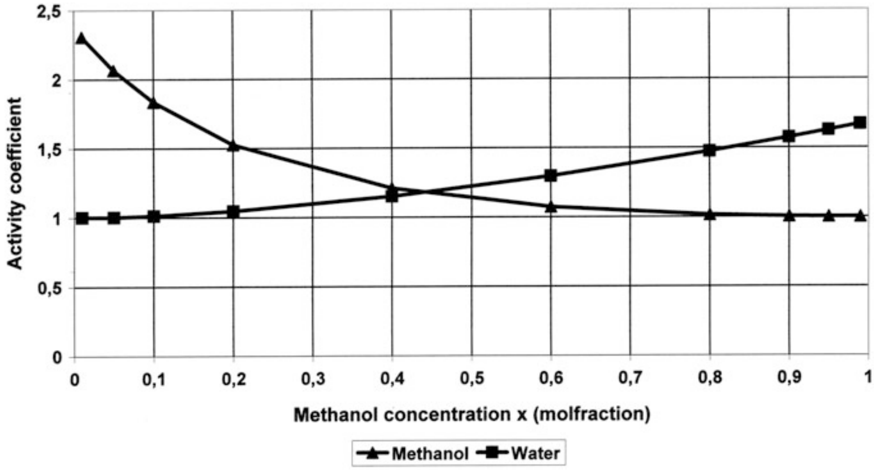


Fig. 2.24 Activity coefficients of methanol and water at 60 °C as a function of the methanol composition in the mixture

ln γ_1 = 0.677 ⇒ γ_1 = 1.968

ln γ^{∞} = 1 - ln 0.371 – 1.033 = 0.958 γ^{∞} = 2.607

γ^{∞} = activity coefficient at infinite dilution.

In Fig. 2.24 the activity coefficients of methanol and water at different compositions are shown.

Example 2.12.2: Calculation of the vapour–liquid equilibrium at 75.7 °C.

Methanol composition x_1 = 0.3909
Water composition x_2 = 0.6091
Methanol vapour pressure p_{01} = 1.526.8 mbar
Water vapour pressure p_{02} = 413.8 mbar
$\Lambda_{1,2}$ = 0.47525
$\Lambda_{2,1}$ = 0.98356
P_{tot} = 1013 mbar

Calculation of the activity coefficient γ_1 of methanol:

$$\ln \gamma_1 = -\ln\left(x_1 + x_2 * \Lambda_{1,2}\right) + x_2 * \left[\frac{\Lambda_{1,2}}{x_1 + x_2 * \Lambda_{1,2}} - \frac{\Lambda_{2,1}}{x_2 + x_1 * \Lambda_{2,1}}\right]$$

$$\ln \gamma_1 = -\ln(0.3909 + 0.6091 * 0.47525)$$

$$+0.6091 * \left[\frac{0.47525}{0.3909 + 0.6091 * 0.47525} - \frac{0.98356}{0.6091 + 0.3909 * 0.98356}\right]$$

$$\ln \gamma_1 = 0.2076 \qquad \gamma_1 = 1.231$$

Calculation of the activity coefficient γ_2 of water:

$$\ln \gamma_2 = -\ln\left(x_2 + x_1 * \Lambda_{2,1}\right) - x_1 * \left[\frac{\Lambda_{1,2}}{x_1 + x_2 * \Lambda_{1,2}} - \frac{\Lambda_{2,1}}{x_1 * \Lambda_{2,1} + x_2}\right]$$

$$\ln \gamma_2 = -\ln(0.6091 + 0.3909 * 0.98356)$$

$$-0.3909 * \left[\frac{0.47525}{0.3909 + 0.6091 * 0.47525} - \frac{0.98356}{0.6091 + 0.3909 * 0.98356}\right]$$

$$\ln \gamma_2 = 0.120359 \quad \gamma_2 = 1.128$$

Calculation of the methanol composition y_1 and the water composition y_2 in the vapour:

$$y_1 = \frac{x_1 * p_{01} * \gamma_1}{P_{\text{tot}}} = \frac{0.3909 * 1526.8 * 1.231}{1013} = 0.72 \text{ molfr.}$$

$$y_2 = \frac{x_2 * p_{02} * \gamma_2}{P_{\text{tot}}} = \frac{0.6091 * 413.8 * 1.128}{1013} = 0.28 \text{ molfr.}$$

Calculation of the vapour composition with relative volatility α:

$$\alpha = \frac{\gamma_1 * p_{01}}{\gamma_2 * p_{02}} = \frac{1.231 * 1526.8}{1.128 * 413.8} = 4.027$$

$$y_1 = \frac{\alpha_{1,2} * x_1}{1 + \left(\alpha_{1,2} - 1\right) * x_1} = \frac{4.027 * 0.3909}{1 + (4.027 - 1) * 0.3909} = 0.72$$

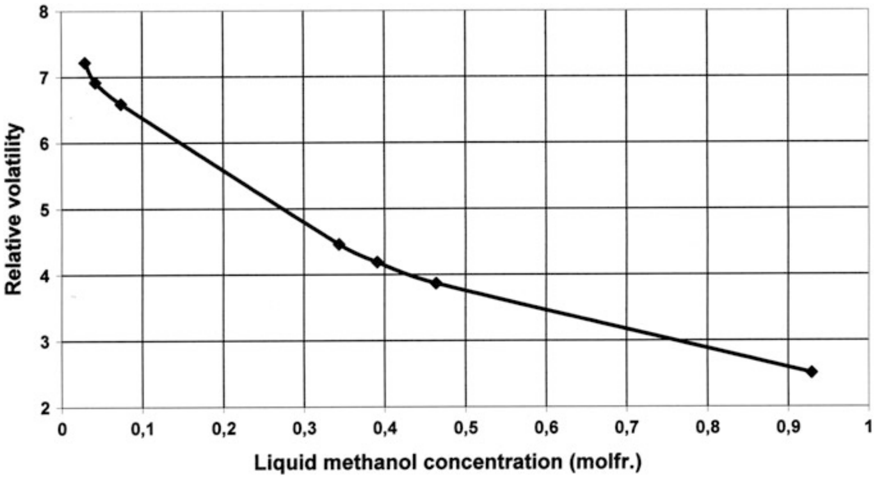


Fig. 2.25 Relative volatility α for methanol–water as function of the methanol composition in the liquid phase

From Fig. 2.25 it can be seen that the separation factor α for the non-ideal mixture methanol–water decreases with increasing methanol composition.

2.12.2 Calculation According to NRTL for Partially Miscible Components with Two Liquid Phases [9]

$$\tau_{12} = \frac{g_{12}}{R * T} \qquad \tau_{21} = \frac{g_{21}}{R * T}$$

$$G_{12} = \exp(-\alpha_{12} * \tau_{12}) \quad G_{21} = \exp(-\alpha_{21} * \tau_{21})$$

$$\ln \gamma_1 = X_2^2 * \left[\tau_{21} * \left(\frac{G_{21}}{X_1 + X_2 + G_{21}}\right)^2 + \frac{\tau_{12} * G_{12}}{(X_2 + X_1 * G_{12})^2}\right]$$

$$\gamma^\infty = \tau_{21} + \tau_{12} * G_{12}$$

Required data:

g_{12} and g_{21} = interaction parameter

$\alpha_{12} = \alpha_{21}$ = non-randomness factor

Example 2.12.2.1: Methanol [1]–water [2] at 30 °C and x_1 = 0.1.

g_{12} = −253.965 cal/mol g_{21} = 845.16 cal/mol α_{12} = 0.299

$$\tau_{12} = \frac{-253.965}{1.987 * 303} = -0.422 \quad \tau_{21} = \frac{845.16}{1.987 * 303} = 1.4$$

$$G_{12} = \exp(-0.299 * -0.422) = 1.134$$

$$G_{21} = \exp(-0.299 * 1.404) = 0.657$$

$$\ln \gamma_1 = 0.9^2 * \left[1.404 * \left(\frac{0.657}{0.1 + 0.9 * 0.657}\right)^2 + \frac{-0.422 * 1.134}{(0.9 + 0.1 * 1.134)^2}\right]$$

$\ln \gamma_1 = 0.65 \Rightarrow \gamma_1 = 1.915$
$\ln \gamma_1^{\infty} = 1.404 + (-0.422) * 1.134 = 0.925 \Rightarrow \gamma_1^{\infty} = 2.522$

2.12.3 Calculation According to Uniquac for Components with a Miscibility Gap

$$\tau_{12} = \exp\left(-\frac{u_{12}}{R * T}\right) \quad \tau_{21} = \exp\left(-\frac{u_{21}}{R * T}\right)$$

$$\varphi_i = \frac{r_i * x_i}{\sum r_i * x_i} \quad \vartheta_i = \frac{q_i * x_i}{\sum q_i * x_i}$$

$$l_i = \frac{z}{2} * (r_i - q_i) - (r_i - 1)$$

$$\ln \gamma_1 = \ln \gamma_{1C} + \ln \gamma_{1R}$$

$$\ln \gamma_{1C} = \ln \frac{\varphi_1}{x_1} + \frac{z}{2} * q_1 * \ln \frac{\vartheta_1}{\varphi_1} + \varphi_2 * (l_1 - \frac{r_1}{r_2} * l_2)$$

$$\ln \gamma_{1R} = -q_1 * \ln(\vartheta_1 + \tau_{21} * \vartheta_2) + \vartheta_2 * q_1 * \left(\frac{\tau_{21}}{\vartheta_1 + \tau_{21} * \vartheta_2} - \frac{\tau_{12}}{\vartheta_2 + \tau_{12} * \vartheta_1}\right)$$

Required data:
u_{12} and u_{21} = interaction parameters.
r = volume parameter (van der Waals).
q = surface parameter (van der Waals).
z = coordination number (mostly = 10).

Example 2.12.3.1: Calculation of activity coefficient of methanol in a methanol–water mixture at 30 °C.

$$u_{12} = -328.451\,\text{cal/mol} \quad u_{21} = 506.088\,\text{cal/mol}$$
$$r_1 = 1.4311 \quad r_2 = 0.92$$
$$q_1 = 1.432 \quad q_2 = 1.40$$

Methanol composition x_{Meth} = 0.1 molfr. = 10 mol%

$$\varphi_1 = \frac{0.1 * 1.4311}{0.1 * 1.4311 + 0.9 * 0.92} = 0.147$$
$$\varphi_2 = 1 - 0.1473 = 0.853$$
$$\vartheta_1 = \frac{0.1 * 1.432}{0.1 * 1.432 + 0.9 * 1.4} = 0.102$$
$$\vartheta_2 = 1 - 0.102 = 0.898$$

l_1 = 10/2 * (1.4311 − 1.432) − (1.4311 − 1) = −0.4356
l_2 = 10/2 * (0.92 − 1.40) − (0.92 − 1) = −2.32

$$\tau_{12} = \exp\left(-\frac{-328.451}{1.987 * 303}\right) = 1.7255$$
$$\tau_{12} = \exp\left(-\frac{506.088}{1.987 * 303}\right) = 0.4314$$

$$\ln \gamma_{1C} = \ln \frac{0.147}{0.1} + \frac{10}{2} * 1.4311 * \ln \frac{0.102}{0.147}$$
$$+ 0.853 * \left[-0.4356 - \frac{1.4311}{0.92} * (-2.32)\right] = 0.471$$

$$\ln \gamma_{1R} = -1.432 * \ln(0.102 + 0.4314 * 0.898) + 0.898 * 1.432$$
$$* \left(\frac{0.4314}{0.102 + 0.898 * 0.4314} - \frac{1.7255}{0.898 + 0.102 * 1.7255}\right) = 0.0908$$

ln γ_1 = 0.477 + 0.0908 = 0.5678 ⇒ **γ_1 = 1.764**

2.12.4 Critical Comparison of the Activity Coefficients Calculated Using Different Models

The available models for equilibria calculations of distillation and absorption plants or the design of condensers and evaporators can be simplified with the use of computer. Substantial discrepancies can be seen if the results of the different calculation methods are compared. This is shown in the following Examples 2.12.4.1 and 2.12.4.2.

Example 2.12.4.1: Activity coefficients for a pentane–toluene mixture.
Composition: 10 mol% Pentane, 90 mol% Toluene

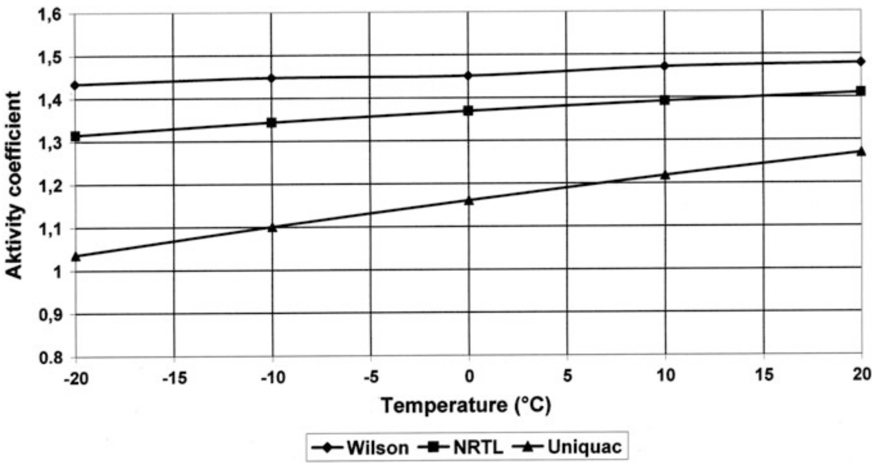


Fig. 2.26 Activity coefficient of pentane in toluene as function of temperature, using different models

Interaction parameters:

Wilson:	$\lambda_{11} = 0$	$\lambda_{12} = -296.9388$	$\lambda_{21} = 1145.5506$	$\lambda_{22} = 0$	
NRTL	$g_{11} = 0$	$g_{12} = 1401.7145$	$g_{21} = -490.4151$	$g_{22} = 0$	$\alpha = 0.298$
Uniquac	$u_{11} = 0$	$u_{12} = 869.1587$	$u_{21} = -436.4687$	$u_{22} = 0$	

Conclusion: The activity coefficients calculated using different models for pentane in toluene deviate considerably (Fig. 2.26). The activity coefficient of pentane becomes greater with increasing temperature. Additionally the non-temperature dependent activity coefficients of pentane are calculated according to Margules and van Laar.

Margules: $\gamma = 1.44$ for Pentane.

van Laar: $\gamma = 1.47$ for Pentane.

The activity coefficient of toluene lies constantly at 1.

Example 2.12.4.2: Activity coefficients for the a hexane, ethyl acetate, and toluene mixture

Composition:

Hexane: $x = 0.3 = 30$ mol%.
Ethyl acetate: $x = 0.3 = 30$ mol%.
Toluene: $x = 0.4 = 40$ mol%.

Interaction parameter	Wilson	Uniquac	NRTL	Alpha
1/1	0	0	0	0
1/2	107.1217	302.7052	427.6309	0.2995
1/3	21.0210	112.6399	130.3146	0.3016
2/1	618.7792	−83.8122	255.6205	0.2995
2/2	0	0	0	0
2/3	135.1766	−62.3228	63.3896	0.3021
3/1	246.4956	−57.7374	131.5420	0.3016
3/2	15.6079	63.3994	86.1714	0.3021
3/3	0	0	0	0

Calculation results:

	Wilson		Uniquac		NRTL	
	20 °C	30 °C	20 °C	30 °C	20 °C	30 °C
Hexane	1.373	1.36	1.37	1.358	1.376	1.363
Ethyl acetate	1.264	1.257	1.251	1.246	1.269	1.26
Toluene	1.031	1.03	1.017	1.018	1.029	1.028

The deviations range 0.2–1%!

2.13 Bubble Point, Dew Point, and Flash Separation for Non-ideal Binary Mixtures

For non-ideal mixtures the influence of the activity coefficient γ must be considered in the calculation of the partial pressure.

Example 2.13.1: Bubble point calculation with the activity coefficient for the methanol [1]**–water** [2] **mixture**.

$$\begin{array}{llll} x_1 = 0.1 & x_2 = 0.9 & t = 87.8\,^\circ\mathrm{C} & P_{\mathrm{tot}} = 1000\,\mathrm{mbar} \\ \gamma_1 = 1.705 & \gamma_2 = 1 & & \\ p_{01} = 2438\,\mathrm{mbar} & p_{02} = 646\,\mathrm{mbar} & & \end{array}$$

$\boldsymbol{P_{\mathrm{boil}} = x_1 * \gamma_1 * p_{01} + x_2 * \gamma_2 * p_{02} = 0.1 * 1.705 * 2438 + 0.9 * 1 * 646 = 997\ \mathrm{mbar} \approx 1\ \mathrm{bar}}$

Cross-check calculation of the bubble point:

$$K_1 = \frac{\gamma_1 * p_{01}}{P_{\mathrm{tot}}} = \frac{1.705 * 2438}{1000} = 4.167 \qquad K_2 = \frac{1 * 646}{1000} = 0.64$$

$\Sigma\, K_i * x_i = 0.1 * 4.167 + 0.9 * 0.64 = 1$

Therefore, the bubble point condition is fulfilled at 87.8 °C!

Without considering the activity coefficient γ a bubble point temperature of 93.1 °C rather than one of 87.8 °C is obtained.

Example 2.13.2: Dew point calculation with the activity coefficient γ for the methanol [1]-water [2] mixture.

$$\begin{array}{llll} y_1 = 0.1 & y_2 = 0.9 & t = 97.1\,^\circ\mathrm{C} & P_{\mathrm{tot}} = 1.000\,\mathrm{mbar} \\ \gamma_1 = 2.2 & \gamma_2 = 1.0 & & \\ p_{01} = 3.343\,\mathrm{mbar} & p_{02} = 910.3\,\mathrm{mbar} & & \end{array}$$

$$\frac{1}{P_{\mathrm{dew}}} = \frac{y_1}{\gamma_1 * p_{01}} + \frac{y_2}{\gamma_2 * p_{02}} = \frac{0.1}{2.2 * 3343} + \frac{0.9}{910.3} = 0.001 \qquad P_{\mathrm{dew}} = 1\ \mathrm{bar}$$

Cross-check calculation of the dew point:

$$K_1 = \frac{2.2 * 3343}{1000} = 7.373 \quad K_2 = \frac{1 * 910.3}{1000} = 0.9125$$

$$\sum \frac{y_i}{K_i} = \frac{0.1}{7.373} + \frac{0.9}{0.9125} = 1$$

Therefore, the dew point condition is fulfilled at 97.1 °C!

Example 2.13.3: Flash calculation for the methanol [1]–water [2] mixture

$$\begin{array}{lll} P_{\mathrm{tot}} = 1\,\mathrm{bar} = 1000\,\mathrm{mbar} & t = 92.1\,^\circ\mathrm{C} & \text{Feed rate} = 100\,\mathrm{kmol/h} \\ \text{Feed compositions:} & z_1 = 0.1\,\mathrm{molfr.} & z_2 = 0.9\,\mathrm{molfr.} \\ & \gamma_1 = 1.848 & \gamma_2 = 1.004 \\ & p_{01} = 2823.7\,\mathrm{mbar} & p_{02} = 758.3\,\mathrm{mbar} \end{array}$$

$$K_1 = \frac{1.848 * 2823.7}{1000} = 5.218 \quad K_2 = \frac{1.004 * 758.3}{1000} = 0.7614$$

$$\frac{V}{F} = \frac{z_1 * \frac{K_1 - K_2}{1 - K_2} - 1}{K_1 - 1} = \frac{0.1 * \frac{5.218 - 0.7614}{1 - 0.7614} - 1}{5.218 - 1} = 0.2058$$

At 92.1 °C 20.58% of the feed is vapour.
Vapour rate $V = 0.2058 * 100 = 20.58$ kmol/h
Liquid rate $L = 100–20.58 = 79.42$ kmol/h

Composition calculation in the liquid and the vapour:

$$x_1 = \frac{1 - K_2}{K_1 - K_2} = \frac{1 - 0.7614}{5.218 - 0.7614} = 0.0535\ \mathrm{molfr.}$$

$$\mathrm{x}_2 = 1 - 0.0535 = 0.9465(\mathrm{molfr.}) = 94.65\,\mathrm{mol\%}$$

$$y_1 = K_1 * x_1 = 5.218 * 0.0535 = 0.279\,\mathrm{molfr.} = 27.9\,\mathrm{mol\%}$$

$$y_2 = K_2 * x_2 = 0.7614 * 0.9465 = 0.721\,\mathrm{molfr.} = 72.1\,\mathrm{mol\%}$$

Without consideration being given to the activity coefficient γ, the following incorrect results at 92.1 °C are obtained:

$$\begin{array}{ll} K_1 = 2.74 & K_2 = 0.758 \\ V = 0 & L = 100\,\text{kmol/h} \end{array}$$

Nothing is vaporized because the bubble point lies with $\gamma = 1$ at 93.1 °C above 92.1 °C.

2.14 Non-ideal Multi-component Mixtures

The equilibria calculation of mixtures with more than two components is very complex and therefore done using computers. The compositions, the temperature, and the Antoine Constants for the vapour pressure and the interaction parameters for the equilibrium must be input. The activity coefficients are strongly dependent on the composition of the liquid phase. Example 2.14.1 shows how strongly the activity coefficient of water increases with decreasing water composition in the liquid phase.

Example 2.14.1: Activity coefficient of water at different compositions.

		Activity coefficient γ	
	x (molfr.)	30 °C	50 °C
n-Heptane	0.2	1.1	1.014
Methyl ethyl ketone	0.2	1.138	1.13
Ethyl acetate	0.2	1.14	1.142
Toluene	0.2	1.63	1.606
Water	0.2	4.287	4.22

		Activity coefficient γ	
	x (molfr.)	30 °C	50 °C
n-Heptane	0.225	1.138	1.128
Methyl ethyl ketone	0.225	1.088	1.087
Ethyl acetate	0.225	1.102	1.104
Toluene	0.225	1.338	1.323
Water	0.1	6.055	5.912

		Activity coefficient γ	
	x (molfr.)	30 °C	50 °C
n-Heptane	0.2475	1.262	1.243
Methyl ethyl ketone	0.2475	1.066	1.07
Ethyl acetate	0.2475	1.096	1.098
Toluene	0.2475	1.133	1.125
Water	0.01	8.912	8.578

Example 2.14.2: Flash calculation for a four-component mixture with different compositions at 1 bar total pressure as function of temperature.

Mixture 1	*x* (molfr.)	Activity coefficient
n-Heptane	0.25	1.65
Methyl ethyl ketone	0.25	1.331
Ethyl acetate	0.25	1.273
Toluene	0.25	0.974
Mixture 2	*x* (molfr.)	Activity coefficient
n-Heptane	0.1	1.83
Methyl ethyl ketone	0.1	1.314
Ethyl acetate	0.4	1.112
Toluene	0.4	1.013

In Fig. 2.27 the flash curves for both of the different compositions are shown.

Figure 2.28 shows how the composition of a non-ideal mixture of *n*-heptane, methyl ethyl ketone, ethyl acetate, and toluene changes in nine consecutive vaporization stages. After four vaporization stages the compositions scarcely change. If toluene is distilled off then the composition of the mixture remains constant:

Ethyl acetate:	45.7 mol%
Methyl ethyl ketone:	37.5 mol%
n-Heptane:	16.8 mol%

The composition curves in Fig. 2.28 result from Fig. 2.29 with the equilibrium constants K of the different components. After four vaporization stages the toluene has vanished and the K values lie at 1. At $K = 1$ the vapour composition y equals the liquid composition x. This is a ternary azeotropic mixture.

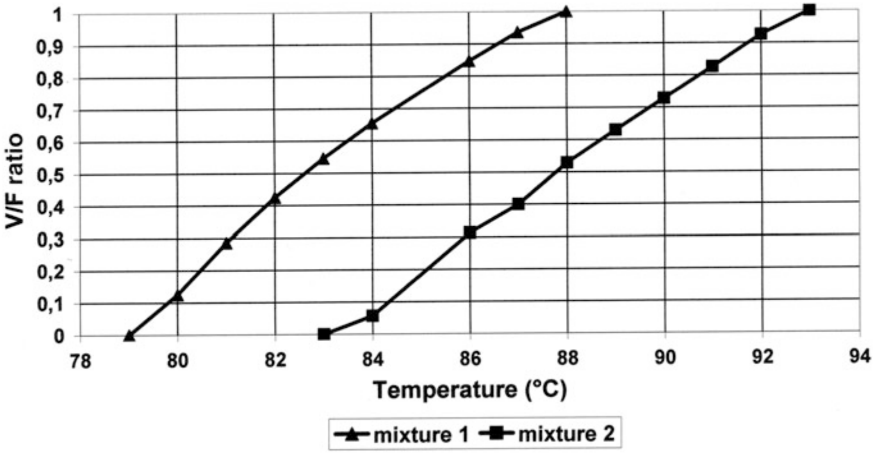


Fig. 2.27 Flash curves for two non-ideal mixtures as a function of temperature

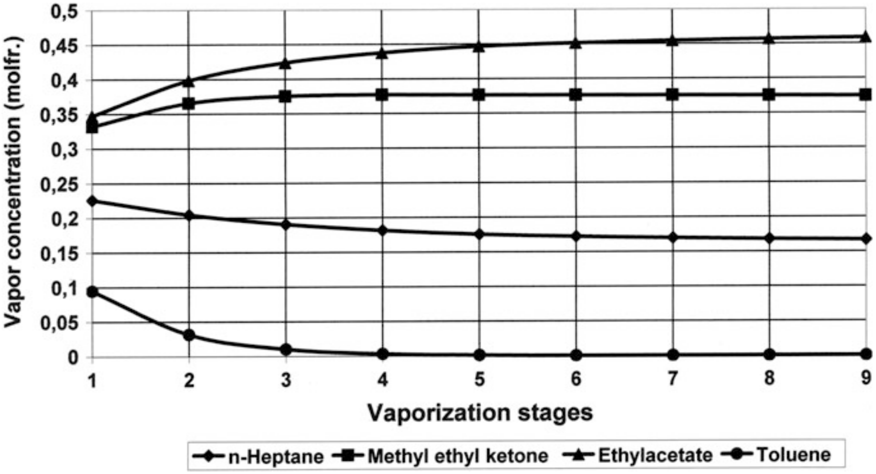


Fig. 2.28 The behaviour of the compositions of the four components with increasing number of vaporization stages

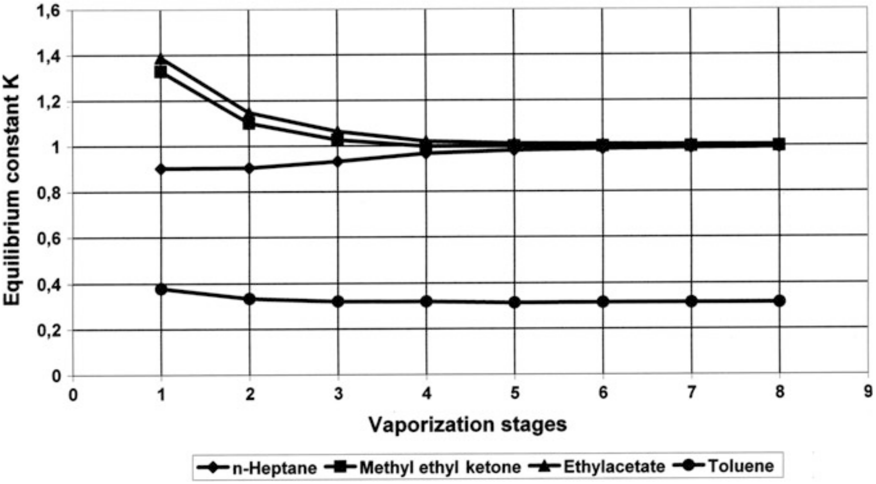


Fig. 2.29 Equilibrium constants of the components as a function of the vaporization stages

Although the three light components have different vapour pressures the separation factor α is set to 1 by the activity coefficient.

The determining factor for the separation is the relative volatility.

	Bubble point (°C)	Mole weight
Ethyl acetate	77	88
Methyl ethyl ketone	80	72
Heptane	98.4	100
Toluene	110.6	92

Example 2.14.3: Calculation of the relative volatility α at 73 °C and P_{tot} = 977 mbar.

		p_0 (mbar)	p_0/P_{tot}	γ	K
1.	*n*-Heptane	448.7	0.459	2.155	0.99
2.	Methyl ethyl ketone	800.5	0.827	1.206	0.998
3.	Ethyl acetate	878.8	0.899	1.117	1.005
4.	Toluene	302.4	0.309	1.017	0.315

$$\alpha_{1/2} = \frac{\gamma_1 * P_{01}}{\gamma_2 * P_{02}} = \frac{2.155 * 448.7}{1.206 * 800.5} = 1$$

$$\alpha_{2/3} = \frac{\gamma_2 * P_{02}}{\gamma_3 * P_{03}} = \frac{1.206 * 800.5}{1.117 * 878.8} = 0.98$$

$$\alpha_{1/3} = \frac{\gamma_1 * P_{01}}{\gamma_3 * P_{03}} = \frac{2.155 * 448.7}{1.117 * 878.8} = 0.985$$

$$\alpha_{3/4} = \frac{\gamma_3 * P_{03}}{\gamma_4 * P_{04}} = \frac{1.117 * 878.8}{1.017 * 302.4} = 3.19$$

$$\alpha_{1/4} = \frac{\gamma_1 * P_{01}}{\gamma_4 * P_{04}} = \frac{2.155 * 448.7}{1.017 * 302.4} = 3.19$$

$$\alpha_{3/4} = \frac{\gamma_2 * P_{02}}{\gamma_4 * P_{04}} = \frac{1.206 * 800.5}{1.017 * 302.4} = 3.19$$

Conclusion

The first three components with a separation factor α = 1 do not allow separation. However, toluene with a separation factor α = 3.19 allows very simple separation.

Figures 2.30 and 2.31 show the calculation results for another non-ideal four-component mixture with non-ideal behaviour.

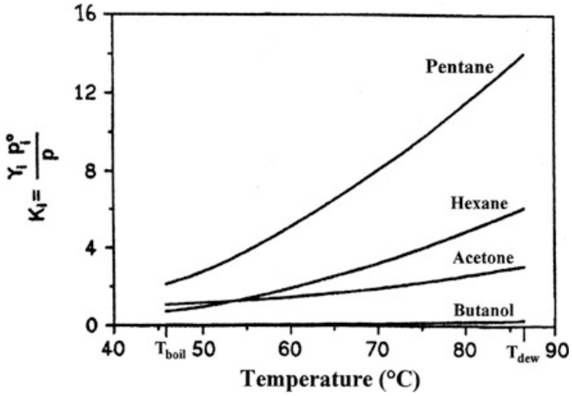
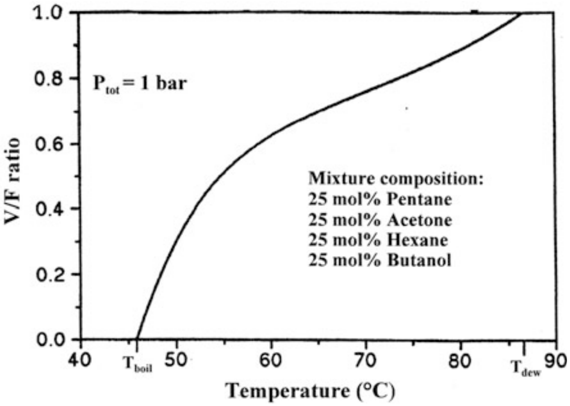


Fig. 2.30 Equilibrium factors *K* for the different components of the mixture dependent of the temperature

Fig. 2.31 Flash *curve* for the non-ideal, four-component mixture as function of temperature



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Chapter 3
Fractionation of Binary Mixtures

3.1 Material Balance

Prior to the design of each new column a material balance should be prepared, considering the specifications of the distillate and bottoms.

$$\mathbf{F} * \mathbf{x_F} = \mathbf{B} * \mathbf{x_B} + \mathbf{D} * \mathbf{x_D} = (\mathbf{F} - \mathbf{D}) * \mathbf{x_B} + \mathbf{D} * \mathbf{x_D}$$

$$D = F * \frac{X_\mathrm{F} - X_\mathrm{B}}{X_\mathrm{D} - X_\mathrm{B}} \quad \frac{B}{D} = \frac{X_\mathrm{D} - X_\mathrm{F}}{X_\mathrm{F} - X_\mathrm{B}}$$

X_F = feed composition (molfr.)
X_B = bottoms composition (molfr.)
X_D = distillate composition (molfr.)
F = feed rate (kmol/h)
B = bottoms rate (kmol/h)
D = distillate rate (kmol/h)

Example 3.1.1: Preparation of a mass balance
A mixture with 33% A in feed is to be enriched in the distillate with 97% of A and should only contain 4% of A in the bottoms.

Feed rate = 100 kmol/h
x_F = 0.33 molfr.
x_D = 0.97 molfr.
x_B = 0.04 molfr.

$$D = 100 * \frac{0.33 - 0.04}{0.97 - 0.04} = 31.2\,\mathrm{kmol/h}$$

$$B = 100 - 31.2 = 68.8\ \mathrm{kmol/h}.$$

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_3

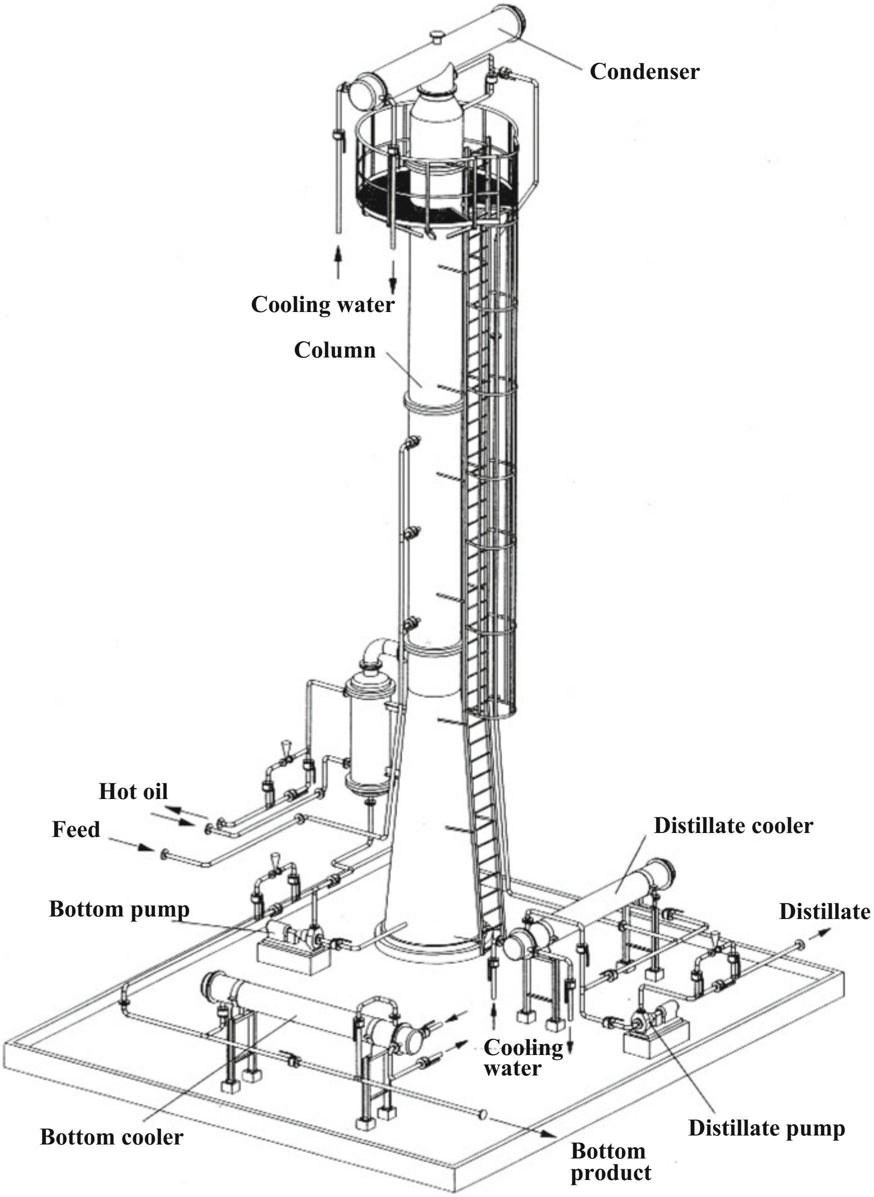


Fig. 3.1 A continuous fractionation column

Cross-check:

$$B = D * \frac{X_D - X_F}{X_F - X_B} = 31.2 * \frac{0.97 - 0.33}{0.33 - 0.04} = 68.8\,\text{kmol/h}$$

The vapour and liquid loadings of the column in the rectification section and the stripping section result from the reflux ratio and the thermal condition of the feed (q value).

3.2 Vapour–Liquid Equilibria

In order to determine the required theoretical stages and the reflux ratio the vapour–liquid equilibrium is needed.

3.2.1 Equilibria of Ideal Mixtures

$$y_1 = \frac{p_1}{P_{\text{tot}}} = \frac{x_1 * p_{01}}{P_{\text{tot}}}$$

$$K_1 = \frac{y_1}{x_1} = \frac{p_{01}}{P_{\text{tot}}} \quad K_2 = \frac{y_2}{x_2} = \frac{p_{02}}{P_{\text{tot}}}$$

P_{tot} = total pressure (mbar)
p_1 = partial pressure of the light component (mbar)
p_{01} = vapour pressure of the light component (mbar)
x_1 = composition of the light component in the liquid (molfr.)
y_1 = composition of the light component in the vapour (molfr.)
p_{02} = vapour pressure of the heavy component (mbar)
x_2 = composition of the heavy component in the liquid (molfr.)
y_2 = composition of the heavy component in vapour (molfr.)
K = equilibrium constant = y/x
α = relative volatility

$$\alpha = \frac{K_1}{K_2} = \frac{p_{01}}{p_{02}}$$

$$y_1 = \frac{\alpha * x_1}{1 + (\alpha - 1) * x_1}$$

$$y_2 = \frac{\alpha * K_2 - 1}{\alpha - 1}$$

$$x_2 = \frac{\alpha * K_2 - 1}{K_2 - \alpha - 1}$$

.

The **relative volatility** α changes with temperature in the column. In general the geometrical average of the top, feed, and bottom temperature is inserted.

$$\alpha = \sqrt[3]{\alpha_{\text{top}} * \alpha_{\text{feed}} * \alpha_{\text{bottom}}}$$

If heavy deviations are present the calculation must be made segment-wise with different α values.

Example 3.2.1.1: Calculation of vapour–liquid equilibrium at P_{tot} = 340 mbar

Component 1	x_1 = 0.7 molfr.	Vapour pressure p_{01} = 400 mbar
Component 2	x_2 = 0.3 molfr.	Vapour pressure p_{02} = 200 mbar

Partial pressure $p_1 = x1 * p_{01} = 0.7 * 400 = 280$ mbar
Partial pressure $p_2 = x_2 * p_{02} = 0.3 * 200 = 60$ mbar
Total pressure $P_{\text{tot}} = p_1 + p_2 = 280 + 60 = 340$ mbar

Calculation of the vapour compositions for $x_1 = 0.7$ and $x_2 = 0.3$ using the partial pressures:

$$y_1 = \frac{p_1}{P_{\text{tot}}} = \frac{280}{340} = 0.82 \quad y_2 = \frac{60}{340} = 0.18$$

Calculation of the relative volatility α from the vapour pressures:

$$\alpha = \frac{P_{01}}{P_{02}} = \frac{400}{200} = 2$$

Calculation of the vapour compositions for $x_1 = 0.7$ using relative volatility:

$$y_1 = \frac{\alpha * x_1}{1 + (\alpha - 1) * x_1} = \frac{2 * 0.7}{1 + (2 - 1) * 0.7} = 0.82$$

Calculation of the equilibrium constant K from the vapour pressure and the total pressure:

$$K_1 = \frac{P_{01}}{P_{\text{tot}}} = \frac{400}{340} = 1.176 \quad K_2 = \frac{P_{02}}{P_{\text{tot}}} = \frac{200}{340} = 0.588$$
$$\text{Relative volatility } \alpha = \frac{K_1}{K_2} = \frac{1.176}{0.588} = 2$$

Calculation of the vapour compositions for $x_1 = 0.7$ and $x_2 = 0.3$ with the equilibrium constants K_1 and K_2:

$$y_1 = K_1 * x_1 = 1.176 * 0.7 = 0.82 \text{ molfr.}$$
$$y_2 = K_2 * x_2 = 0.588 * 0.3 = 0.18 \text{ molfr.}$$

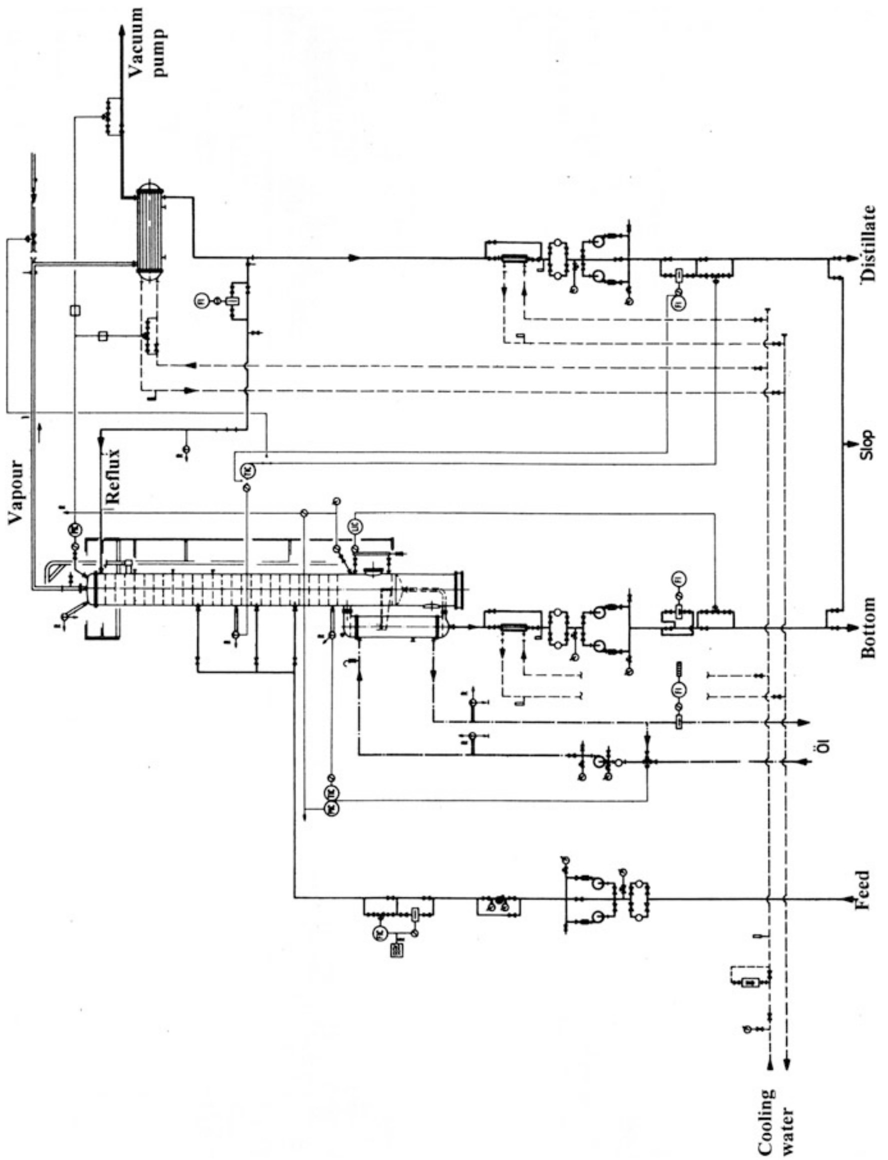


Fig. 3.2 Flow sheet for a continuous fractionation unit

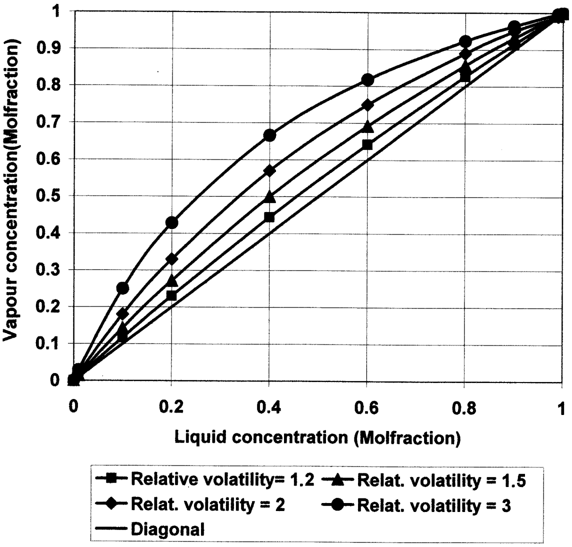


Fig. 3.3 Vapour–liquid equilibrium for an ideal mixture with different relative volatilities

Calculation of the total equilibrium curve using the constant relative volatility $\alpha = 2$:

x_1	0.01	0.05	0.1	0.20	0.40	0.6	0.8	0.9	0.950	0.99
y_1	0.02	0.10	0.18	0.33	0.57	0.75	0.89	0.95	0.97	0.99

The relative volatility α changes less with temperature than the equilibrium constants K, and is therefore more suitable for the preparation of an equilibrium curve. The equilibrium curves for different relative volatilities α are given in Fig. 3.3.

3.2.2 Equilibria of Non-ideal Mixtures

With non-ideal mixtures, for instance alcohol/water, the specific activity coefficients γ for each component pair must be considered additionally. The partial pressure of the component and the vapour–liquid equilibrium is influenced by mutual interaction.

$$P_{\text{tot}} = \gamma_1 * x_1 * p_{01} + \gamma_2 * x_2 * p_{02}$$

$$y_1 * P_{\text{tot}} = \gamma_1 * x_1 * p_{01}$$

In the calculation of the vapour–liquid equilibrium the activity coefficient γ must be considered and it is found to be strongly dependent on the composition in the liquid phase.

$$
\begin{aligned}
y_1 &= \frac{\gamma_1 * x_1 * p_{01}}{P_{\text{tot}}} \\
K_1 &= \frac{y_1}{x_1} = \frac{\gamma_1 * p_{01}}{P_{\text{tot}}} \\
K_2 &= \frac{y_2}{x_2} = \frac{\gamma_2 * p_{02}}{P_{\text{tot}}} \\
\alpha &= \frac{K_1}{K_2} = \frac{\gamma_1 * p_{01}}{\gamma_2 * p_{02}} - \frac{y_1 * (1 - x_1)}{x_1 * (1 - y_1)}
\end{aligned}
$$

Example 3.2.2.1: Calculation of the methanol vapour composition of a methanol–water solution at 92.1 °C and P_{tot} = 1000 mbar

$$
\begin{array}{llll}
P_{\text{tot}} = 1000\,\text{mbar}. & & & \\
\text{Methanol}: & x_1 = 0.0535\,\text{molfr.} & \text{Water}: & x_2 = 0.9465\text{ molfr.} \\
 & \gamma_1 = 1.848 & & \gamma_2 = 1.004 \\
 & p_{01} = 2816.7\,\text{mbar} & & p_{02} = 756.4\,\text{mbar}
\end{array}
$$

$$
\begin{aligned}
y_1 &= \frac{1.848 * 0.0535 * 2816.7}{1000} = 0.279 \\
y_2 &= \frac{1.004 * 0.9465 * 756.4}{1000} = 0.721 \\
K_1 &= \frac{1.848 * 281.6}{1000} = 5.218 \\
K_2 &= \frac{1.004 * 756.4}{1000} = 0.761 \\
\alpha &= \frac{K_1}{K_2} = \frac{5.218}{0.761} = 6.853
\end{aligned}
$$

In comparison the ideal relative volatility without activity coefficients from the vapour pressures is calculated:

$$
\alpha_{\text{ideal}} = \frac{p_{01}}{p_{02}} = \frac{281.6}{756.4} = 3.724
$$

Conclusion: the influence of γ is severe!

The relative volatility is almost doubled by the activity coefficients when going from ideal α = 3.724 to non-ideal α = 6.853.

The activity coefficient γ is dependent on the temperature and is very strongly dependent **on the concentration in the liquid phase.**

3.3 Minimum Number of Trays and Minimum Reflux Ratio

This calculation is valid for ideal mixtures with a constant relative volatility α in the column. In order to separate a mixture by fractionation a minimum number of stages at infinite reflux and a minimum reflux ratio at infinite number of stages is needed. Using these calculation parameters the required actual number and the reflux ratio for a separation task can be determined very easily.

Calculation of the **minimum number of stages** for a separation at infinite reflux [1]:

$$N_{\min} = \frac{\lg\left[\left(\frac{x_1}{x_2}\right)_{\mathrm{D}} * \left(\frac{x_2}{x_1}\right)_{\mathrm{B}}\right]}{\lg \alpha}$$

x_1 = Light boiling component composition (molfr.)
x_2 = Heavy boiling component composition (molfr.)
D = Composition in the distillate
B = Composition in the bottoms

Minimum number of stages for the rectification section:

$$N_{\min\mathrm{V}} = \frac{\lg\left[\left(\frac{x_1}{x_2}\right)_{\mathrm{D}} * \left(\frac{x_2}{x_1}\right)_{\mathrm{F}}\right]}{\lg \alpha}$$

D = composition in the distillate
F = composition in the feed

Minimum number of stages for the stripping section:

$$N_{\min\mathrm{A}} = \frac{\lg\left[\left(\frac{x_1}{x_2}\right)_{F} * \left(\frac{x_2}{x_1}\right)_{B}\right]}{\lg \alpha}$$

B = composition in the bottoms draw.

Calculation of the **minimum reflux ratio** at an infinite number of stages [2]:

$$R_{\min} = \frac{1}{\alpha - 1} * \left[\left(\frac{x_{\mathrm{D}}}{x_{\mathrm{F}}}\right)_1 - \alpha * \left(\frac{x_{\mathrm{D}}}{x_{\mathrm{F}}}\right)_2\right]$$

$$R_{\min} = \frac{x_{\mathrm{D}} - y_{\mathrm{F}}}{y_{\mathrm{F}} - x_{\mathrm{F}}} \qquad y_{\mathrm{F}} = \frac{\alpha * x_{\mathrm{F}}}{1 + (\alpha - 1) * x_{\mathrm{F}}}$$

x_D = composition in the distillate (molfr.)
x_F = liquid composition in the feed (molfr.)
y_F = corresponding vapour composition to x_F (molfr.)
$(x_D/x_F)_1$ = ratio of the distillate composition to feed composition for the light boiling component

Remark: In non-ideal equilibrium lines the minimum reflux ratio can be graphically calculated from the coordinates of the intersection point between the equilibrium and the operating line.

$$\left(\frac{L}{V}\right)_{\min} = \frac{R_{\min}}{R_{\min}+1} = \quad \text{Minimum slope of operating line}$$

L = liquid rate in the rectification section (kmol/h)
V = vapour rate in the rectification section (kmol/h)

Example 3.3.1: Calculation of the minimum number of stages and the minimum reflux ratio for a given separation task

$$\text{Relative volatility } \alpha = 2. \quad \text{Feed rate} = 100\,\text{kmol/h}.$$

Separation task:

Component	Feed molfr.	Distillate molfr.	Bottoms draw molfr.
A	0.5	0.95	0.05
B	0.5	0.05	0.95

Mass balance: Distillate $D = 100 * \frac{0.5-0.05}{0.95-0.05} = 50$ kmol/h

Calculation of the minimum number of stages for the separation:

$$N_{\min} = \frac{\lg\left(\frac{0.95}{0.05} * \frac{0.95}{0.05}\right)}{\lg 2} = 8.5$$

$$N_{\min V} = \frac{\lg\left(\frac{0.95}{0.05} * \frac{0.95}{0.05}\right)}{\lg 2} = 4.25$$

$$N_{\min A} = \frac{\lg\left(\frac{0.5}{0.5} * \frac{0.95}{0.05}\right)}{\lg 2} = 4.25$$

Required minimum reflux ratio

$$R_{\min} = \frac{1}{2-1} * \left(\frac{0.95}{0.5} - 2 * \frac{0.05}{0.5}\right) = 1.7$$

$$x_F = 0.5 \quad y_F = \frac{2 * 0.5}{1 + (2-1) * 0.5} = 0.67$$

$$R_{\min} = \frac{0.95 - 0.67}{0.67 - 0.5} = 1.7$$

3.4 Conversion of the Minimum Number of Trays to the Actual Number of Trays [3]

The calculated minimum number of theoretical stages is only valid for an infinite reflux ratio without distillate draw and the minimum reflux ratio for a column with an infinite number of stages. The determined values must therefore be converted to actual process conditions for the existing number of stages and a chosen reflux ratio. The following approximations are used for the conversion.

$$\boxed{\begin{gathered} \tfrac{N-N_{\min}}{N+1} = Y \\ Y = 0.75 - 0.75 * X^{0.5668} \\ \tfrac{R-R_{\min}}{R+1} = X \\ X = \left(\tfrac{0.75-Y}{0.75}\right)^{1/0.5668} \end{gathered}}$$

Example 3.4.1: Determination of the required number of theoretical stages for *R* = 2

From Example 3.3.1: $R_{\min} = 1.7 \quad N_{\min} = 8.5 \quad \text{Chosen}: R = 2$

$$X = \frac{2 - 1.7}{3} = 0.1$$

$$Y = 0.75 * 0.75 * 1^{0.5668} = 0.547$$

$$N - N_{\min} = 0.547N + 0.547$$

$$0.453N = 8.5 + 0.547 = 9.047 \Rightarrow \mathbf{N = 20}$$

Therefore, 20 theoretical stages are required for a reflux ratio *R* = 2.

3.5 Determination of the Feed Tray According to Kirkbride [4]

The ratio of the rectification trays N_V to the stripping trays N_A is calculated according to the method of Kirkbride.

$$\frac{N_V}{N_A} = \left[\left(\frac{x_A}{x_B}\right) * \left(\frac{x_{AB}}{x_{BD}}\right)^2 * \frac{B}{D}\right]^{0.206}$$

Example 3.5.1: Determination of the feed stage for the separation task in Example 3.3.1

$$\frac{N_V}{N_A} = \left(\frac{0.5}{0.5} * \left(\frac{0.05}{0.05}\right)^2\right)^{0.206} = 1$$

$$N_V = \frac{1}{2} * 20 = 10$$

The feed stream should be fed to the 10th theoretical tray of the column.

3.6 Graphical Determination of the Number of Trays According to Mcabe–Thiele (Fig. 3.4)

Required Information

- Relative volatility α or the vapour–liquid equilibrium.
- Feed composition x_F.
- Desired distillate composition x_D.
- Required bottoms composition x_B.
- Reflux ratio R.
- Thermal condition of the feed (q value).

Figures 3.5 and 3.6 show how to graphically determine the required theoretical trays for a given fractionation task in the Mcabe–Thiele diagram.

First, the **equilibrium curve y = f(x)** must be drawn. These are the calculated values for y and x using the relative volatility or measured equilibrium values for the mixture which is to be separated. Subsequently the q-line is drawn in from the intersection point of x_F with the diagonal. The q-line is vertical, if the product is introduced into the feed tray at boiling temperature. Next, the **operating lines in the rectification and stripping section are drawn in for the chosen reflux ratio R**.

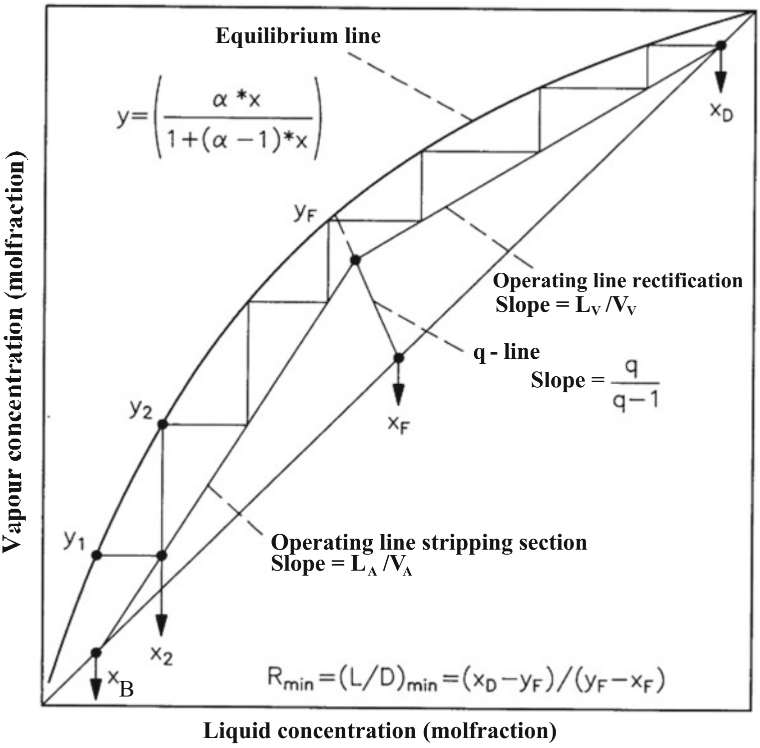


Fig. 3.4 Mcabe–Thiele diagram for the determination of the theoretical number of trays

Rectification line: From x_D with a slope $L_V/V_V = R/R + 1$.

L_V = liquid rate in the rectification section of the column (kmol/h)
V_V = rising vapour in the rectification section of the column (kmol/h)

Stripping line: From x_B with a slope $L_A/V_A = R_A/R_A - 1$.

L_A = liquid rate in the stripping section of the column (kmol/h)
V_A = rising vapour in the stripping section of the column (kmol/h)

First the slopes of the rectification line and the stripping line are determined considering the thermal condition q of the feed. Starting from x_D and x_B the theoretical trays are then drawn between the equilibrium curve and the operating lines.

Advantages of this method

Illustrative method for different reflux ratios.
Considers different feed conditions (q values).
Offers direct steam heating without a reboiler.
Considers side draws and the influence of the feed tray.

Suitable for changing α values and non-ideal mixtures as well as non-equal molar latent heat using a corresponding correction.

Disadvantages

Time consuming and inaccurate for small α values and very high end-concentrations of distillate or bottoms products.
No temperatures considered.
Correction is required at different molar latent heats.

Example 3.6.1: Graphical determination of the required theoretical stages for *R* = 3

Feed composition	$x_F = 0.5$ molfr.	Required distillate composition	$x_D = 0.95$ molfr.
Relative volatility	$\alpha = 2.4$	Total pressure $P_{tot} = 1$ bar	$R = 3$

Thermal condition $q = 1$ slope of the q-line = ∞

$$\text{Slope of the reflux line } \frac{L}{V} = \frac{R}{R+1} = \frac{3}{4} = 0.75$$

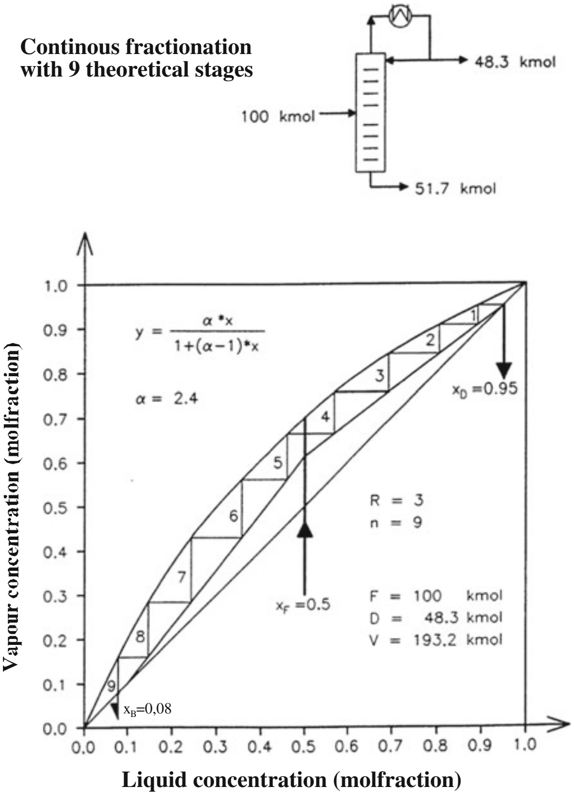


Fig. 3.5 Graphical determination of the number of theoretical stages for *R* = 3

From figure Bild 3.5 it can be seen that with **9 theoretical trays at a reflux ratio of R = 3** the bottoms product exits with a composition of $x_B = 0.08$ molfr.

Mass balance:

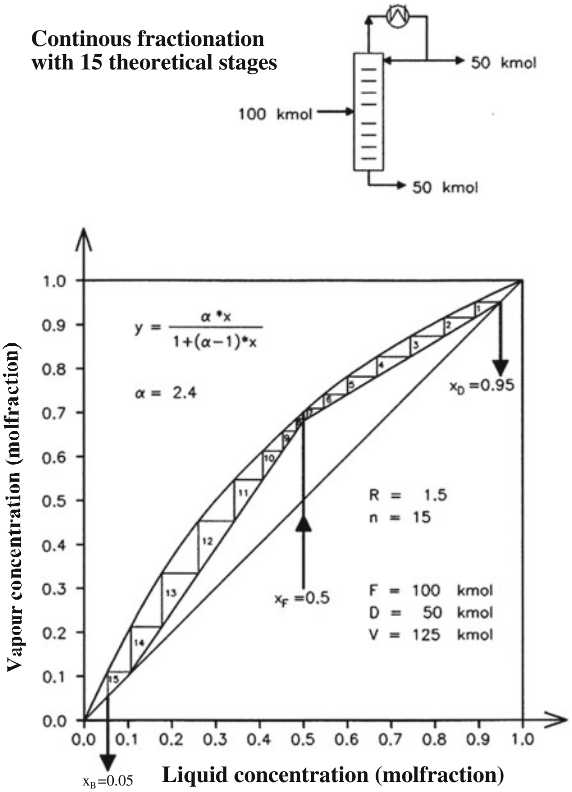
Feed rate $F = 100$ kmol/h.

$$D = F * \frac{x_F - x_B}{x_D - x_B} = \frac{0.5 - 0.08}{0.95 - 0.08} = 48.3 \text{ kmol/h}$$

Bottoms draw rate $B = 51.7$ kmol/h

Required total vaporization $V = (R + 1) * D = 4 * 48.3 = 193.7$ kmol/h

Fig. 3.6 Graphical determination of the number of trays for $R = 1.5$



Example 3.6.2: Graphical determination of the number of theoretical stages for *R* = 1.5

Feed composition	$x_F = 0.5$ molfr.	Required distillate composition	$x_D = 0.95$ molfr.
Relative volatility	$\alpha = 2.4$	Total pressure $P_{tot} = 1$ bar	$R = 1.5$

Thermal condition $q = 1 \rightarrow$ slope of the q-line = ∞

$$\text{Slope of the reflux line } \frac{L}{V} = \frac{R}{R+1} = \frac{1.5}{2.5} = 0.6$$

From Fig. 3.6 it can be seen that with 15 theoretical trays at a reflux ratio of $R = 1.5$ the bottoms product exits with a composition of $x_S = 0.05$ molfr.

Mass balance:

Feed rate $F = 100$ kmol/h.

$$D = F * \frac{x_F - x_B}{x_D - x_B} = 100 * \frac{0.5 - 0.05}{0.95 - 0.05} = 50 \text{ kmol/h}$$

Bottoms draw rate $B = 50$ kmol/h

Required total vaporization $V = (R + 1) * D = 2.5 * 50 = 125$ kmol/h.

3.7 Calculation of the Number of Trays Using the McCabe–Thiele Method [5]

Starting from the distillate composition the compositions for the trays are calculated from top down. When the feed composition is achieved the calculation must be switched from the rectification calculation to the stripping calculation.

Required information: see Sect. 3.6 and the ratio D/F.

D = distillate rate (kmol/h)
F = feed rate (kmol/h)
L_A = liquid rate in the stripping section (kmol/h)
B = bottoms draw rate (kmol/h)

Advantages

No drawing/plotting required.
More precise at high concentrations in the distillate and bottoms.

Disadvantages

Less illustrative.
Only valid for $q = 1$ and equal molar latent heats.

Recommendation: Estimate the reflux ratio beforehand using approximation methods.

Procedure for calculating the rectification section of the column

$$A = \frac{L}{V} = \frac{R}{R+1} \quad B = \frac{x_\mathrm{D}}{R+1}$$

Starting at $x_\mathrm{D} = y_1$ at the top, the corresponding liquid composition x_1 of the uppermost top tray to this vapour composition is calculated.

$$x_1 = \frac{\frac{x_D}{\alpha * (1-x)}}{1 + \frac{x_D}{\alpha(1-x_\mathrm{D})}}$$

V = vapour rate rectification (kmol/h)
L = liquid rate rectification (kmol/h)
x_D = distillate composition (molfr.)

The rising vapour from tray 2 at the top then has the following composition:

$$y_2 = A * x_1 + B = \frac{R}{R+1} * x_1 + \frac{x_\mathrm{D}}{R+1}$$

Consequently, x_2 is calculated for tray 2 from the top:

$$x_2 = \frac{\frac{y_2}{\alpha * (1-y)}}{1 + \frac{y_2}{\alpha * (1-y_2)}}$$

This calculation is repeated until the liquid concentration is less than the feed composition x_F.

Calculation for the stripping section of the column

$$C = \frac{R_\mathrm{A}}{R_\mathrm{A} - 1} \quad D = \frac{x_\mathrm{B}}{R_\mathrm{A} - 1} \quad R_\mathrm{A} = \frac{L_\mathrm{A}}{B}$$

Starting from x_F or the last x value from the rectification calculation, the rising vapour composition $y_{\mathrm{A}1}$ from the first stripping tray below the feed tray is calculated:

$$y_{\mathrm{A}1} = C * x - D = \frac{R_\mathrm{A}}{R_\mathrm{A} - 1} * x - \frac{x_\mathrm{B}}{R_\mathrm{A} - 1}$$

The liquid composition x_{A1} on the first stripping tray is calculated as follows:

$$x_{\mathrm{A1}} = \frac{\frac{y_{\mathrm{A1}}}{\alpha*(1-y_{\mathrm{A1}})}}{1+\frac{y_{\mathrm{A1}}}{\alpha*(1-y_{\mathrm{A1}})}}$$

The calculation is repeated until the liquid composition gets below the desired bottoms composition.

Remark: The α values can be varied in the calculations for different trays. Efficiencies can also be considered [6].

Example 3.7.1: Determination of the number of trays by calculation according to Mcabe–Thiele

$x_{\mathrm{F}} = 0.5$	$x_{\mathrm{D}} = 0.95$	$x_{\mathrm{B}} = 0.05$	$R = 2$	$D/F = 0.5$	$\alpha = 2$
$q = 1$	$F = 100$ kmol/h		$D = 50$ kmol/h	$B = 50$ kmol/h	
$V = (2 + 1) * 50 = 150$ kmol/h$L_{\mathrm{V}} = 2 * 50 = 100$ kmol/h$L_{\mathrm{A}} = 200$ kmol/h					

Calculation for the rectification section from top down to the feed tray:

$$x_1 = \frac{\frac{0.95}{2*(1-0.95)}}{1+\frac{0.95}{2*(1-0.95)}} = 0.9048$$

$$A = \frac{L}{V} = \frac{R}{R+1} = \frac{2}{3} \qquad B = \frac{x_D}{R+1} = \frac{0.95}{3}$$
$$y_2 = \frac{2}{3} * 0.9048 + \frac{0.95}{3} = 0.9198 \quad x_2 = 0.8516$$
$$y_3 = 0.8844 \quad x_3 = 0.7927$$
$$y_4 = 0.8452 \quad x_4 = 0.7318$$
$$y_{10} = 0.6567 \quad x_{10} = 0.4888$$

For the 10th tray from the top the calculated liquid concentration is:

$$\mathbf{x} = \mathbf{0.4888} < \mathbf{x_F} = \mathbf{0.5}.$$

Calculation for the stripping section of the column from the feed tray to the bottom:

$$R_A = \frac{L_A}{B} = \frac{200}{50} = 4$$
$$\frac{L_A}{V_A} = \frac{200}{150} = \frac{R_A}{R_A - 1} = \frac{4}{4-1} = 1.33$$
$$D = \frac{x_S}{R_A - 1} = \frac{0.05}{4-1} = 0.0167$$
$$y_{A1} = 1.33 * 0.4888 - 0.0167 = 0.6351$$
$$x_{A1} = \frac{\frac{0.6351}{2*(1-0.6351)}}{1+\frac{0.6351}{2*(1-0.6351)}} = 0.4653$$
$$y_{A2} = 0.6037 \qquad x_{A2} = 0.4324$$
$$y_{A3} = 0.5599 \qquad x_{A3} = 0.3888$$

Calculated compositions of the trays according to McCabe–Thiele

Trays	Vapour composition (molfr.)	Liquid composition (molfr.)
1	0.9500 ($x_D = 0.95$)	0.9048
2	0.9198	0.8516
3	0.8844	0.7927
4	0.8452	0.7318
5	0.8046	0.6730
6	0.7653	0.6199
7	0.7299	0.5747
8	0.6998	0.5383
9	0.6755	0.5100
10	0.6567	0.4888 ($x_F = 0.5$)
11	0.6351	0.4653
12	0.6037	0.4321
13	0.5599	0.3888
14	0.5017	0.3348
15	0.4298	0.2737
16	0.3483	0.2109
17	0.2645	0.1524
18	0.1865	0.1029
19	0.1205	0.0641
20	0.0688	0.0356 ($x_B < 0.05$)

The graphical determination of the number of trays in Fig. 3.7 gives the same result as the calculated method.

3.8 Tray to Tray—Calculation Using the Flow Rates and Relative Volatility α [6]

In this calculation the component mass balance is combined with the equilibrium calculation.

Required information

Vapour and liquid rates in the rectification section and the stripping section.
Distillate rate d and bottoms rate b.
Relative volatility α or equilibrium factors K_1 and K_2.

Advantages

The flows and compositions are determined.
Adequate for different q-values.

Calculation procedure

The calculation is started from condenser down and from the reboiler up and is continued from tray to tray until the compositions overlap.

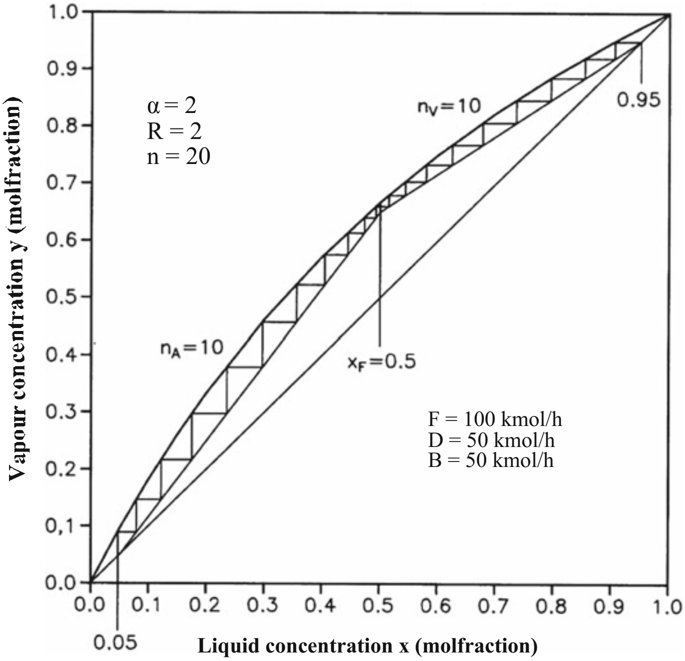


Fig. 3.7 Graphical determination of the number of trays in Example 3.7.1

Rectification

(a) Make a list of distillate flows d and relative volatilities α.

(b) Calculate d/α and Σ d/α.

(c) Determine the liquid rates l of both components and their sums Σ*l*.

$$I = \frac{(\mathrm{d}/\alpha) * L}{\Sigma(\mathrm{d}/\alpha)}$$

$$L = \text{reflux rate (kmol/h)} = R * D$$

(d) Determine of the vapour rate $v = l + d$ rising from the next tray.

Example 3.8.1: Determination of the number of trays in the rectification section using *R* = 2

$\text{Distillate D} = 50\,\text{kmol/h} \quad \text{Reflux L} = 100\,\text{kmol/h} \quad x_F = 0.5$

	From condenser			Tray 1 below the condenser		
Component	d (kmol/h)	α	d/α	*l* (kmol/h)	*v* (kmol/h)	*y* (molfr.)
A	47.5	2	23.75	90.5	138	0.92
B	2.5	1	2.5	9.5	12	0.08
			26.25	100	150	1.0

Stripping

(a) Make a list of bottoms draw rates b with a separation factor α.
(b) Calculate $b * \alpha$ and $\Sigma b * \alpha$.
(c) Determine vapour rates v of the components and the sum

$$v = \frac{(\alpha * b) * V}{\Sigma(\alpha * b)}$$

$V = V_A$ = the rising vapour rate from the reboiler (kmol/h).
(d) Determine the liquid rate running down from the next tray $l = v + b$.

Example 3.8.2: Determination of the number of trays in the stripping section

Bottoms draw $B = 50\,\text{kmol/h} \quad V = 150\,\text{kmol/h}$

	From reboiler			Bottom draw above reboiler	
Components	b (kmol/h)	α	$\alpha * b$	v (kmol/h)	l (kmol/h)
A	2.5	2	5	14.3	16.8
B	47.5	1	47.5	135.7	183.2
	68.8		52.5	150	200

Remark: Both calculations starting from the top and bottom do not meet each other at one point. The compositions are drawn over the numbers of trays and the point of intersection of the liquid concentration calculated from the top and the bottom, with the feed composition $x_F = 0.5$, is chosen as a feed tray (see Fig. 3.8).

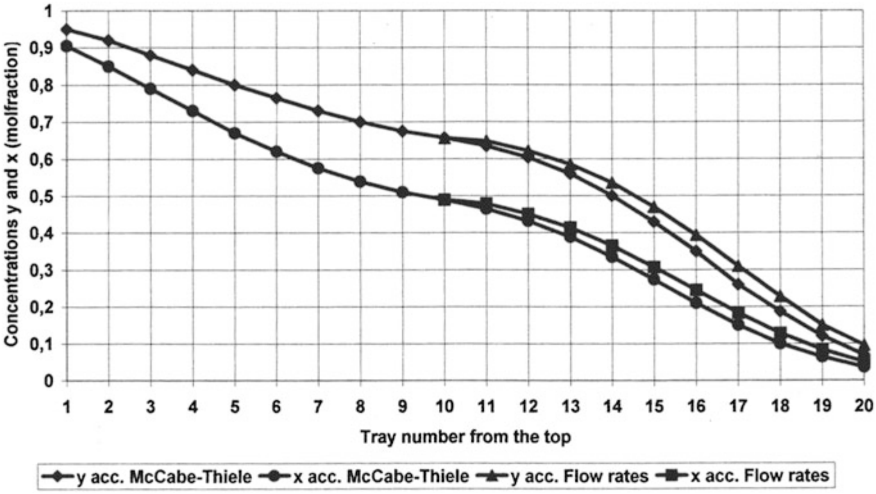


Fig. 3.8 Calculated vapour and liquid compositions on the theoretical trays according to the Mcabe–Thiele and flow rate calculations

Results of the tray-to-tray-calculation with flows and compositions

From column top to the feed tray

Tray number	1	2	3	4	8	9	10	11
v_1 (kmol/h)	47	138	133	127	105	101	98.5	96
v_2 (kmol/h)	**2.5**	12	17	23	45	49	51.5	54
y_1 (molfr.)	0.95	0.919	0.884	0.845	0.699	0.675	0.657	0.643
l_1 (kmol/h)	90.5	85	80	73	54	51	49	47
l_2 (kmol/h)	9.5	15	20	27	46	49	51	53
x_1 (molfr.)	0.905	0.852	0.793	0.732	0.538	0.51	0.489	0.473

From reboiler to the feed tray

Tray number	20	19	18	17	14	13	12	11	10
v_1 (kmol/h)	14.3	23.2	34.2	46.5	80.3	87.8	93.3	97.2	99.8
v_2 (kmol/h)	135.7	126.8	115.8	103.5	69.7	62.2	56.7	52.8	50.2
y_1 (molfr.)	0.095	0.155	0.228	0.31	0.535	0.586	0.622	0.648	0.665
l_1 (kmol/h	2.5	16.8	25.7	36.7	73	82.8	90.3	95.8	99.7
l_2 (kmol/h	47.5	183.2	174.3	163.3	127	117.2	109.7	104.2	100.3
x_1 (molfr.)	0.05	0.084	0.129	0.183	0.365	0.414	0.452	0.479	0.498

On tray 10 the vapour rates and the liquid composition of the light component are almost the same:

	Rectification	Stripping
v_1	98.5	99.8
v_2	51.5	50.2
x_1	0.489	0.498

3.9 Analytical Calculation According to Smoker [7–10]

Starting with a given reflux ratio and the compositions x_F, x_D, and x_B, as well as the relative volatility α, rectification and stripping trays are calculated.

Advantages

Quick method, especially for small α values with many separation stages in the corners of the diagram.
More accurate than the determination of the minimum tray number according to Fenske.

The calculation method is well described in the essays of Stage and Juilfs [9].

Example 3.9.1: Calculation of the required number of trays n for the rectification according to Smoker

Data: see Example 3.6.1 $x_F = 0.5 \quad x_D = 0.95 \quad \alpha = 2 \quad R = 2$

$A = \alpha - 1 = 2 - 1 = 1$
$B = A * x_F = 1 * 0.5 = 0.5$
$D = A * x_D = 1 * 0.95 = 0.95$
$E = A * R = 1 * 2 = 2$

$$V = \frac{E + \alpha - D}{2} = \frac{2 + 2 - 0.95}{2} = 1.525 \qquad V^2 = 2.326$$

$W^2 = V^2 - D * R = 2.326 - 0.95 * 2 = 0.426 \; W = 0.652$
$K_1 = V - W = 1.525 - 0.652 = 0.873$
$K_2 = K_1/R = 0.873/2 = 0.437$
$c = K_2 + 1 = 0.437 + 1 = 1.437 \quad d = c^2 = 2.064$
$G = D - K_2 = 0.95 - 0.437 = 0.513$
$H = B - K_2 = 0.5 - 0.437 = 0.063$

$$\beta = \frac{\alpha * (R + 1)}{d * R} = \frac{2 * 3}{2.064 * 2} = 1.453$$

$F = c * (\beta - 1) = 1.437 * 0.453 = 0.652$
$N = F - G = 0.652 - 0.513 = 0.139$
$M = F - H = 0.652 - 0.063 = 0.589$

$$\gamma = \frac{G * M}{H * N} = \frac{0.513 * 0.589}{0.063 * 0.139} = 34.5 \quad n = \frac{\lg \gamma}{\lg \beta} = \frac{\lg 34.5}{\lg 1.453} = 9.5$$

Required rectification trays: 10 theoretical trays.

3.10 Thermal Condition of the Feed [10]

The thermal condition of the feed is characterized by the ***q*-value**.

In the following it is shown how the *q*-value is determined and what influence this has on the fractionation and the vapour and liquid loading of the column.

(a) **Cold feed with a temperature T_F below the boiling temperature T_S of the feed**

$$\mathbf{T_{feed} < T_S = T_{boil} \rightarrow q > 0} \quad q = 1 + \frac{c_{Fl} * (T_S - T_F)}{r}$$

(b) **Feed at boiling temperature $\mathbf{T_{feed} = T_S = T_{boil} \rightarrow q = 1}$**
(c) **Feed of a vapour–liquid mixture $\mathbf{\rightarrow 0 < q < 1 \Rightarrow q =}$ liquid fraction**

(d) **Saturated vapour at the dew point** $T_{\mathbf{feed}} = \mathbf{T_{dew}} \quad \rightarrow \mathbf{q = 0}$

(e) **Overheated vapour with feed temperature** $\mathbf{T_F}$

$$\mathbf{T_{feed}} > \mathbf{T_{dew}} \quad \rightarrow \quad \mathbf{q < 0} \quad q = \frac{-c_D * (T_F - T_{\text{dew}})}{r}$$

Using the q-value the equation of the q-line is determined:

$$y = -\frac{q}{1-q} * x + \frac{x_F}{1-q}$$

$$\text{Slope of the } q - \text{line } = \frac{q}{1-q}$$

T_F = feed temperature (°C)
T_S = boiling temperature (°C)
T_{dew} = dew point temperature (°C)
c_D = specific heat capacity of the vapour (Wh/kgK)
c_{Fl} = specific heat capacity of the liquid (Wh/kgK)
r = latent heat of the feed mixture (Wh/kg)

Example 3.10.1: Calculation of the slope of the *q*-line

(a) **Subcooled feed with $\mathbf{T_F}$ = 20 °C**

$$T_S = 95.3\,°\text{C} \quad c_{Fl} = 0.79\,\text{Wh/kgK} \quad r = 161\,\text{Wh/kg}$$

$$q = 1 + \frac{0.79 * (95.3 - 20)}{161} = 1.37$$

Slope of the *q*-line = 1.37/0.37 = 3.7

(b) **Feed = 66% vapour ⇒ q = 0.34**

Slope of the *q*-line = 0.34/0.34 – 1 = – 0.51

(c) **Feed = saturated vapour ⇒ q = 0**

Slope of the *q*-line = 0/1 – 0 = 0

(d) **Feed = overheated vapour with $\mathbf{T_F}$ = 130 °C**

$$T_{\text{dew}} = 100\,°\text{C} \quad c_D = 0.3\,\text{Wh/kgK} \quad r = 120\,\text{Wh/kg}$$

$$q = \frac{-0.3 * (130 - 100)}{120} = -0.075$$

The *q*-value influences

- The vapour and liquid loading in the column.
- The optimal feed tray.
- The number of trays and required reflux ratio.

In **mass balance in the rectification and stripping sections** the q-value must absolutely be considered. The vapour and liquid loadings in the column are calculated as follows:

$$
\begin{aligned}
&V_V = (R+1)*D && L_V = R*D \\
&V_A = V_V - (1-q)*F && V_V - V_A = (1-q)*F \\
&V_V = V_A + (1-q)*F && \\
&L_A = L_V + q*F && L_A - L_V = (1-q)*F
\end{aligned}
$$

F = feed rate (kmol/h)
D = distillate rate (kmol/h)
R = reflux ratio
V_A = vapour rate in the stripping section of the column (kmol/h)
L_A = liquid rate in the stripping section (kmol/h)
V_V = vapour rate in the rectification section (kmol/h)
L_V = liquid rate in the rectification section (kmol/h)

Example 3.10.2: Mass balances in the rectification and stripping sections at different q-values

$$\mathrm{F} = 100\,\mathrm{kmol/h} \quad \mathrm{D} = 30\,\mathrm{kmol/h} \quad \mathrm{B} = 70\,\mathrm{kmol/h} \quad R = 3$$

(a) **Feed at boiling temperature ⇒ q = 1**

$$
\begin{aligned}
&V_V = 4*30 = 120\,\mathrm{kmol/h} && L_V = 3*30 = 90\,\mathrm{kmol/h} \\
&V_V = V_A = 120\,\mathrm{kmol/h} && L_A = 90+100 = 190\,\mathrm{kmol/h}
\end{aligned}
$$

(b) **Subcooled feed ⇒ q = 1.5**

V_V = 120 kmol/h L_V = 90 kmol/h
V_A = 120 – (1 – 1.5) * 100 = 170 kmol/h
V_A = 240 – 70 = 170 kmol/h
L_A = 90 + 1.5 * 100 = 240 kmol/h

(c) **Vapour feed ⇒ q = 0**

L_A = L_V = 90 kmol/h
V_A = 120 – 100 = 20 kmol/h
V_V = V_A + F = 20 + 100 = 120 kmol/h
V_A = 90 – 70 = 20 kmol/h

(d) **Feed = vapour–liquid mixture with 50% vapour ⇒ q = 0.5**

L_A = 90 + 50 = 140 kmol/h
V_A = 120 – 50 = 70 kmol/h
V_V = 70 + 50 = 120 kmol/h

Figure 3.9 show the **influence of q on the required number of trays and the correct feed tray**.

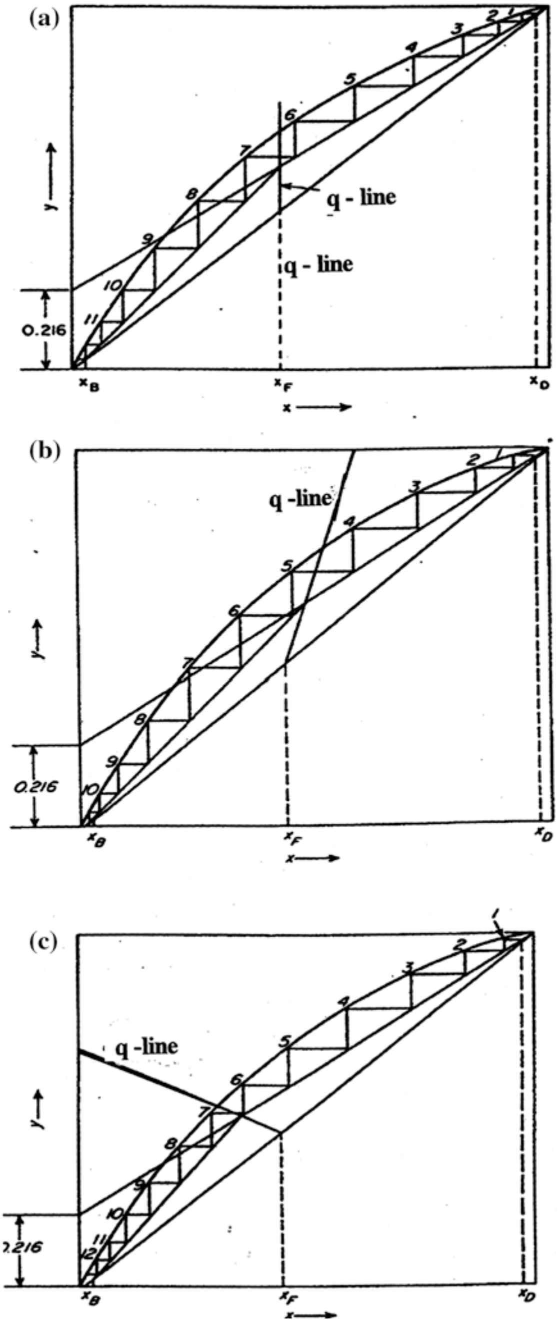


Fig. 3.9 **a** Feed with boiling temperature ⇒ $q = 1$. Required number of trays: 11. Feed tray: seventh tray from the *top*. **b** Subcooled feed ⇒ $q = 1.37$. Required number of trays: 10. Feed trays: fifth tray from the *top*. **c** Feed = 2/3 vapour ⇒ $q = 1/3$. Required number of trays: 12. Feed tray: seventh tray from the *top*

3.11 Column Loading in the Rectification and Stripping Section

The vapour and liquid rates in the rectifying and stripping section of the column result from the mass balance, the reflux ratio, and the thermal condition of the feed or the q-value.

F = feed rate (kmol/h)
D = distillate rate (kmol/h)
B = bottoms rate (kmol/h)
V_V = vapour rate in the rectification section (kmol/h)
L_V = liquid rate in the stripping section (kmol/h)
V_A = vapour rate in the stripping section (kmol/h)
L_A = liquid rate in the stripping section (kmol/h)
$R = L_V/D$ = reflux ratio in the rectification section
$R_A = L_A/B$ = reflux ratio in the stripping section

Rectification section

$$V_V = (R + 1) * D \quad L_V = R * D$$

Slope of the operating line for the rectification section = L_V/V_V

$$\frac{L_V}{V_V} = \frac{R}{R + 1}$$

Stripping section

$V_A = V_V - (1 - q) * F = L_A - B$
$L_A = L_V + q * F = R * D + q * F = R_A * B$

Slope of the operating line for the stripping section = L_A/V_A

$$\frac{L_A}{V_A} = \frac{R_A}{R_A - 1}$$

Example 3.11.1: Vapour and liquid loadings in the rectification and stripping sections

(a) $\mathbf{q = 1 \quad R = 3.05 \quad F = 100\ kmol/h \quad D = 31.2\ kmol/h}$

Rectification section

$V_V = (3.05 + 1) * 31.2 = 126.36$ kmol/h
$L_V = 3.05 * 31.2 = 95.16$ kmol/h
$L_V/V_V = 95.16/126.36 = 0.753 = 3.05/4.05$ = slope of the rectification operating line

Stripping section

L_A = 95.16 + 1 * 100 = 195.16 kmol/h
V_A = 126.36 – (1) * 100 = 126.36 kmol/h
L_A/V_A = 195.16/126.36 = 1.54 = slope of the stripping operating line

(b) $\mathbf{q = 1.25 \quad R = 3.05 \quad F = 100\ kmol/h \quad D = 31.2\ kmol/h}$

Rectification section

V_V = 4.05 * 31.2 = 126.36 kmol/h
L_V = 3.05 * 31.2 = 95.16 kmol/h
L_V/V_V = 0.753 = slope of the rectification operating line

Stripping section

L_A = 95.16 + 1.25 * 100 = 220.16 kmol/h
V_A = 126.36 – (1 – 1.25) * 100 = 151.36 kmol/h
L_A/V_A = 1.45 = slope of the stripping operating line

3.12 Design Data for the Column Internals

From the calculated column loading in kmol/h the vapour and liquid flows in kg/h and m^3/h must be determined using the average mole weights and the vapour or liquid densities at column temperature and the column pressure:

$$\text{Vapour rate} = \frac{V*M_a}{\varrho_V} \quad (\text{m}^3/\text{h}) \quad \text{Liquid rate} = \frac{L*M_a}{\varrho_L} \quad (\text{m}^3/\text{h})$$

M_a = average mole weight of the mixture
V = vapour loading (kmol/h)
L = liquid loading (kmol/h)
ϱ_L = liquid density (kg/m^3)
ϱ_V = vapour density (kg/m^3)

Example 3.11.1: Separation of a benzene–toluene mixture with relative volatility α = 2

Component	x_F (molfr.)	x_D (molfr.)	x_B (molfr.)
Benzene	0.5	0.9734	0.0266
Toluene	0.5	0.0266	0.9734

Rate (kmol/h)	100	50	50
Rate (kg/h)	8512.7	3924.44	4588.26
Average *M*	85.13	78.49	91.77
Temperatures	91.7 °C	80.2 °C	108.9 °C

Feed at boiling temperature ⇒ **q = 1**

Calculation of the minimum number of trays

$$N_{\min} = \frac{\lg\left(\frac{0.9734}{0.0266} * \frac{0.9734}{0.0266}\right)}{\lg 2.4} = 8.22$$

$$N_{\min V} = \frac{\lg\left(\frac{0.9734}{0.0266} * \frac{0.5}{0.5}\right)}{\lg 2.4} = 4.11$$

Calculation of the minimum reflux ratio

$$R_{\min} = \frac{1}{2.4 - 1} * \left(\frac{0.9734}{0.5} - 2.4 * \frac{0.0266}{0.5}\right) = 1.3$$

Required number of theoretical trays at the chosen reflux ratio R = 1.5

$$X = \frac{R - R_{\min}}{R + 1} = \frac{1.5 - 1.3}{2.5} = 0.08$$

$$Y = 0.75 - 0.75 * X^{0.5668} = 0.75 - 0.75 * 0.08^{0.5668} = 0.57$$

$$N = 20.4$$

Calculated number or trays according to McCabe–Thiele

Total number of trays	$n_{\text{tot}} = 20$
Rectification trays	$n_{\text{V}} = 10$
Stripping trays	$n_{\text{A}} = 10$
Feed tray	$n_{\text{F}} = 10$

Column loading at q = 1 without heat losses

V_{V} = (1.5 + 1) * 50 = 125 kmol/h
V_{V} = 125 * M_m = 125 * 78.49 = 9811 kg/h
L_{V} = 1.5 * 50 = 75 kmol/h
L_{V} = 75 * 78.49 = 5886 kg/h
V_{A} = 125 kmol/h = 125 * 85.13 = 10.641 kg/h
L_{A} = 75 + 100 = 175 kmol/h
L_{A} = 175 * 85.13 = 14.898 kg/h

Design data for the column internals

Rectification	**Stripping**
$\varrho_V = 2.66$ kg/m^3 at 1 bar	$\varrho_V = 2.8$ kg/m^3
$V_V = 9811$ kg/h = 3688 m^3/h	$V_A = 10.641$ kg/h = 3800 m^3/h
$\varrho_L = 814$ kg/m^3	$\varrho_L = 780$ kg/m^3
$L_V = 5886$ kg/h = 7.23 m^3/h	$L_A = 14.898$ kg/h = 19.1 m^3/h

Example 3.11.2: Influence of the *q*-value on the separation in Example 3.11.1
The separation effort at the fractionation of a benzene–toluene mixture is strongly influenced by the thermal condition of the feed.

(a) **Feed at boiling temperature ⇒ q = 1**

$V_V = 125$ kmol/h	$L_V = 75$ kmol/h	
$V_A = 125$ kmol/h	$L_A = 175$ kmol/h	
$x_F = 0.50$ molfr.	$x_D = 0.9734$ molfr.	$x_B = 0.0266$ molfr.

(b) **Feed subcooled to 30 °C ⇒ q = 1.287**

$V_V = 125$ kmol/h	$L_V = 75$ kmol/h	
$V_A = 154$ kmol/h	$L_A = 200$ kmol/h	
$x_F = 0.5$ molfr.	$x_D = 0.9847$ molfr.	$x_B = 0.0153$ molfr.

Conclusion: The separation is lightly better!

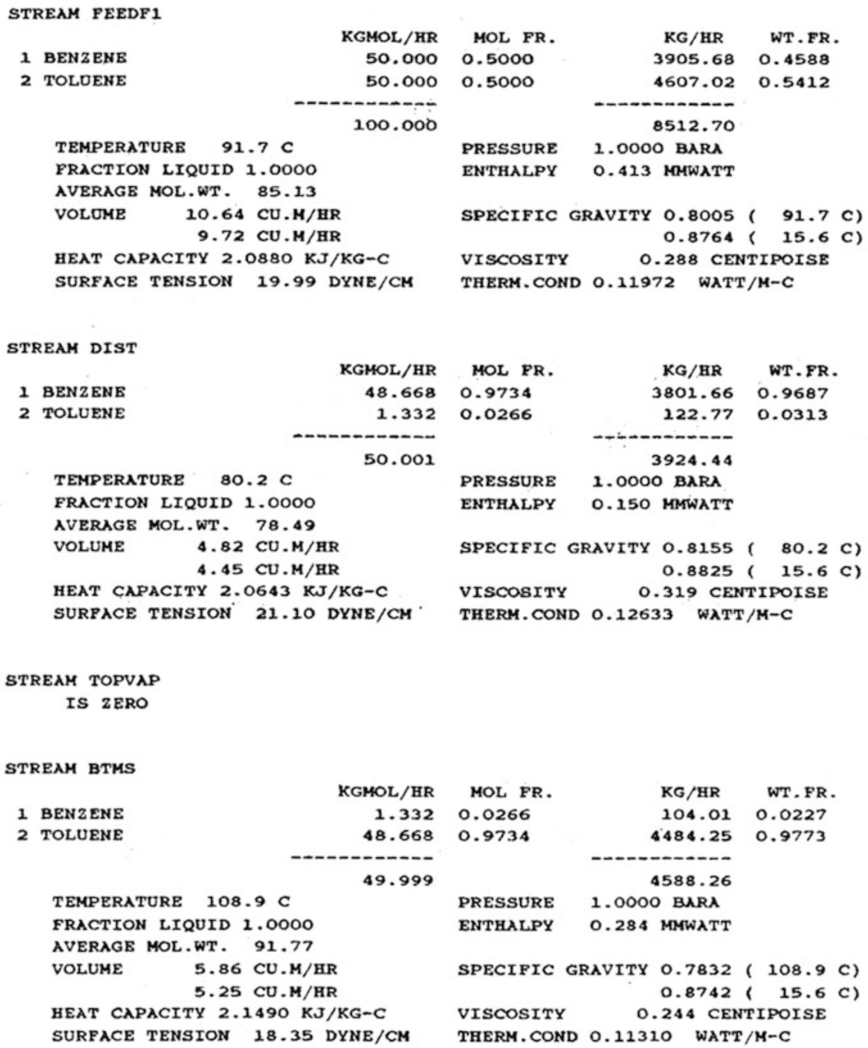
(c) **Feed as overheated vapour at 120 °C**

$V_V = 125$ kmol/h	$L_V = 75$ kmol/h	
$V_A = 14$ kmol/h	$L_A = 64$ kmol/h	
$x_F = 0.5$ molfr.	$x_D = 0.7768$ molfr.	$x_B = 0.2232$ molfr.

Conclusion: The separation is clearly worse!

For comparison, the output of a computer simulation for Example 3.11.1 is shown in Figs. 3.10 and 3.11.

The results are nearly identical. The great advantage of the computer calculation is the output of data for many components, needed for **fluid-dynamic design and calculation of the condenser and the reboiler.** Using computer programs the column design is made easier because the components are included in the program



```
STREAM FEEDF1
                                KGMOL/HR   MOL FR.         KG/HR    WT.FR.
 1 BENZENE                        50.000   0.5000        3905.68   0.4588
 2 TOLUENE                        50.000   0.5000        4607.02   0.5412
                            ------------             ------------
                                 100.000                 8512.70
    TEMPERATURE    91.7 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000             ENTHALPY    0.413 MMWATT
    AVERAGE MOL.WT.   85.13
    VOLUME       10.64 CU.M/HR         SPECIFIC GRAVITY 0.8005 (   91.7 C)
                  9.72 CU.M/HR                          0.8764 (   15.6 C)
    HEAT CAPACITY 2.0880 KJ/KG-C       VISCOSITY       0.288 CENTIPOISE
    SURFACE TENSION   19.99 DYNE/CM    THERM.COND 0.11972   WATT/M-C

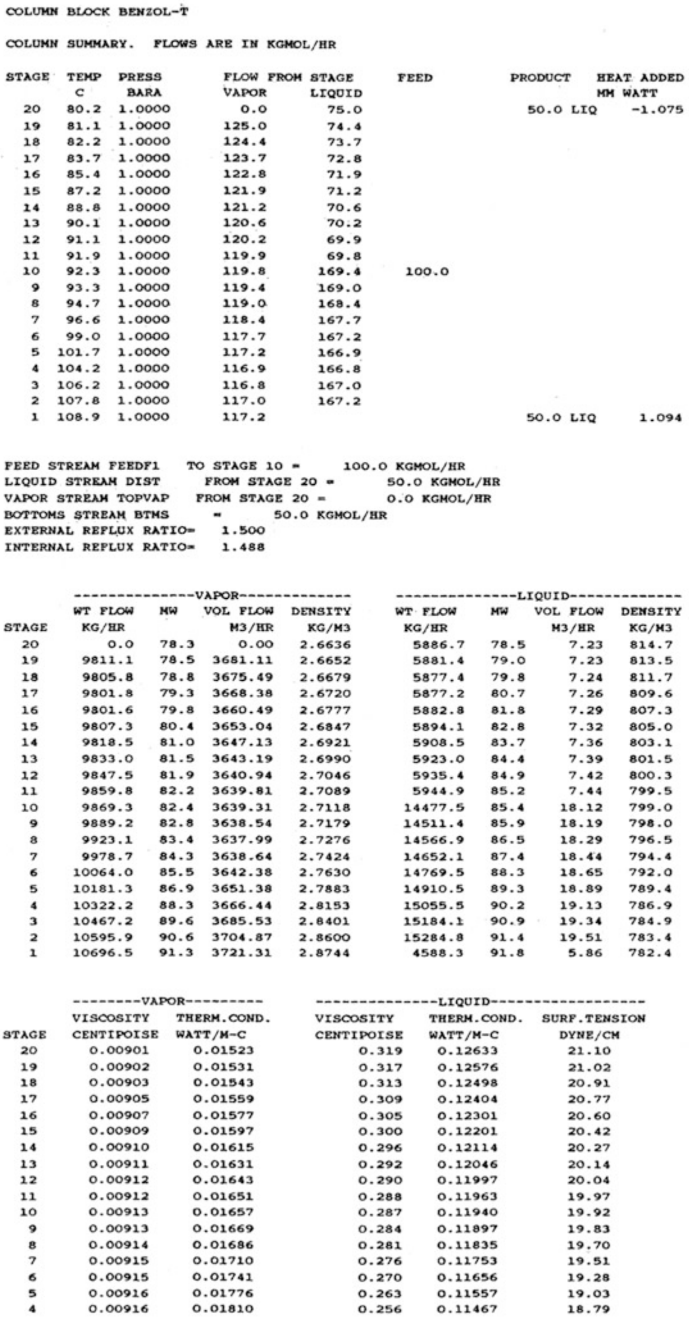

STREAM DIST
                                KGMOL/HR   MOL FR.         KG/HR    WT.FR.
 1 BENZENE                        48.668   0.9734        3801.66   0.9687
 2 TOLUENE                         1.332   0.0266         122.77   0.0313
                            ------------             ------------
                                  50.001                 3924.44
    TEMPERATURE    80.2 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000             ENTHALPY    0.150 MMWATT
    AVERAGE MOL.WT.   78.49
    VOLUME        4.82 CU.M/HR         SPECIFIC GRAVITY 0.8155 (   80.2 C)
                  4.45 CU.M/HR                          0.8825 (   15.6 C)
    HEAT CAPACITY 2.0643 KJ/KG-C       VISCOSITY       0.319 CENTIPOISE
    SURFACE TENSION   21.10 DYNE/CM    THERM.COND 0.12633   WATT/M-C


STREAM TOPVAP
     IS ZERO


STREAM BTMS
                                KGMOL/HR   MOL FR.         KG/HR    WT.FR.
 1 BENZENE                         1.332   0.0266         104.01   0.0227
 2 TOLUENE                        48.668   0.9734        4484.25   0.9773
                            ------------             ------------
                                  49.999                 4588.26
    TEMPERATURE   108.9 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000             ENTHALPY    0.284 MMWATT
    AVERAGE MOL.WT.   91.77
    VOLUME        5.86 CU.M/HR         SPECIFIC GRAVITY 0.7832 ( 108.9 C)
                  5.25 CU.M/HR                          0.8742 (   15.6 C)
    HEAT CAPACITY 2.1490 KJ/KG-C       VISCOSITY       0.244 CENTIPOISE
    SURFACE TENSION   18.35 DYNE/CM    THERM.COND 0.11310   WATT/M-C
```

Fig. 3.10 Computer simulation of the benzene–toluene separation, Part 1

along with the equilibria. Therefore, the sometimes laborious generation of physical properties is no longer necessary. It is important to **critically check computer results.** From the computer output the influence of the *q*-value, reflux ratio, side draw, and feed tray on the required separation effort can not be seen as it can in the McCabe–Thiele diagram.



```
COLUMN BLOCK BENZOL-T

COLUMN SUMMARY.  FLOWS ARE IN KGMOL/HR

STAGE  TEMP  PRESS       FLOW FROM STAGE     FEED          PRODUCT   HEAT ADDED
         C    BARA       VAPOR      LIQUID                             MM WATT
  20   80.2  1.0000        0.0        75.0                 50.0 LIQ    -1.075
  19   81.1  1.0000      125.0        74.4
  18   82.2  1.0000      124.4        73.7
  17   83.7  1.0000      123.7        72.8
  16   85.4  1.0000      122.8        71.9
  15   87.2  1.0000      121.9        71.2
  14   88.8  1.0000      121.2        70.6
  13   90.1  1.0000      120.6        70.2
  12   91.1  1.0000      120.2        69.9
  11   91.9  1.0000      119.9        69.8
  10   92.3  1.0000      119.8       169.4    100.0
   9   93.3  1.0000      119.4       169.0
   8   94.7  1.0000      119.0       168.4
   7   96.6  1.0000      118.4       167.7
   6   99.0  1.0000      117.7       167.2
   5  101.7  1.0000      117.2       166.9
   4  104.2  1.0000      116.9       166.8
   3  106.2  1.0000      116.8       167.0
   2  107.8  1.0000      117.0       167.2
   1  108.9  1.0000      117.2                             50.0 LIQ     1.094

FEED STREAM FEEDF1    TO STAGE 10 =      100.0 KGMOL/HR
LIQUID STREAM DIST      FROM STAGE 20 =       50.0 KGMOL/HR
VAPOR STREAM TOPVAP   FROM STAGE 20 =       0.0 KGMOL/HR
BOTTOMS STREAM BTMS      =       50.0 KGMOL/HR
EXTERNAL REFLUX RATIO=   1.500
INTERNAL REFLUX RATIO=   1.488

        --------------VAPOR-------------     -------------LIQUID------------
        WT FLOW    MW   VOL FLOW  DENSITY    WT FLOW    MW   VOL FLOW  DENSITY
STAGE   KG/HR              M3/HR    KG/M3    KG/HR              M3/HR    KG/M3
  20       0.0    78.3     0.00    2.6636     5886.7   78.5      7.23    814.7
  19    9811.1    78.5  3681.11    2.6652     5881.4   79.0      7.23    813.5
  18    9805.8    78.8  3675.49    2.6679     5877.4   79.8      7.24    811.7
  17    9801.8    79.3  3668.38    2.6720     5877.2   80.7      7.26    809.6
  16    9801.6    79.8  3660.49    2.6777     5882.8   81.8      7.29    807.3
  15    9807.3    80.4  3653.04    2.6847     5894.1   82.8      7.32    805.0
  14    9818.5    81.0  3647.13    2.6921     5908.5   83.7      7.36    803.1
  13    9833.0    81.5  3643.19    2.6990     5923.0   84.4      7.39    801.5
  12    9847.5    81.9  3640.94    2.7046     5935.4   84.9      7.42    800.3
  11    9859.8    82.2  3639.81    2.7089     5944.9   85.2      7.44    799.5
  10    9869.3    82.4  3639.31    2.7118    14477.5   85.4     18.12    799.0
   9    9889.2    82.8  3638.54    2.7179    14511.4   85.9     18.19    798.0
   8    9923.1    83.4  3637.99    2.7276    14566.9   86.5     18.29    796.5
   7    9978.7    84.3  3638.64    2.7424    14652.1   87.4     18.44    794.4
   6   10064.0    85.5  3642.38    2.7630    14769.5   88.3     18.65    792.0
   5   10181.3    86.9  3651.38    2.7883    14910.5   89.3     18.89    789.4
   4   10322.2    88.3  3666.44    2.8153    15055.5   90.2     19.13    786.9
   3   10467.2    89.6  3685.53    2.8401    15184.1   90.9     19.34    784.9
   2   10595.9    90.6  3704.87    2.8600    15284.8   91.4     19.51    783.4
   1   10696.5    91.3  3721.31    2.8744     4588.3   91.8      5.86    782.4

        --------VAPOR---------      ---------------LIQUID-----------------
        VISCOSITY   THERM.COND.     VISCOSITY    THERM.COND.   SURF.TENSION
STAGE   CENTIPOISE  WATT/M-C        CENTIPOISE   WATT/M-C        DYNE/CM
  20     0.00901     0.01523             0.319    0.12633          21.10
  19     0.00902     0.01531             0.317    0.12576          21.02
  18     0.00903     0.01543             0.313    0.12498          20.91
  17     0.00905     0.01559             0.309    0.12404          20.77
  16     0.00907     0.01577             0.305    0.12301          20.60
  15     0.00909     0.01597             0.300    0.12201          20.42
  14     0.00910     0.01615             0.296    0.12114          20.27
  13     0.00911     0.01631             0.292    0.12046          20.14
  12     0.00912     0.01643             0.290    0.11997          20.04
  11     0.00912     0.01651             0.288    0.11963          19.97
  10     0.00913     0.01657             0.287    0.11940          19.92
   9     0.00913     0.01669             0.284    0.11897          19.83
   8     0.00914     0.01686             0.281    0.11835          19.70
   7     0.00915     0.01710             0.276    0.11753          19.51
   6     0.00915     0.01741             0.270    0.11656          19.28
   5     0.00916     0.01776             0.263    0.11557          19.03
   4     0.00916     0.01810             0.256    0.11467          18.79
```

Fig. 3.11 Computer simulation of the benzene–toluene separation, Part 2

3.13 Fractionation of Non-ideal Binaries

With the distillation calculations for ideal mixtures you can calculate, to a large extent, with a constant relative volatility α. This makes the calculation easy. With the fractionation of non-ideal mixtures the relative volatility in the column changes from tray to tray because the activity coefficient γ strongly depends on the concentration. Much more time is needed for a distillation calculation because the compositions vary inside the column and for each new composition the activity coefficient for the equilibrium has to be determined once again. Figure 3.12 shows the curve of the activity coefficients for a methanol–water mixture depends on the methanol composition.

Figure 3.13 shows how the relative volatility for the methanol–water mixture varies on the different theoretical trays. In the design of a column there needs to be made an iterative calculation until the equilibrium corresponds to the tray composition. First of all the composition of a tray is sized up using the equilibrium of the previous theoretical tray. Then the activity coefficient for the new composition is determined and the new equilibrium on the theoretical tray is calculated until the right equilibrium for the composition on the tray is determined. Much time is needed for this calculation. Therefore, such calculations are completed using a computer. Figure 3.14 depicts the curve for the composition in a column for the separation of methanol and water.

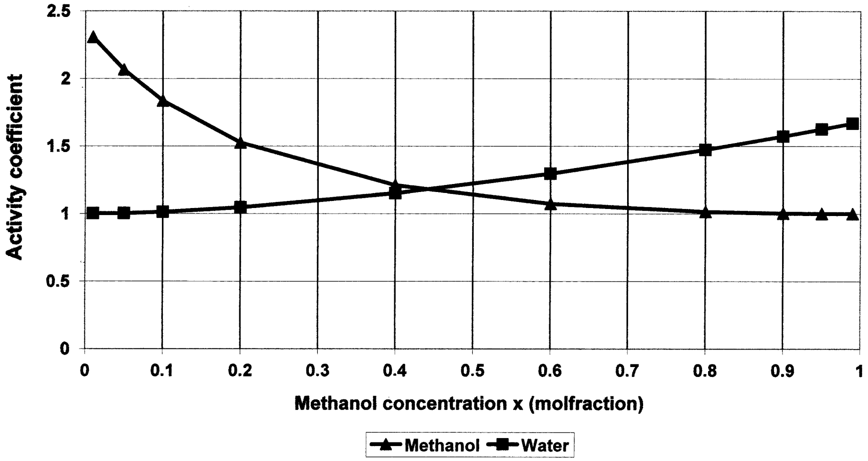


Fig. 3.12 Activity coefficients of methanol and water as a function of methanol concentration in the liquid phase

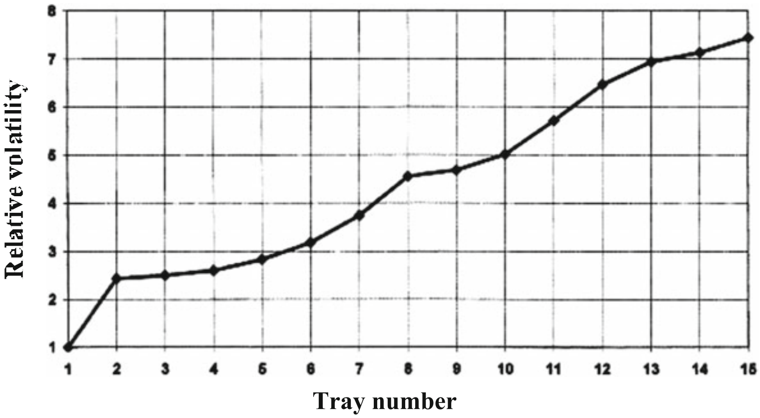


Fig. 3.13 Relative volatility on different trays of a methanol–water column

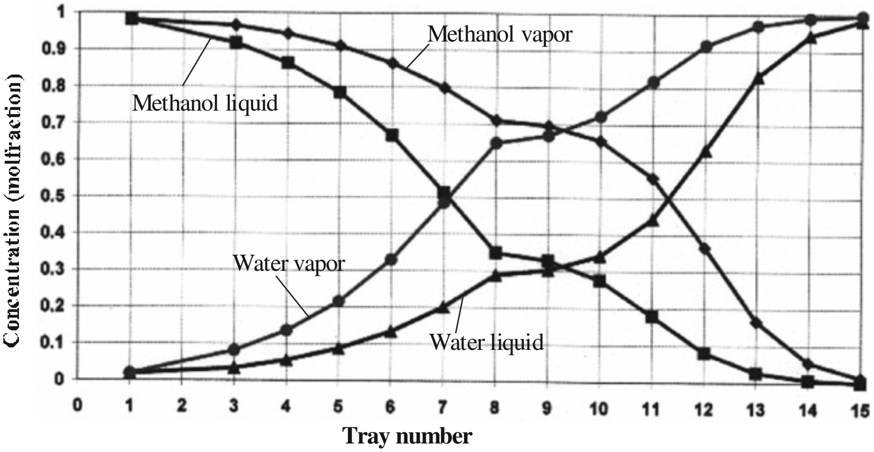


Fig. 3.14 Composition of methanol and water on the column trays

The graphical design of a column for a non-ideal, two-component mixture is very easy. The vapour–liquid equilibrium and an A3-sheet paper is all that is needed. The application is shown in Example 3.12.6 and Fig. 3.15.

Example 3.12.6: Distillative separation effort for an isopropanol–water mixture

IPA-feed composition:	50 weight% = 23.06 mol%
IPA-distillate composition:	>86.1 weight% = 65 mol%
IPA-bottoms composition:	<14.93 weight% = 5 mol%

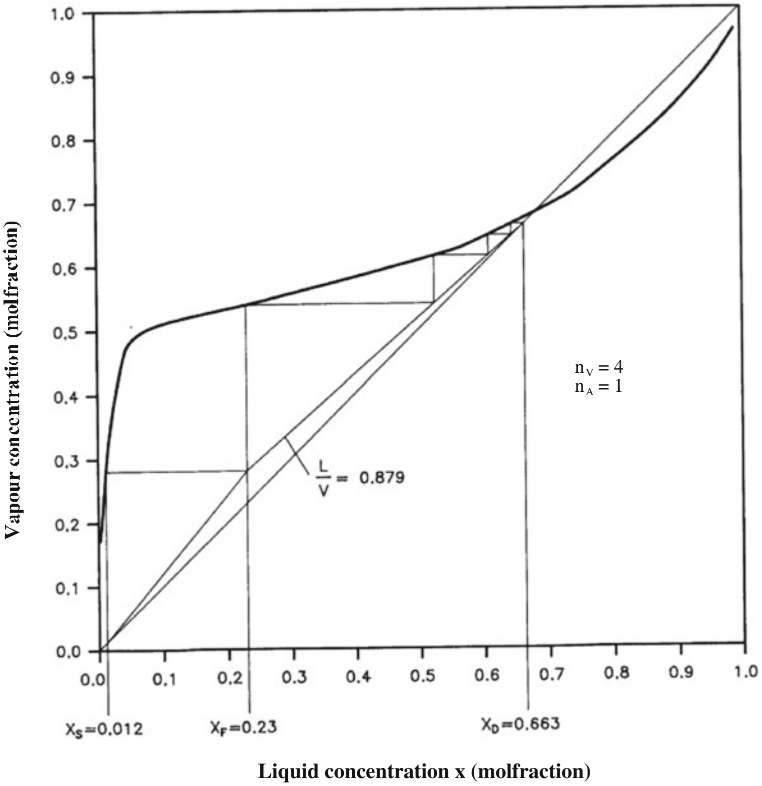


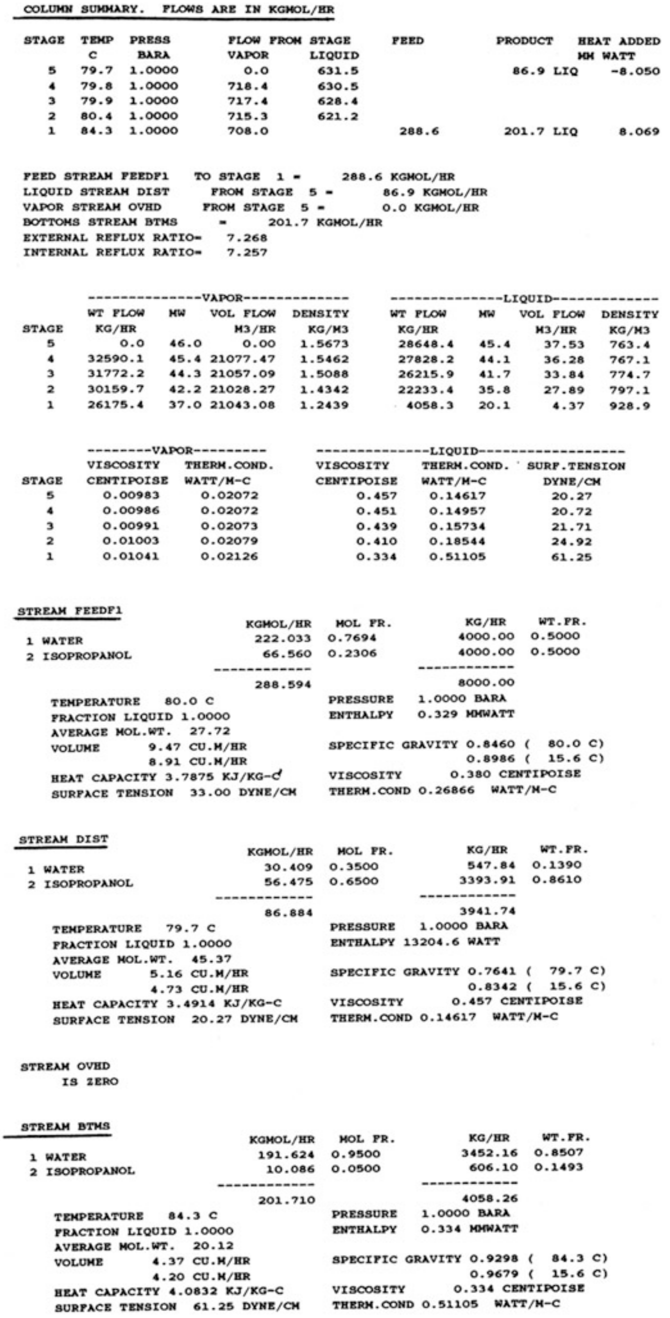
Fig. 3.15 Graphical design of a column for isopropanol–water separation

From the McCabe–Thiele diagram shown below the following separation conditions result:

$$\frac{L}{V} = 0.879 = \frac{R}{R+1} \quad R = 0.879 * R + 0.879 \quad R = \frac{0.879}{0.121} = 7.26$$

Required rectification trays: 4	Required stripping trays: 1
Total number of theoretical trays: 5	

The following computer simulation of Example 3.12.6 in Fig. 3.16 gives the same result as the graphical design.



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COLUMN SUMMARY.  FLOWS ARE IN KGMOL/HR

STAGE  TEMP   PRESS          FLOW FROM STAGE      FEED         PRODUCT    HEAT ADDED
        C      BARA          VAPOR      LIQUID                             MM WATT
  5    79.7   1.0000           0.0       631.5                 86.9 LIQ     -8.050
  4    79.8   1.0000         718.4       630.5
  3    79.9   1.0000         717.4       628.4
  2    80.4   1.0000         715.3       621.2
  1    84.3   1.0000         708.0                    288.6     201.7 LIQ     8.069

FEED STREAM FEEDF1    TO STAGE  1 =      288.6 KGMOL/HR
LIQUID STREAM DIST      FROM STAGE  5 =       86.9 KGMOL/HR
VAPOR STREAM OVHD      FROM STAGE  5 =       0.0 KGMOL/HR
BOTTOMS STREAM BTMS       =     201.7 KGMOL/HR
EXTERNAL REFLUX RATIO=   7.268
INTERNAL REFLUX RATIO=   7.257

          --------------VAPOR-------------    --------------LIQUID------------
          WT FLOW    MW    VOL FLOW   DENSITY   WT FLOW     MW    VOL FLOW   DENSITY
STAGE      KG/HR                M3/HR     KG/M3     KG/HR               M3/HR      KG/M3
  5           0.0    46.0       0.00    1.5673   28648.4    45.4      37.53     763.4
  4       32590.1    45.4   21077.47    1.5462   27828.2    44.1      36.28     767.1
  3       31772.2    44.3   21057.09    1.5088   26215.9    41.7      33.84     774.7
  2       30159.7    42.2   21028.27    1.4342   22233.4    35.8      27.89     797.1
  1       26175.4    37.0   21043.08    1.2439    4058.3    20.1       4.37     928.9

          --------VAPOR---------          --------------LIQUID------------------
          VISCOSITY    THERM.COND.        VISCOSITY    THERM.COND.   SURF.TENSION
STAGE     CENTIPOISE   WATT/M-C           CENTIPOISE   WATT/M-C        DYNE/CM
  5        0.00983      0.02072               0.457     0.14617          20.27
  4        0.00986      0.02072               0.451     0.14957          20.72
  3        0.00991      0.02073               0.439     0.15734          21.71
  2        0.01003      0.02079               0.410     0.18544          24.92
  1        0.01041      0.02126               0.334     0.51105          61.25

STREAM FEEDF1
                                KGMOL/HR   MOL FR.          KG/HR     WT.FR.
 1 WATER                         222.033   0.7694          4000.00   0.5000
 2 ISOPROPANOL                    66.560   0.2306          4000.00   0.5000
                             ------------              ------------
                                 288.594                   8000.00
   TEMPERATURE    80.0 C                   PRESSURE    1.0000 BARA
   FRACTION LIQUID 1.0000                  ENTHALPY    0.329 MMWATT
   AVERAGE MOL.WT.   27.72
   VOLUME          9.47 CU.M/HR            SPECIFIC GRAVITY 0.8460 (   80.0 C)
                   8.91 CU.M/HR                             0.8986 (   15.6 C)
   HEAT CAPACITY 3.7875 KJ/KG-C            VISCOSITY        0.380 CENTIPOISE
   SURFACE TENSION   33.00 DYNE/CM         THERM.COND 0.26866   WATT/M-C

STREAM DIST
                                KGMOL/HR   MOL FR.          KG/HR     WT.FR.
 1 WATER                          30.409   0.3500           547.84   0.1390
 2 ISOPROPANOL                    56.475   0.6500          3393.91   0.8610
                             ------------              ------------
                                  86.884                   3941.74
   TEMPERATURE    79.7 C                   PRESSURE    1.0000 BARA
   FRACTION LIQUID 1.0000                  ENTHALPY 13204.6 WATT
   AVERAGE MOL.WT.   45.37
   VOLUME          5.16 CU.M/HR            SPECIFIC GRAVITY 0.7641 (   79.7 C)
                   4.73 CU.M/HR                             0.8342 (   15.6 C)
   HEAT CAPACITY 3.4914 KJ/KG-C            VISCOSITY        0.457 CENTIPOISE
   SURFACE TENSION   20.27 DYNE/CM         THERM.COND 0.14617   WATT/M-C

STREAM OVHD
    IS ZERO

STREAM BTMS
                                KGMOL/HR   MOL FR.          KG/HR     WT.FR.
 1 WATER                         191.624   0.9500          3452.16   0.8507
 2 ISOPROPANOL                    10.086   0.0500           606.10   0.1493
                             ------------              ------------
                                 201.710                   4058.26
   TEMPERATURE    84.3 C                   PRESSURE    1.0000 BARA
   FRACTION LIQUID 1.0000                  ENTHALPY    0.334 MMWATT
   AVERAGE MOL.WT.   20.12
   VOLUME          4.37 CU.M/HR            SPECIFIC GRAVITY 0.9298 (   84.3 C)
                   4.20 CU.M/HR                             0.9679 (   15.6 C)
   HEAT CAPACITY 4.0832 KJ/KG-C            VISCOSITY        0.334 CENTIPOISE
   SURFACE TENSION   61.25 DYNE/CM         THERM.COND 0.51105   WATT/M-C
```

Fig. 3.16 Computer simulation of isopropanol–water separation

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Chapter 4
Calculation of Multi-component Fractionation Plants

4.1 Basic Data for the Design

4.1.1 Mass Balance for the Separation Task

First a preliminary mass balance for the specified separation task is prepared:

- Feed composition.
- Distillate composition.
- Bottoms composition.

These compositions are required in order to determine the bubble point temperatures of the feed and bottoms product and the dew point at the column top in order to determine the average relative volatility α for the given fractionation task.

The calculation method is essentially reduced to the separation of two key components, i.e., the light key (LK) and the heavy key (HK) components.

Example 4.1.1: Mass balance for a four-component mixture

Component		Feed			Distillate			Bottoms		
	M									
	kg/kmol	kg/h	kmol/h	x_E	kg/h	kmol/h	x_D	kg/h	kmol/h	x_B
Light	78	1952	25	0.25	1952	25	0.48	0.0	0.0	0
LK	92.1	2303	25	0.25	2081	22.6	0.44	219	2.4	0.05
HK	106.1	2652	25	0.25	228	2.15	0.04	2425	22.85	0.48
Heavy	104.1	2602	25	0.25	239	2.3	0.04	2580	24.77	0.47
		9508	100	1.0	4500	52.05		5008	47.95	1.0

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_4

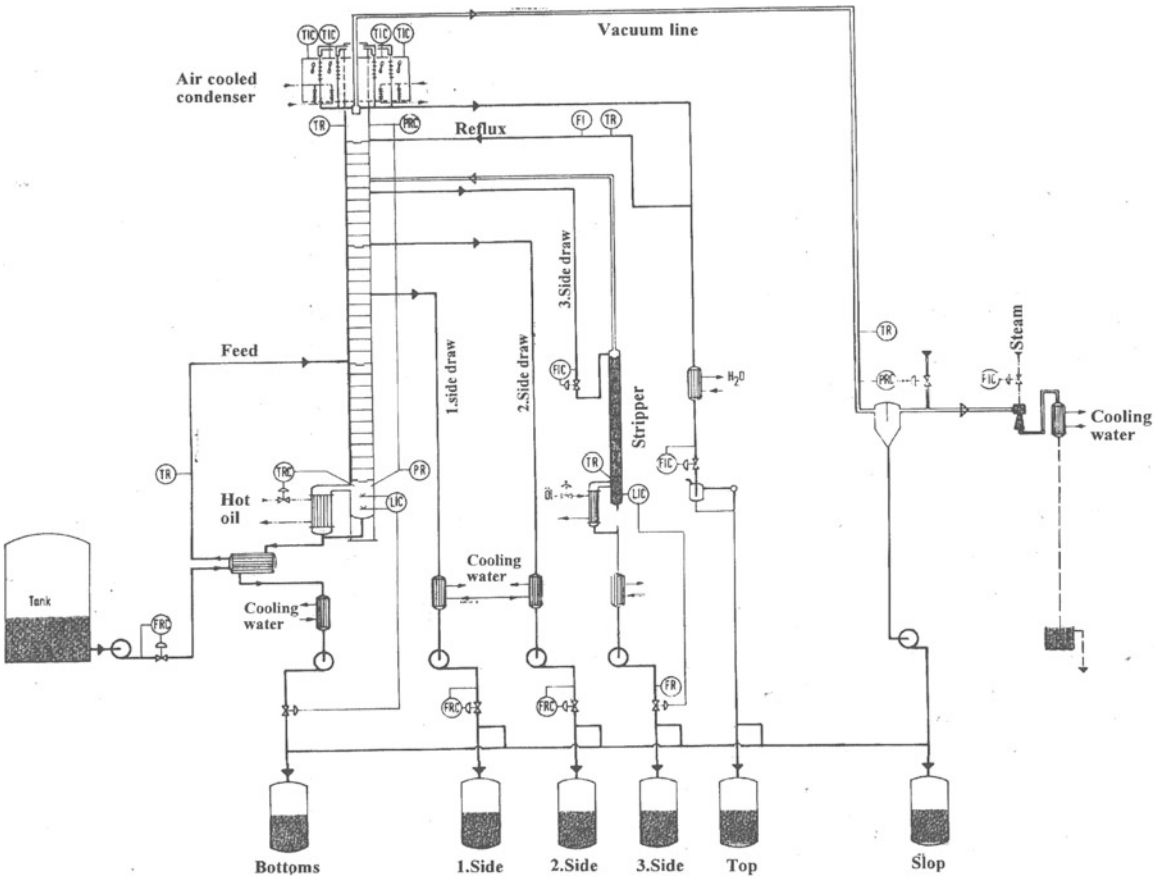


Fig. 4.1 Continous fractionation column with side draws and a side stripper

Average mole weight $M_m = \sum x_i * M_i$

$$\text{Feed:} M_m = 95.075 \quad \text{Distillate:} M_m = 86.37 \quad \text{Bottoms:} M_m = 104.46$$

HK = heavy key component.
LK = light key component.
M = molecular weight (kg/kmol).
x_E = feed composition (molfraction).
x_D = distillate composition (molfraction).
x_B = bottoms composition (molfraction).

4.1.2 Calculation of the Average Relative Volatility α for Ideal Mixtures

For the determination of the averaged relative volatility, the temperatures at the column top, in the column bottom, and at the feed stage are required in order to determine the averaged relative volatilities for the different temperatures at the top, the feed stage and the bottom.

Calculation of the bubble points and dew points is shown in Chap. 2.

Bubble Point Equation:

$$\sum y_i = 1 = \sum K_i * x_i = \sum \frac{x_i * \gamma_i * p_{0i}}{P_{\text{tot}}}$$

Dew Point Equation:

$$\sum x_i = 1 = \sum \frac{y_i}{K_i} = \sum \frac{y_i * P_{\text{tot}}}{\gamma_i * p_{0i}}$$

The **activity coefficient** γ must be considered for non-ideal mixtures!

P_{tot} = total pressure (mbar).
P_{0i} = vapour pressure of component i.
x_i = composition of component i in the liquid (molfraction).
γ_i = activity coefficient of component i.
y_i = vapour composition of component i (molfraction).
K = equilibrium constant = y/x.

In multi-component mixtures the relative volatility α is derived from the vapour pressures and is based on the HK component.

$$\text{Relative volatility of component 1: } \alpha_1 = \frac{p_{01}}{p_{0\mathrm{HK}}}$$

$$\text{Relative volatility of component 2: } \alpha_2 = \frac{p_{02}}{p_{0\mathrm{HK}}}$$

$$\text{Relative volatility of component LK: } \alpha_{LK} = \frac{p_{0\mathrm{LK}}}{p_{0\mathrm{HK}}}$$

p_{01} = vapour pressure of component 1.
α_1 = relative volatility of component 1.
p_{02} = vapour pressure of component 2.
α_2 = relative volatility of component 2.
$p_{0\mathrm{LK}}$ = vapour pressure of the LK component.
$p_{0\mathrm{HK}}$ = vapour pressure of the HK component.

The vapour pressures at different temperatures are calculated and hence the average relative volatilities α_m derived:

$$\alpha_m = \sqrt[3]{\alpha_{\mathrm{top}} * \alpha_{\mathrm{feed}} * \alpha_{\mathrm{bottom}}}$$

Example 4.1.2.1: Determination of the Relative volatilities for a benzene/toluene/ethyl benzene/styrene mixture

	Top		Bottom		Feed	
Temperature (°C)	101		138.1		108	
	p_0	α	p_0	α	p_0	α
Component	mbar	–	mbar	–	mbar	–
Benzene	1387	5.20	3398	4.25	1690	4.99
Toluene	573.4	2.15	1562	1.95	715.2	2.11
Ethylbenz	265.7	1.0	800	1.0	338.8	1.0
Styrene	199.8	0.75	627.5	0.78	257.3	0.76

$$\text{Benzene: } \alpha_{m1} = \sqrt[3]{5.2 * 4.25 * 4.99} = 4.79$$

$$\text{Toluene: } \alpha_{m2} = \sqrt[3]{2.15 * 1.95 * 2.11} = 2 \ \ \text{LK}$$

$$\text{Ethylbenzene: } \alpha_{m3} = \sqrt[3]{1 * 1 * 1} = 1 \ \ \text{HK}$$

$$\text{Styrene: } \alpha_{m4} = \sqrt[3]{0.75 * 0.78 * 0.76} = 0.76$$

Below are the chosen average relative volatilities for the determination of the required theoretical stages N and the required reflux ratio R:

Light boiling benzene: $\alpha_m = 4.79$
LK component toluene: $\alpha_m = 2.0$
HK component ethyl benzene: $\alpha_m = 1.0$
High boiling styrene: $\alpha_m = 0.76$.

4.1.3 Component Distribution According to Relative Volatilities [1, 6]

After the relative volatilities are determined the preliminary mass balance, with component distribution, is prepared according to the method of Hengstebeck–Geddes [1].

$$\lg \frac{d_i}{b_i} = a + b * \lg \ \alpha_i$$

f_i = feed flow rate of component i (kmol/h).
d_i = distillate flow rate of component i (kmol/h).
b_i = bottoms flow rate of component i (kmol/h).
α_i = relative volatility of component i based on the HK component.

$$a = -\lg\left(\frac{b_{\mathrm{HK}}/f_{\mathrm{HK}}}{1 - b_{\mathrm{HK}}/f_{\mathrm{HK}}}\right)$$

$$b = \frac{\lg\left[\frac{d_{\mathrm{LK}}/f_{\mathrm{LK}}}{1-d_{\mathrm{LK}}/f_{\mathrm{LK}}} * \frac{b_{\mathrm{HK}}/f_{\mathrm{HK}}}{1-b_{\mathrm{HK}}/f_{\mathrm{HK}}}\right]}{\lg \ \alpha_{\mathrm{LK}}}$$

$$\frac{d_i}{f_i} = \frac{10^a * \alpha^b}{1 + 10^a * \alpha^b}$$

$$\frac{b_i}{f_i} = \frac{1}{1 + 10^a * \alpha^b}$$

Example 4.1.3.1: Calculation of Components Distribution

Component		Volatility	Feed
	M	α	(kmol/h)
Light	78	4.79	25
LK	92.1	2	25
HK	106.1	1	25
Heavy	104.1	0.75	25
			100

Required separation: $\boldsymbol{b_{\mathrm{HK}} = 22.85\ \mathrm{kmol/h}} \quad \boldsymbol{d_{\mathrm{LK}} = 22.6\ \mathrm{kmol/h}}$

$$a = -\log\frac{b_{\mathrm{HK}}/f_{\mathrm{HK}}}{1 - b_{\mathrm{HK}}/f_{\mathrm{HK}}} = -\log\frac{22.85/25}{1 - 22.85/25} = -1.0264$$

$$b = \frac{\log\left[\frac{d_{\mathrm{LK}}/f_{\mathrm{LK}}}{1-d_{\mathrm{LK}}/f_{\mathrm{LK}}} * \frac{b_{\mathrm{HK}}/f_{\mathrm{HK}}}{1-b_{\mathrm{HK}}/f_{\mathrm{HK}}}\right]}{\log \alpha_{\mathrm{LK}}} = \frac{\log\left[\frac{22.6/25}{1-22.6/25} * \frac{22.85/25}{1-22.85/25}\right]}{\log 2} = 6.645$$

Calculation of the distillate and bottoms flow rate for the HK component:

$$d_{\mathrm{HK}} = \frac{10^a * \alpha^b}{1 + 10^a * \alpha^b} * f_{\mathrm{HK}} = \frac{10^{-1.0264} * 1^{6.645}}{1 + 10^{-1.0264} * 1^{6.645}} * 25 = 0.086 * 25 = 2.15\ \mathrm{kmol}$$

$$b_{\mathrm{HK}} = \frac{1}{1 + 10^a * \alpha^b} * f_{\mathrm{HK}} = \frac{1}{1 + 10^{-1.0264} * 1^{6.645}} * 25 = 0.914 * 25 = 22.85\ \mathrm{kmol}$$

Result of the Distribution Calculation:

Component	Feed	Distillate	Bottoms
	(molfr.)	(kmol/h)	(kmol/h)
Benzene	0.25	24.99	0.01
Toluene	0.25	22.6	2.4
Ethyl benzine	0.25	2.15	22.85
Styrene	0.25	0.34	24.66

4.2 Short-Cut Method for Ideal Multi-component Mixtures [2–7]

With the short-cut method both the required minimum number of trays N_{min} at total reflux and the required minimum reflux ratio R_{min} at infinite number of trays is determined. Using a simple conversion the required number of theoretical stages for a certain reflux ratio R is determined. The method is very simple and illustrates the difficulty level of a separation. However, the short-cut method is not suitable for non-ideal vapour–liquid equilibria because the relative volatility strongly changes with concentration for non-ideal mixtures.

4.2.1 *Calculation of the Minimum Number of Trays* N_{min} *for a Given Component Distribution According to Fenske [8]*

The minimum number of stages at total reflux for the separation of the LK and HK components is calculated. The compositions for the calculation are taken from the components distribution according to Hengstebeck–Geddes, described in Sect. 4.1.3. Alternatively, the minimum number of trays for an estimated components distribution can be performed and then the mass balance can be determined according to Sect. 4.2.2. The determination of the required relative volatilities is shown in Sect. 4.1.2.

$$N_{\min} = \frac{\lg\left[\left(\frac{x_{\mathrm{LK}}}{x_{\mathrm{HK}}}\right)_{\mathrm{top}} * \left(\frac{x_{\mathrm{HK}}}{x_{LK}}\right)_{\mathrm{bottom}}\right]}{\lg \alpha_{\mathrm{LK}}}$$

α_{LK} = relative volatility of the LK component based on the HK component.
x_{LK} = composition of the LK component at the top and the bottom.
x_{HK} = composition of the HK component at the top and the bottom.

4.2.2 *Calculation of the Components Distribution at the Minimum Number of Trays* N$_{min}$

The flow distribution according to the relative volatilities for the calculated minimum number of trays is determined:

$$A = \alpha_i^{N_{\min}} * \left(\frac{d_{\mathrm{HK}}}{b_{\mathrm{HK}}}\right) \qquad B = A + 1$$

$$d_i = \frac{A}{B} * f_i \qquad b_i = \frac{f_i}{B} \qquad f_i = d_i + b_i$$

b_i = bottoms flow rate of component i (kmol/h).
d_i = distillate flow rate of component i (kmol/h).
f_i = feed flow rate of component i (kmol/h).
α_i = relative volatility of component i based on HK component.
$\left(\frac{d}{b}\right)_{\mathrm{HK}}$ = distribution of the HK component to the distillate and bottoms.

4.2.3 *Determination of the Minimum Reflux Ratio* R$_{min}$ *According to Underwood [9]*

First the operand Θ for the feed composition and the thermal condition of the feed, characterized by the q-value, is determined. Then, with the help of the Θ-value, which is determined iteratively by trial and error, the minimum reflux ratio $R_{\min}$ is calculated.

$$1 - q = \sum \frac{\alpha_i * x_{iF}}{\alpha_i - \Theta}$$
$$R_{\min} + 1 = \sum \frac{\alpha_i * x_{iD}}{\alpha_i - \Theta}$$

4.2.4 Conversion to the Real Number of Trays at a Real Reflux Ratio R [10]

The calculated minimum number of trays is valid for an infinite reflux ratio without distillate draw and the minimum reflux ratio for a column with an infinite number of trays. The derived values must therefore be converted to realistic operating conditions for a definite number of trays and a definite reflux ratio. The following approximation formula can be used for the conversion:

$$\frac{N - N_{\min}}{N + 1} = Y$$
$$Y = 0.75 - 0.75 * X^{0.5668}$$
$$\frac{R - R_{\min}}{R + 1} = X$$
$$X = \left(\frac{0.75 - Y}{0.75}\right)^{1/0.5668}$$

4.2.5 Determination of the Feed Tray According to Kirkbride [11]

The ratio of the rectification trays N_V to the stripping trays N_A is calculated.

$$\frac{N_V}{N_A} = \left[\left(\frac{x_{HKF}}{x_{LKF}}\right) * \left(\frac{x_{LKB}}{x_{HKD}}\right)^2 * \frac{B}{D}\right]^{0.206}$$
$$N_V = \frac{N_V/N_A}{1 + N_V/N_A} * N_{tot}$$
$$N_A = N_{tot} - N_V.$$

4.3 Vapour and Liquid Loading of the Column

The vapour and liquid flow rates in the rectification and stripping sections result from the mass balance, the reflux ratio, and the thermal condition of the feed or the q-value (see Chap. 3). The thermal condition of the feed mixture is characterized by the q-value.

Feed of a liquid at boiling temperature $T_{\text{feed}} = T_{\text{boil}} \Rightarrow q = 1$
Feed of a cold liquid with $T_{\text{feed}} < T_{\text{boil}} \Rightarrow q > 1$
Feed of vapour at dew point $T_{\text{feed}} = T_{\text{dew}} \Rightarrow q = 0$
Feed of overheated vapour with $T_{\text{feed}} > T_{\text{dew}} \Rightarrow q < 0$

The q-value is required for the determination of the vapour and liquid flow rates in the column. For instance, the liquid flow rate in the stripping section is increased with a cold liquid feed.

Rectification section:

$$\text{Vapour flow rate } V_{\text{V}} = (R+1) * D \quad \text{Liquid flow rate } L_{\text{V}} = R * D$$

Slope of the operating line for rectification

$$\frac{L_{\text{V}}}{V_{\text{V}}} = \frac{R}{R+1}$$

Stripping section:

$$\text{Vapour flow rate } V_{\text{A}} = V_{\text{V}} - (1-q) * F = L_{\text{A}} - B$$

$$\text{Liquid flow rate } L_{\text{A}} = L_{\text{V}} + q * F = R * D + q * F = R_{\text{A}} * B$$

Slope of the operating line for stripping

$$\frac{L_{\text{A}}}{V_{\text{A}}} = \frac{R_{\text{A}}}{R_{\text{A}} - 1}$$

F = feed flow rate (kmol/h).
D = distillate flow rate (kmol/h).
B = bottoms flow rate (kmol/h).
V_{V} = vapour flow rate in the rectification section (kmol/h).
L_{V} = liquid flow rate in the rectification section (kmol/h).
V_{A} = vapour flow rate in the stripping section (kmol/h).
L_{A} = liquid flow rate in the stripping section (kmol/h).
$R = L_{\text{V}}/D$ = reflux ratio in the rectification section.
$R_{\text{A}} = L_{\text{A}}/B$ = reflux ratio in the stripping section.

Example 4.3.1: Column Loading at different *q*-Values

(a) Feed of liquid with bubble point temperature: $T_{feed} = T_{boil}$

$$\mathbf{q = 1 \quad R = 3.05 \quad F = 100\,kmol/h \quad D = 31.2\,kmol/h}$$

Rectification:

$V_V = (3.05 + 1) * 31.2 = 126.36$ kmol/h
$L_V = 3.05 * 31.2 = 95.16$ kmol/h
Slope of the rectifying line $L_V/V_V = 95.16/126.36 = 0.753$

Stripping:

$L_A = 95.16 + 1 * 100 = 195.16$ kmol/h
$V_A = 126.36 - (1 - 1) * 100 = 126.36$
Slope of the stripping line $L_A/V_A = 195.16/126.36 = 1.54$

(b) Feed of cold liquid: $T_{feed} < T_{boil}$

$$\mathbf{q = 1.25 \quad R = 3.05 \quad F = 100\,kmol/h \quad D = 31.2\,kmol/h}$$

Rectification:

$V_V = 4.05 * 31.2 = 126.36$ kmol/h
$L_V = 3.05 * 31.2 = 95.16$ kmol/h
Slope of the rectifying line $L_V/V_V = 0.753$

Stripping:

$L_A = 95.16 + 1.25 * 100 = 220.16$ kmol/h
$V_A = 126.36 - (1 - 1.25) * 100 = 151.36$ kmol/h
Slope of the stripping line $L_A/V_A = 1.45$

From the calculated column loading in kmol/h the vapor and liquid flow rates in kg/h must be calculated using the average mole weights and the vapour and liquid densities at column temperature:

$$\text{Vapor flow rate} = \frac{V * M_m}{\rho_V}\ (\mathrm{m^3/h})$$

$$\text{Liquid flow rate} = \frac{L * M_m}{\rho_L}\ (\mathrm{m^3/h})$$

M_m = average mole weight of the mixture.
V = vapour loading (kmol/h).
L = liquid loading (kmol/h).
ϱ_L = liquid density (kg/m^3).
ϱ_V = vapour density (kg/m^3).

The described "short-cut" or approximation methods for the determination of the required theoretical stages, the required reflux ratio, the feed stage, as well as the flow distribution for the different streams according to Fenske, Underwood, Gililand, and Kirkbride are particularly suitable for the design of fractionation plants for ideal homogeneous mixtures, such as:

Hydrocarbons.
Aromatic mixtures.
Fatty alcohols, fatty acids, and fatty acid methyl ester.
Nitrochlorid- and nitroparaffin components.

In the separation of non-ideal, multi-component mixtures with activity coefficients a computer program is needed because the composition changes for every tray and the activity coefficient is strongly concentration dependent. This is an enormous calculation task. Often, however, the problem can be reduced to a binary component separation and hence can be graphically solved according to Mcabe–Thiele. With unknown mixtures additional pilot plant fractionation is recommended. This is particularly true for aceotropic and extractive distillations as well as for hybrid plants with intermediate membrane permeation.

Example 4.3.2: Column Calculation for a Mixture of Benzene, Toluene, Ethyl benzene and Styrene
The following mixture is to be separated such that **90.49% of the LK** component toluene is produced at the top and **91.39% of the HK** component ethyl benzene is produced at the bottom.

Feed flow rate: 100 kmol/h.

1. Component Distribution according to Hengstebeck–Geddes with Relative Volatilities

$$a = -1.0264 \quad b = 6.645$$

Component	Feed	Distillate		Bottoms	
	(molfr.)	(kmol/h)	(x_D)	(kmol/h)	(x_B)
Benzene	0.25	24.99	0.499	0.01	0.000
Toluene LK	0.25	22.6	0.451	2.4	0.048
Ethylb HK	0.25	2.15	0.043	22.85	0.458
Styrene	0.25	0.34	0.007	24.66	0.494
	1	50.08	1	49.92	1

2. Calculation of the minimum number of trays $N_{\min}$ with relative volatility α = 2 for the separation of toluene/ethyl benzene

$$N_{\min} = \frac{\lg\left(\frac{0.451}{0.043} * \frac{0.458}{0.048}\right)}{\lg\ 2} = 6.65$$

3. Calculation of the component distribution at $N_{\min}$

$$N_{\min} = 6.65 \quad (b/f)_{\mathrm{HK}} = 22.85/25 = 0.9139 \quad (d/b)_{\mathrm{HK}} = 2.15/22.85 = 0.094$$

Component	Feed	Distillate		Bottom	
	(kmol/h)	(kmol/h)	(kmol/h)	A	B
Benzene	25	24.99	0.01	3143.1	3144.1
Toluene	25	22.6	2.4	9.44	10.44
Ethyl benzine	25	2.15	22.85	0.094	1.094
Styrene	25	0.34	24.66	0.014	1.014
	100	50.08	49.92		

4. Minimum reflux ratio according to Underwood

Calculation using the estimate Θ = 1.33 for q = 1

$$\sum \frac{\alpha_i * x_{i\mathrm{F}}}{\alpha_i - \Theta} = 1 - q = 1 - 1 = 0$$

	α	x_{F}	$\alpha * x_{\mathrm{F}}$	Θ	$\frac{\alpha_i * x_{i\mathrm{F}}}{\alpha_i - \theta}$
Benzene	4.79	0.25	1.1975	1.33	0.3461
Toluene	2	0.25	0.50	1.33	0.7463
Ethyl benzene	1	0.25	0.25	1.33	−0.7576
Styrene	0.76	0.25	0.19	1.33	−0.3333
					0.0015

Calculation of $R_{\min}$ with Θ = 1.33

$$\sum \frac{\alpha_i * x_{i\mathrm{F}}}{\alpha_i - \Theta} = R_{\min} + 1$$

$$R_{\min} = 1.9 - 1 = 0.9 \quad \boldsymbol{R_{\min} = 0.9}$$

x_{D}	$x_{\mathrm{D}} * \alpha$	$\frac{x_{\mathrm{D}} * \alpha}{\alpha - \theta}$
0.503	2.409	0.696
0.451	0.902	1.346
0.040	0.040	−0.121
0.007	0.005	−0.009
		1.9

5. Required number of trays at R = 1

$$X = \tfrac{1-0.9}{1.9} = 0.05 \quad \Rightarrow Y = 0.613$$

$$N - N_{\mathrm{min}} = 0.613\,N + 0.613$$

$$0.387\,N = 0.613 + 6.65 \quad N = \mathbf{19\ at}\ \boldsymbol{R} = \mathbf{1}$$

With a reflux ratio of R = 1 you require 19 theoretical trays.

6. Determination of the feed stage for N_{tot} = 19

$$\frac{N_{\mathrm{V}}}{N_{\mathrm{A}}} = \left[\frac{0.25}{0.25} * \left(\frac{0.051}{0.039}\right)^2 * \frac{50.3}{49.7}\right]^{0.206} = 1.11 \qquad N_V = \frac{1.11}{2.11} * 19 = 10$$

$$N_{\mathrm{A}} = N_{\mathrm{tot}} - N_{\mathrm{V}} = 19 - 10 = 9$$

Therefore, 10 rectification trays (N_{V}) and 9 stripping trays (N_{A}) are required.

7. Column loading at q = 1

Feed = 100 kmol/h.
Distillate = 50 kMol/h.
Bottoms = 50 kMol/h.
Total vapor flow rate rectification = (R + 1) * D = (1 + 1) * 50 = 100 kmol/h.
Liquid flow rate rectification = R * D = 1 * 50 = 50 kmol/h.
Vapor flow rate stripping = (R + 1) * D – (1 – q) * F = 2 * 50 − (1 − 1) * 100 = 100 kmol/h at q = 1.
Liquid flow rate stripping = R * D + q * F = 1 * 50 + 1 * 100 = 150 kmol/h at q = 1.

8. Design data for the column internals

Rectification:

$$\varrho_{\mathrm{V}} = 2.8\ \mathrm{kg/m^3} \quad M = 89.2$$

$$V_{\mathrm{V}} = 100 * 89.2 = 8.920\ \mathrm{kg/h} = 8.920/2.8 = \mathbf{3.186\ m^3/h}$$

$$\varrho_{\mathrm{L}} = 784\ \mathrm{kg/m^3} \quad \mathrm{M} = 94.3$$

$$L_{\mathrm{V}} = 50 * 94.3 = 4.715\ \mathrm{kg/h} = 4.715/784 = \mathbf{6.01\ m^3/h}$$

Stripping:

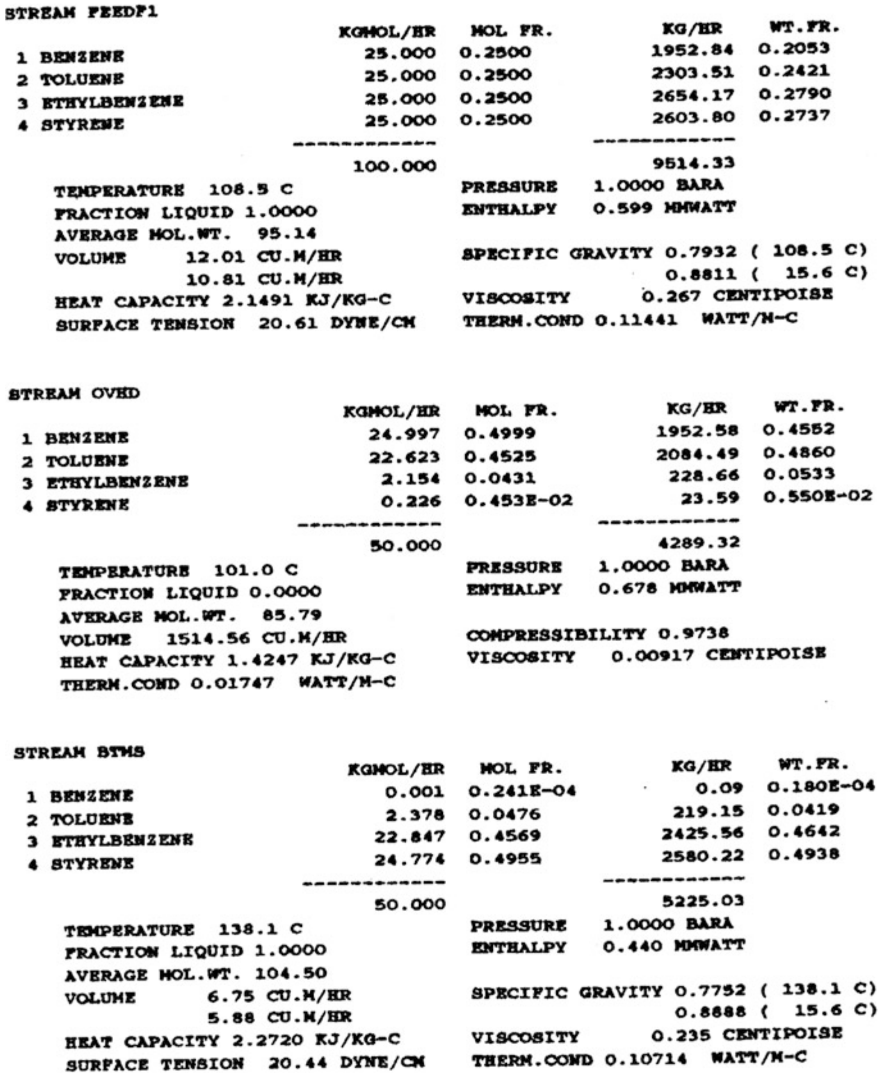
$$\varrho_V = 2.9\ \text{kg/m}^3 \quad M = 96.4$$

$$V_A = 100 * 96.4 = 9.640\ \text{kg/h} = 9.640/2.9 = \mathbf{3.324\ m^3/h}$$

$$\varrho_L = 778\ \text{kg/m}^3 \quad M = 100.8$$

$$L_A = 150 * 100.8 = 15.120\ \text{kg/h} = 15.120/778 = \mathbf{19.43\ m^3/h}$$

The computer calculation below, in Figs. 4.2 and 4.3, gives the same result as the short-cut approximation method for Example 4.3.2.

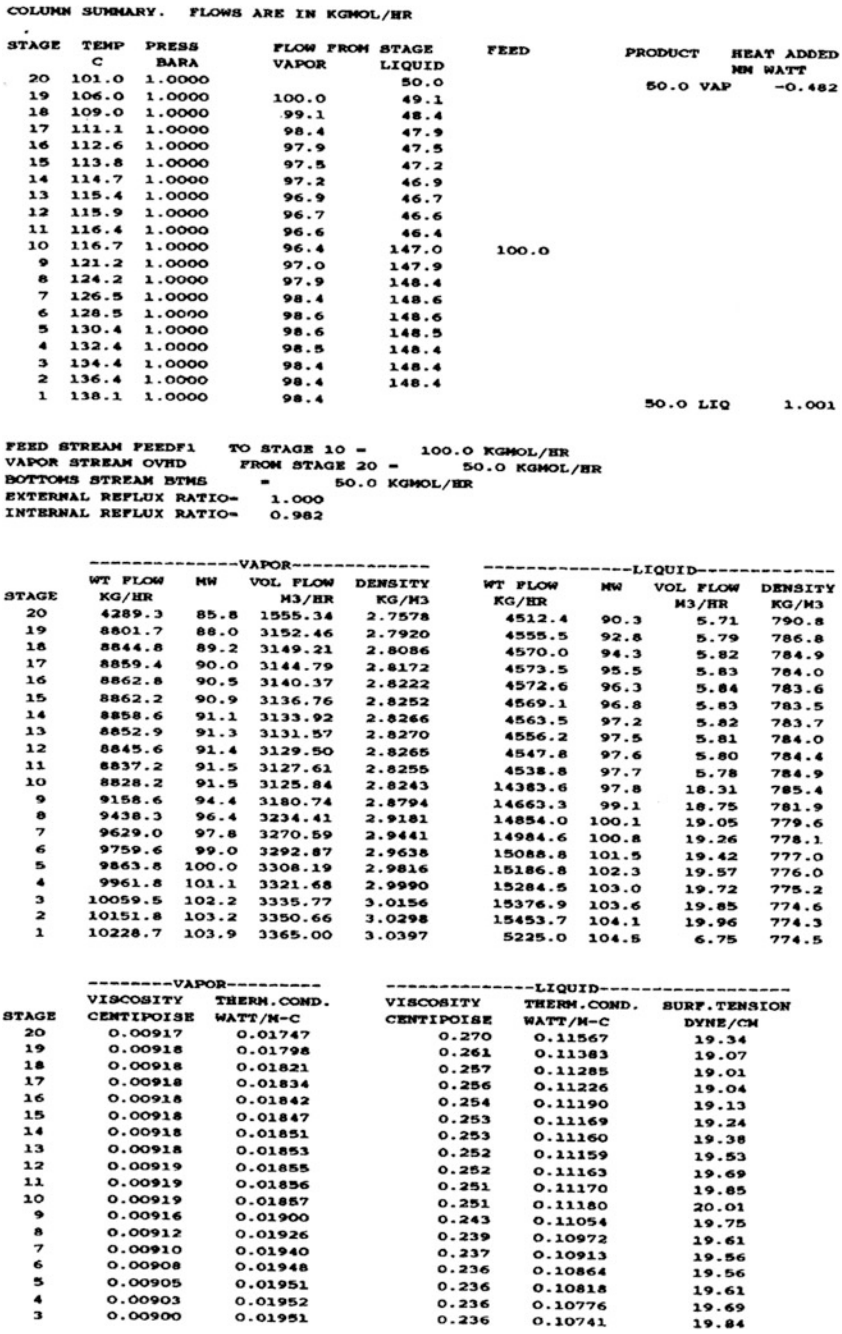


```
STREAM FEEDF1
                                KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 BENZENE                        25.000   0.2500         1952.84   0.2053
 2 TOLUENE                        25.000   0.2500         2303.51   0.2421
 3 ETHYLBENZENE                   25.000   0.2500         2654.17   0.2790
 4 STYRENE                        25.000   0.2500         2603.80   0.2737
                            ------------              -----------
                                 100.000                  9514.33
    TEMPERATURE   108.5 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000             ENTHALPY    0.599 MMWATT
    AVERAGE MOL.WT.   95.14
    VOLUME        12.01 CU.M/HR        SPECIFIC GRAVITY 0.7932 ( 108.5 C)
                  10.81 CU.M/HR                         0.8811 (  15.6 C)
    HEAT CAPACITY 2.1491 KJ/KG-C       VISCOSITY        0.267 CENTIPOISE
    SURFACE TENSION   20.61 DYNE/CM    THERM.COND 0.11441   WATT/M-C

STREAM OVHD
                                KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 BENZENE                        24.997   0.4999         1952.58   0.4552
 2 TOLUENE                        22.623   0.4525         2084.49   0.4860
 3 ETHYLBENZENE                    2.154   0.0431          228.66   0.0533
 4 STYRENE                         0.226   0.453E-02        23.59   0.550E-02
                            ------------              -----------
                                  50.000                  4289.32
    TEMPERATURE   101.0 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 0.0000             ENTHALPY    0.678 MMWATT
    AVERAGE MOL.WT.   85.79
    VOLUME    1514.56 CU.M/HR          COMPRESSIBILITY 0.9738
    HEAT CAPACITY 1.4247 KJ/KG-C       VISCOSITY    0.00917 CENTIPOISE
    THERM.COND 0.01747   WATT/M-C

STREAM BTMS
                                KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 BENZENE                         0.001   0.241E-04         0.09   0.180E-04
 2 TOLUENE                         2.378   0.0476          219.15   0.0419
 3 ETHYLBENZENE                   22.847   0.4569         2425.56   0.4642
 4 STYRENE                        24.774   0.4955         2580.22   0.4938
                            ------------              -----------
                                  50.000                  5225.03
    TEMPERATURE   138.1 C              PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000             ENTHALPY    0.440 MMWATT
    AVERAGE MOL.WT. 104.50
    VOLUME         6.75 CU.M/HR        SPECIFIC GRAVITY 0.7752 ( 138.1 C)
                   5.88 CU.M/HR                         0.8688 (  15.6 C)
    HEAT CAPACITY 2.2720 KJ/KG-C       VISCOSITY        0.235 CENTIPOISE
    SURFACE TENSION   20.44 DYNE/CM    THERM.COND 0.10714   WATT/M-C
```

Fig. 4.2 Computer simulation for Example 4.3.2



```
COLUMN SUMMARY.  FLOWS ARE IN KGMOL/HR
 .
STAGE  TEMP   PRESS        FLOW FROM STAGE     FEED          PRODUCT    HEAT ADDED
         C     BARA        VAPOR     LIQUID                             MM WATT
  20   101.0  1.0000                  50.0                   50.0 VAP    -0.482
  19   106.0  1.0000       100.0      49.1
  18   109.0  1.0000        99.1      48.4
  17   111.1  1.0000        98.4      47.9
  16   112.6  1.0000        97.9      47.5
  15   113.8  1.0000        97.5      47.2
  14   114.7  1.0000        97.2      46.9
  13   115.4  1.0000        96.9      46.7
  12   115.9  1.0000        96.7      46.6
  11   116.4  1.0000        96.6      46.4
  10   116.7  1.0000        96.4     147.0     100.0
   9   121.2  1.0000        97.0     147.9
   8   124.2  1.0000        97.9     148.4
   7   126.5  1.0000        98.4     148.6
   6   128.5  1.0000        98.6     148.6
   5   130.4  1.0000        98.6     148.5
   4   132.4  1.0000        98.5     148.4
   3   134.4  1.0000        98.4     148.4
   2   136.4  1.0000        98.4     148.4
   1   138.1  1.0000        98.4                                 50.0 LIQ     1.001

FEED STREAM FEEDF1     TO STAGE 10 -      100.0 KGMOL/HR
VAPOR STREAM OVHD       FROM STAGE 20 -       50.0 KGMOL/HR
BOTTOMS STREAM BTMS         -       50.0 KGMOL/HR
EXTERNAL REFLUX RATIO-    1.000
INTERNAL REFLUX RATIO-    0.982
```

```
         --------------VAPOR-------------      --------------LIQUID-------------
         WT FLOW    MW    VOL FLOW  DENSITY    WT FLOW     MW    VOL FLOW   DENSITY
STAGE    KG/HR               M3/HR    KG/M3    KG/HR                M3/HR     KG/M3
  20      4289.3   85.8   1555.34   2.7578       4512.4   90.3       5.71     790.8
  19      8801.7   88.0   3152.46   2.7920       4555.5   92.8       5.79     786.8
  18      8844.8   89.2   3149.21   2.8086       4570.0   94.3       5.82     784.9
  17      8859.4   90.0   3144.79   2.8172       4573.5   95.5       5.83     784.0
  16      8862.8   90.5   3140.37   2.8222       4572.6   96.3       5.84     783.6
  15      8862.2   90.9   3136.76   2.8252       4569.1   96.8       5.83     783.5
  14      8858.6   91.1   3133.92   2.8266       4563.5   97.2       5.82     783.7
  13      8852.9   91.3   3131.57   2.8270       4556.2   97.5       5.81     784.0
  12      8845.6   91.4   3129.50   2.8265       4547.8   97.6       5.80     784.4
  11      8837.2   91.5   3127.61   2.8255       4538.8   97.7       5.78     784.9
  10      8828.2   91.5   3125.84   2.8243      14383.6   97.8      18.31     785.4
   9      9158.6   94.4   3180.74   2.8794      14663.3   99.1      18.75     781.9
   8      9438.3   96.4   3234.41   2.9181      14854.0  100.1      19.05     779.6
   7      9629.0   97.8   3270.59   2.9441      14984.6  100.8      19.26     778.1
   6      9759.6   99.0   3292.87   2.9638      15088.8  101.5      19.42     777.0
   5      9863.8  100.0   3308.19   2.9816      15186.8  102.3      19.57     776.0
   4      9961.8  101.1   3321.68   2.9990      15284.5  103.0      19.72     775.2
   3     10059.5  102.2   3335.77   3.0156      15376.9  103.6      19.85     774.6
   2     10151.8  103.2   3350.66   3.0298      15453.7  104.1      19.96     774.3
   1     10228.7  103.9   3365.00   3.0397       5225.0  104.5       6.75     774.5
```

```
         --------VAPOR---------         --------------LIQUID------------------
         VISCOSITY   THERM.COND.        VISCOSITY    THERM.COND.   SURF.TENSION
STAGE    CENTIPOISE  WATT/M-C           CENTIPOISE   WATT/M-C         DYNE/CM
  20       0.00917     0.01747             0.270      0.11567          19.34
  19       0.00918     0.01798             0.261      0.11383          19.07
  18       0.00918     0.01821             0.257      0.11285          19.01
  17       0.00918     0.01834             0.256      0.11226          19.04
  16       0.00918     0.01842             0.254      0.11190          19.13
  15       0.00918     0.01847             0.253      0.11169          19.24
  14       0.00918     0.01851             0.253      0.11160          19.38
  13       0.00918     0.01853             0.252      0.11159          19.53
  12       0.00919     0.01855             0.252      0.11163          19.69
  11       0.00919     0.01856             0.251      0.11170          19.85
  10       0.00919     0.01857             0.251      0.11180          20.01
   9       0.00916     0.01900             0.243      0.11054          19.75
   8       0.00912     0.01926             0.239      0.10972          19.61
   7       0.00910     0.01940             0.237      0.10913          19.56
   6       0.00908     0.01948             0.236      0.10864          19.56
   5       0.00905     0.01951             0.236      0.10818          19.61
   4       0.00903     0.01952             0.236      0.10776          19.69
   3       0.00900     0.01951             0.236      0.10741          19.84
```

Fig. 4.3 Computer simulation for Example 4.3.2

Example 4.3.3 Separation of an aromatic mixture with low relative volatilities α
A five-component aromatic mixture is to be separated by fractionation.

Requirements for the separation:

m-xylene yield in the distillate: 99.5%
o-xylene yield in the bottoms: 97.5%

Feed flow rate and composition:

Component	kg/h	α	M	kmol/h	mol%
Ethyl benzene	215	1.23	106	2.028	21.5
p-xylene	180	1.17	106	1.698	18.0
m-xylene (LK)	400	1.145	106	3.774	40.0
o-xylene (HK)	200	1.0	106	1.887	20.0
Cumene	5	0.815	120	0.042	0.5
	1000			9.429	100

1. Component Distribution according to Hengstebeck–Geddes

Component	Feed	Distillate	Bottoms
	(molfr.)	(molfr.)	(molfr.)
Ethyl benzene	0.215	0.2695	$4.7 * 10^{-5}$
p-xylene	0.18	0.2254	0.0011
m-xylene	0.40	0.4989	0.0099
o-xylene	0.20	0.0063	0.9643
Cumene	0.005	$2.1 * 10^{-10}$	0.0247

2. Mininum number of stages $N_{\min}$

$$N_{\min} = \frac{\lg\left(\frac{0.4989}{0.0063} * \frac{0.9643}{0.0099}\right)}{\lg\ 1.145} = 66.1$$

3. Component distribution at total reflux

$$N_{\min} = 66.1 \quad d/b = 1 - 0.975 = 0.025$$

Component	Feed	Distillate	Bottoms
	(kmol/h)	(kmol/h)	(kmol/h)
Ethyl benzene	2.028	2.028	$9 * 10^{-5}$
p-xylene	1.698	1.696	0.002
m-xylene	3.774	3.755	0.019
o-xylene	1.887	0.046	1.841
Cumene	0.042	$1.4 * 10^{-9}$	0.042
	9.429	7.525	1.904

	Feed	Distillate	Bottoms
Average M	106.23	106.17	106.48
Flow rate (kg/h)	1001.64	798.91	202.73

4. Minimum Reflux Ratio according to Underwood

$$\Theta = 1.030 \quad \Rightarrow R_{\min} = 7.28$$

Figure 4.4 shows how the required number of stages as function of the quotient $R/R_{\min}$ changes.

5. Required number of stages for *R* = 15

$$N = 89.6 \quad \text{Chosen}: N_{\text{tot}} = 90\,\text{stages}$$

At reflux *R* = 15 the requirement is 90 theoretical stages.

6. Determination of the feed stage for N_{tot} = 90

$$D = \frac{0.0995 * 3.774}{0.4989} = \frac{3.755}{0.4989} = 7.524\ \text{kMol/h}$$

$$B = \frac{0.975 * 1.887}{0.9643} = 1.905\ \text{kMol/h}$$

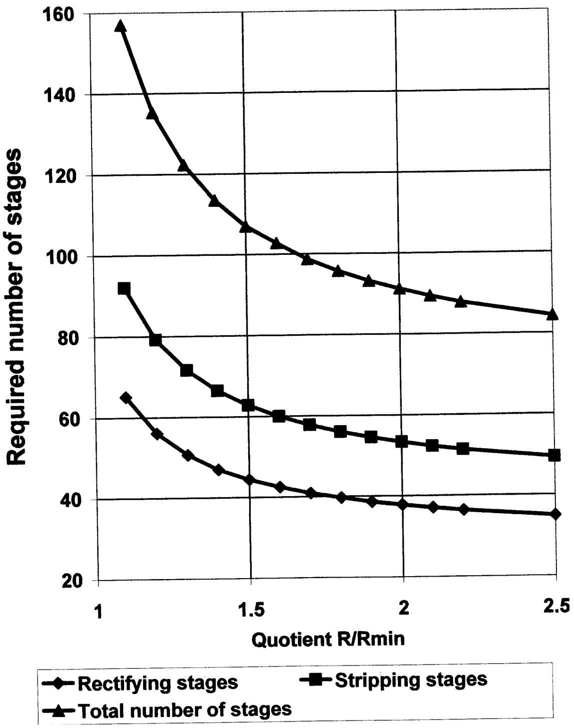
$$\frac{N_V}{N_A} = \left[\frac{0.2}{0.4} * \left(\frac{0.0099}{0.0063}\right)^2 * \frac{1.905}{7.524}\right]^{0.206} = 0.787$$

$$N_V = \frac{0.787}{1.787} * 89.6 = 39.5$$

$$N_V = 40\,\text{stages} \quad \Rightarrow N_A = N_{\text{tot}} - N_V = 90 - 40 = 50\,\text{stages}$$

The feed stage is the 50th from the bottom.

Fig. 4.4 Required theoretical stages as a function of $R/R_{\min}$



7. **Column loading at $q = 1$**

In the **rectification section** above the feed stage:

Vapor flow rate = (15 + 1) * 7.525 = 120.4 kmol/h = 12790 kg/h

Liquid flow rate = 15 * 7.525 = 112.875 kmol/h = 11970 kg/h

In the **stripping section** below the feed stage:

Vapor flow rate = vapor flow rate rectification = 120.4 kmol/h = 12790 kg/h

Liquid flow rate = 112.8 + 9.429 = 122.304 kmol/h = 12976 kg/h

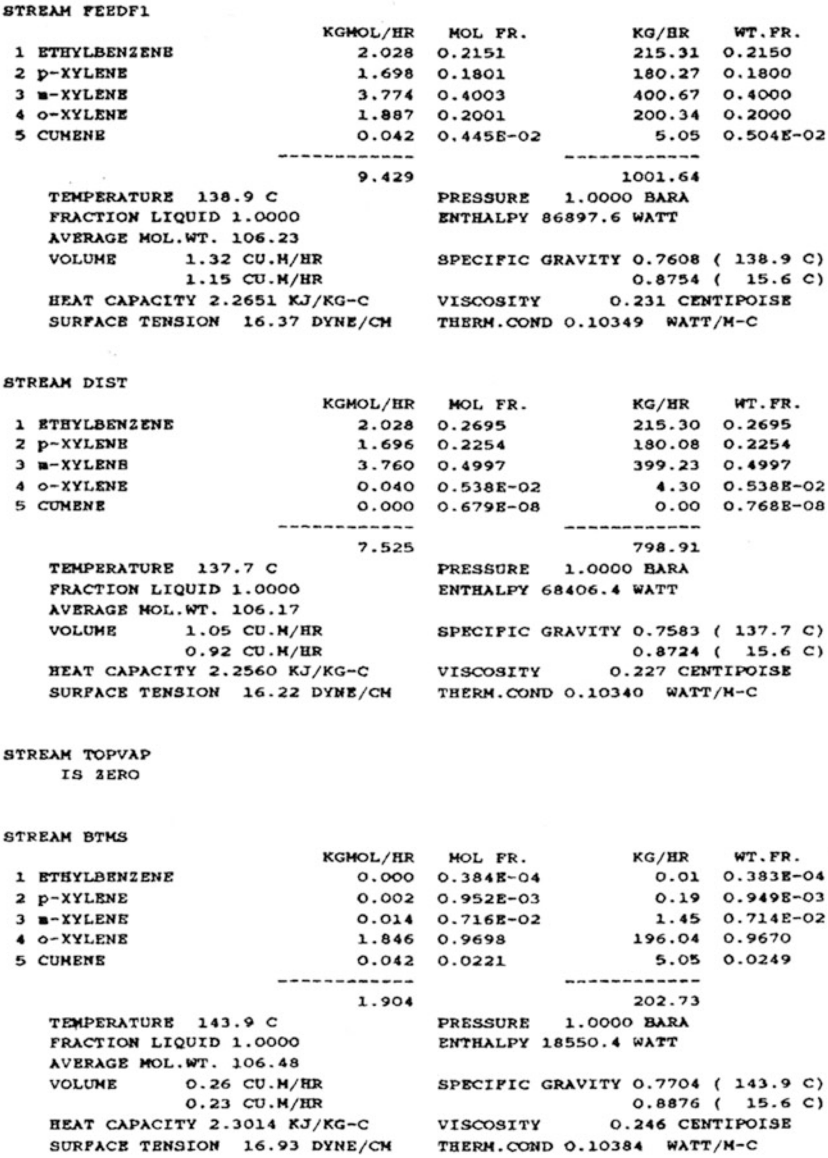
The computer simulation of Example 4.3.3 in Fig. 4.4 gives the same results as the short-cut approximation method.

Result:

Number of stages = 90
Feed stage = 50th from the bottom
Reflux ratio = 15

The mass balances of both of the designs (short-cut and computer) are identical. The mass balance of the computer simulation is given below in Fig. 4.5.

	"Short-cut"	Computer calculation
Feed flow rate (kg/h)	1001.64	1001.64
Distillate flow rate (kg/h)	798.91	798.91
Bottoms flow rate (kg/h)	202.73	202.73



```
STREAM FEEDF1
                                  KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 ETHYLBENZENE                      2.028  0.2151           215.31  0.2150
 2 p-XYLENE                          1.698  0.1801           180.27  0.1800
 3 m-XYLENE                          3.774  0.4003           400.67  0.4000
 4 o-XYLENE                          1.887  0.2001           200.34  0.2000
 5 CUMENE                            0.042  0.445E-02          5.05  0.504E-02
                              ------------             ------------
                                     9.429                  1001.64
    TEMPERATURE  138.9 C                PRESSURE   1.0000 BARA
    FRACTION LIQUID 1.0000              ENTHALPY 86897.6 WATT
    AVERAGE MOL.WT. 106.23
    VOLUME       1.32 CU.M/HR           SPECIFIC GRAVITY 0.7608 ( 138.9 C)
                 1.15 CU.M/HR                            0.8754 (  15.6 C)
    HEAT CAPACITY 2.2651 KJ/KG-C        VISCOSITY      0.231 CENTIPOISE
    SURFACE TENSION  16.37 DYNE/CM      THERM.COND 0.10349  WATT/M-C

STREAM DIST
                                  KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 ETHYLBENZENE                      2.028  0.2695           215.30  0.2695
 2 p-XYLENE                          1.696  0.2254           180.08  0.2254
 3 m-XYLENE                          3.760  0.4997           399.23  0.4997
 4 o-XYLENE                          0.040  0.538E-02          4.30  0.538E-02
 5 CUMENE                            0.000  0.679E-08          0.00  0.768E-08
                              ------------             ------------
                                     7.525                   798.91
    TEMPERATURE  137.7 C                PRESSURE   1.0000 BARA
    FRACTION LIQUID 1.0000              ENTHALPY 68406.4 WATT
    AVERAGE MOL.WT. 106.17
    VOLUME       1.05 CU.M/HR           SPECIFIC GRAVITY 0.7583 ( 137.7 C)
                 0.92 CU.M/HR                            0.8724 (  15.6 C)
    HEAT CAPACITY 2.2560 KJ/KG-C        VISCOSITY      0.227 CENTIPOISE
    SURFACE TENSION  16.22 DYNE/CM      THERM.COND 0.10340  WATT/M-C

STREAM TOPVAP
     IS ZERO

STREAM BTMS
                                  KGMOL/HR   MOL FR.          KG/HR    WT.FR.
 1 ETHYLBENZENE                      0.000  0.384E-04          0.01  0.383E-04
 2 p-XYLENE                          0.002  0.952E-03          0.19  0.949E-03
 3 m-XYLENE                          0.014  0.716E-02          1.45  0.714E-02
 4 o-XYLENE                          1.846  0.9698           196.04  0.9670
 5 CUMENE                            0.042  0.0221             5.05  0.0249
                              ------------             ------------
                                     1.904                   202.73
    TEMPERATURE  143.9 C                PRESSURE   1.0000 BARA
    FRACTION LIQUID 1.0000              ENTHALPY 18550.4 WATT
    AVERAGE MOL.WT. 106.48
    VOLUME       0.26 CU.M/HR           SPECIFIC GRAVITY 0.7704 ( 143.9 C)
                 0.23 CU.M/HR                            0.8876 (  15.6 C)
    HEAT CAPACITY 2.3014 KJ/KG-C        VISCOSITY      0.246 CENTIPOISE
    SURFACE TENSION  16.93 DYNE/CM      THERM.COND 0.10384  WATT/M-C
```

Fig. 4.5 Computer mass balance for Example 4.3.3

Example 4.3.4: Short-cut calculation for a hydrocarbon mixture at 27.6 bar Compositions and relative volatility:

Component	x_F	α	x_D	x_B
Methane	0.05	18.03	0.123	0
Ethane (LK)	0.35	5.125	0.847	0.01
Propylene (HK)	0.15	2.45	0.02	0.239
Propane	0.2	2.2	0.01	0.33
i-butane	0.1	1.243	0	0.168
n-butane	0.15	1	0	0.253

Feed flow rate F = 100 kmol/h
Distillate flow rate: D = 40.6 kmol/h
Bottoms draw B = 59.4 kmol/h

Liquid feed with bubble point temperature (q = 1): $R_{\min} = 1.42$ $N_{\min} = 9.38$
Chosen: $R/R_{\min}$ = 1.2 ➔ R = 1.71

Rectification section:

G_V = 2.71 * 40.6 = 110 kmol/h
L_V = 1.71 * 40.6 = 69.3 kmol/h
N_V = 9.2 theoretical stages

Stripping section:

G_A = 110 kmol/h
L_a = 110 + 59.4 = 169 kmol/h
N_A = 12.8 theoretical stages

Vapour feed with dew point temperature (q = 0): $R_{\min} = 2.87$ $N_{\min} = 9.38$
Chosen: $R/R_{\min}$ = 1.2 ➔ R = 3.45

Rectification section:

G_V = 4.45 * 40.6 = 180 kmol/h
L_V = 3.45 * 40.6 = 140 kmol/h
N_V = 8.7 theoretical stages

Stripping section:

G_A = 180 – 100 = 80 kmol/h
L_a = 140 + 0 = 140 kmol/h
N_A = 12.1 theoretical stages

	Liquid feed (q = 1)			Vapour feed (q = 0)		
R/R_{min}	N_V	N_A	N_{tot}	N_V	N_A	N_{tot}
1.2	9.2	12.5	21.7	8.7	12.1	20.8
1.4	7.8	10.8	18.6	7.3	10.1	17.4
1.6	7	9.7	16.7	6.5	9.1	15.6
1.8	6.4	8.9	15.3	6.1	8.4	14.5
2.0	6.1	8.4	14.5	5.7	8	13.7

4.4 Calculation of the Compositions on Theoretical Stages [12, 13]

The concentration of the individual components of a multi-component mixture on the stages in the column can be determined for a given reflux ratio according to the Lewis–Matheson method with the relative volatilities α of the components for a given vapour and liquid loading.

For the **rectification section** the calculation is made from the condenser down until the feed composition is reached.

Required data:

Required concentration in the top product.
Distillate flow rate of the individual components.
Relative volatilities based on the HK component.
Liquid flow rate in the rectification section.

For the **stripping section** the calculation is made from the reboiler up to the feed composition.

Required data:

Required concentration in the bottoms product.
Bottoms draw flow rates of the individual components.
Relative volatilities.
Vapour flow rate in the stripping section.

The intersection of the concentrations of both key components, from the downwards calculation from the top and upwards calculation from the bottoms, is chosen as the feed stage. The components which are lighter than the LK components vanish very quickly under the feed stage and the components which are heavier than the HK component vanish very quickly above the feed stage. In practice it is only a matter of the separation of the two key components. In the paper of Bakowski [13] the calculation procedure for the determination of the compositions on the stages for different stage efficiencies is shown with examples.

Scheme for the calculation of the compositions in the rectification section from the condenser down:

The liquid concentration which is in equilibrium with the vapour streaming upward is calculated.

$$\text{Liquid concentration } x = \frac{y/\alpha}{\sum y/\alpha}$$

$$\text{Vapor rate } v = x * L_V + d$$

$$\text{Vapor concentration } y = \frac{v}{\sum v}$$

L_V = Liquid rate in the rectification section (kmol/h)

d = Distillate rate of the component (kmol/h)

Example 4.4.1: Concentration calculation for the stages below the condenser Problem definition with basic data:

	x_F	F	D	α	y_D	x_B	B
Benzene	0.25	25	25	4.79	0.5	0	0
Toluene	0.25	25	22.6	2	0.45	0.048	2.4
Ethyl benzene	0.25	25	2.2	1	0.04	0.456	22.8
Styrene	0.25	25	0.2	0.76	0.01	0.496	24.8
			50		1	1	50

$$R = 1 \quad V_V = 50 \text{ kmol/h} \quad q = 1 \quad L_V = 50 \text{ kmol/h} \quad L_A = 150 \text{ kmol/h}$$

Concentration calculation:

	α	d	y_D	y_D/α	x_1	v	y_1
Benzene	4.79	25	0.50	0.104	0.273	38.6	0.386
Toluene	2	22.6	0.45	0.225	0.588	52	0.52
Ethyl benzene	1	2.2	0.04	0.04	0.104	7.4	0.074
Styrene	0.76	0.2	0.01	0.013	0.034	2	0.02
	50	1	0.382	1.0	1.0	100	1.0

	y_1/α	x_2	v	y_2	x_3	x_4
Benzene	0.0806	0.1828	34.2	0.3416	0.1490	0.3245
Toluene	0.26	0.5897	52.1	0.5213	0.5445	0.4982
Ethyl benzene	0.074	0.1678	10.6	0.1064	0.2222	0.1331
Styrene	0.0263	0.0597	3.1	0.0307	0.0843	0.0442
	0.4409	1.0	100	1.0	1.0	1.0

Scheme for the calculation of the concentration profile in the stripping section from the reboiler upward:

The vapour composition, which is in equilibrium with the liquid streaming downward, is determined.

$$\text{Vapor concentration } y = \frac{x * \alpha}{\sum x * \alpha}$$

$$\text{Liquid rate (kmol/h) } l = y * V_A + b$$

$$\text{Liquid concentration } x = \frac{l}{\sum l}$$

V_A = Vapor rate in the stripping section (kmol/h)

b = Bottoms draw rate of the component (kmol/h)

Example 4.4.2: Concentration calculation on the stages above the evaporator V_A = 100 kmol/h.

	α	1	x_0	$x * \alpha$	y_0	1	x_1	x_2
Benzene	4.79	0	0.0	0.0	0.0	0	0	0
Toluene	2	2.4	0.048	0.096	0.1033	12.7	0.0849	0.1315
Ethyl benzene	1	22.8	0.456	0.456	0.4909	71.9	0.4792	0.4779
Styrene	0.76	*24.8*	*0.496*	*0.377*	*0.4058*	*65.4*	*0.4359*	*0.3906*
		50	1	0.929	1	150	1	1

The calculated liquid compositions on the individual stages in Examples 4.4.1 and 4.4.2 are shown in Fig. 4.6 (stage 1 is the bottom of the column, stage 21 is the top of the column). The intersection point of the composition curves with the feed composition of the key components x_F = 0.25 lies approximately on stage 10. This is identical to the short-cut calculation in Example 4.3.2.

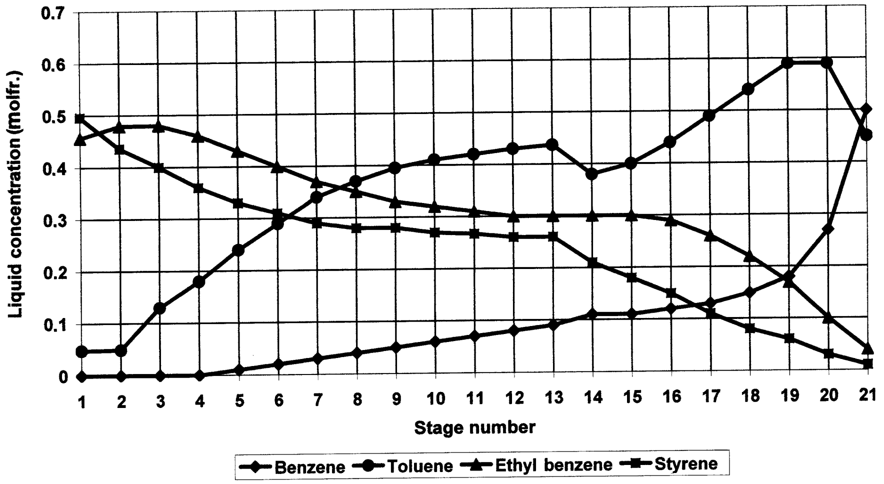
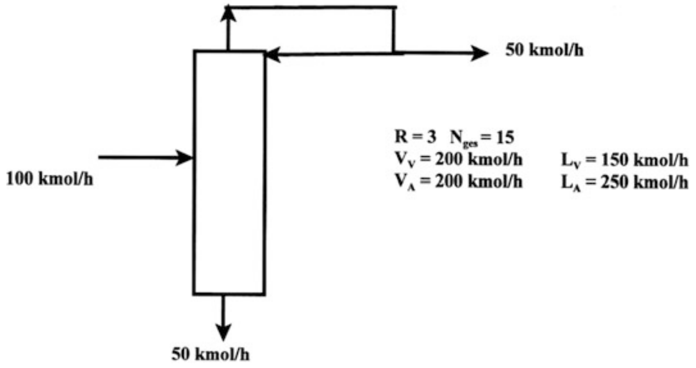


Fig. 4.6 Composition curve for benzene, toluene, ethyl benzene, and styrene in the column

Example 4.4.3: Calculation of the concentrations on the stages



Problem definition:

Component	α	x_F	x_D	Distillate	x_B	Bottoms
		(molfr.)	(molfr.)	(kmol/h)	(molfr.)	(kmol/h)
A	4	0.25	0.5	25	0.0001	0.0001
B	2	0.25	0.49	24.5	0.1	0.5
C	1	0.25	0.01	0.5	0.49	24.5
D	0.5	0.25	0.0001	0.0001	0.5	25

Calculation results:

Stage	15	14	13	12	11	10	9	8
x_A	0.5	0.222	0.162	0.128	0.105	0.086	0.066	0.049
x_B	0.45	0.723	0.738	0.7	0.618	0.492	0.34	0.21
x_C	0.01	0.053	0.094	0.15	0.22	0.28	0.299	0.25
x_D	0.0005	0.0019	0.006	0.02	0.056	0.14	0.294	0.49

Stage	0	1	2	3	4	5	6	7	8
x_A	0.0001	0.0004	0.0016	0.006	0.018	0.05	0.13	0.27	0.43
x_B	0.01	0.023	0.046	0.08	0.135	0.2	0.25	0.26	0.21
x_C	0.49	0.61	0.68	0.693	0.66	0.58	0.46	0.33	0.23
x_D	0.5	0.36	0.27	0.22	0.19	0.17	0.15	0.14	0.13

Stage 15 = column top with distillate.
Stage 0 = column bottoms with bottoms draw.

In Fig. 4.7 the results of the composition calculations for the individual stages are shown. The concentrations of the key components *B* and *C* intersect the feed composition of $x_F = 0.25$ on stage 8.

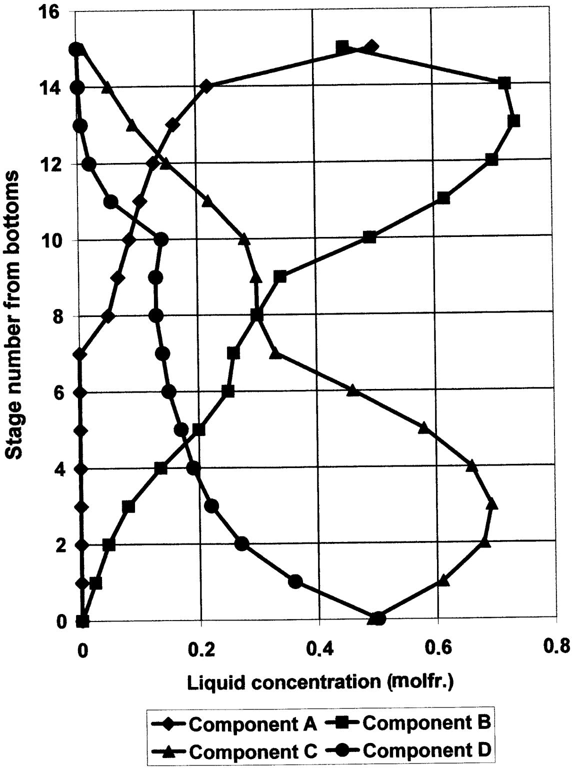


Fig. 4.7 Composition curve for the individual stages of the column

Cross-check calculation using the short-cut method:

$$N_{\min} = 7.9\,\text{theoretical stages} \quad R_{\min} = 1.06$$

The short-cut calculation confirms the composition calculation from stage to stage. At a reflux ratio $R = 3$ you require 8 rectification stages and 8 stripping stages.

$R/R_{\min}$	N_V	N_A	N_{ges}
1.2	13.4	13.4	26.8
1.4	11.4	11.4	22.8
1.6	10.2	10.2	20.4
1.8	9.5	9.5	19
2	8.9	8.9	17.8
2.2	8.5	8.5	17
2.5	8.1	8.1	16.2
3	8	8	16

4.5 Fractionation of Non-ideal, Multi-component Mixtures

For ideal systems with an almost constant relative volatility α the calculation of the composition curve of the different components in the column according to Lewis–Matheson or Thiele–Geddes is relatively simple. The calculations start from the top down and from the bottom up. At the feed stage the concentration curves of both key components intersect the feed composition x_F of both LK and HK components.

For non-ideal systems the calculation must be iteratively performed until the composition on the stage corresponds to the vapour–liquid equilibrium for the liquid composition. A computer program is needed to complete the great number of computations. The operation of these simulation programs is described in Ref. [14].

Required data:

Antoine Constants of all components for the vapour pressure determination: *A*, *B*, and *C*.

Binary interaction parameters pertaining to the equilibrium models for all components contained in the mixture, for instance for the Wilson model.

Interaction parameters:

$\boldsymbol{\lambda_{12} - \lambda_{13} - \lambda_{14}}$
$\boldsymbol{\lambda_{21} - \lambda_{23} - \lambda_{24}}$
$\boldsymbol{\lambda_{31} - \lambda_{32} - \lambda_{34}}$
$\boldsymbol{\lambda_{41} - \lambda_{42} - \lambda_{43}}$
Mole volumina: $\boldsymbol{v_1, v_2, v_3, v_4}$

In the following the application of a computer program for a fractionation task is shown. The task is that 99% methanol is to be separated from a mixture of ethanol, isopropanol, n-butanol, and water.

Example 4.5.1: Distillation for the production of 99% methanol
Feed stage 12:

Component	Flow rate (kg/h)	weight (%)
Methanol	600	60
Ethanol	100	10
Isopropanol	100	10
n-butanol	100	10
Water	100	10
	1000	100

Specifications for the separation task:

Distillate with 99 weight% methanol and 99% methanol yield.

Uniquac interaction parameters are entered for the equilibrium calculations.

The physical properties, for instance vapour pressures, molecular weights, and physical data are supplied with the program.

The specifications for the separation must be input (i.e., top composition of methanol and methanol yield in the distillate or number of stages and reflux and feed stage).

This gives as its result the composition curve for the stages from bottoms (stage 1) to the top of the column (stage 20), as shown in Fig. 4.8.

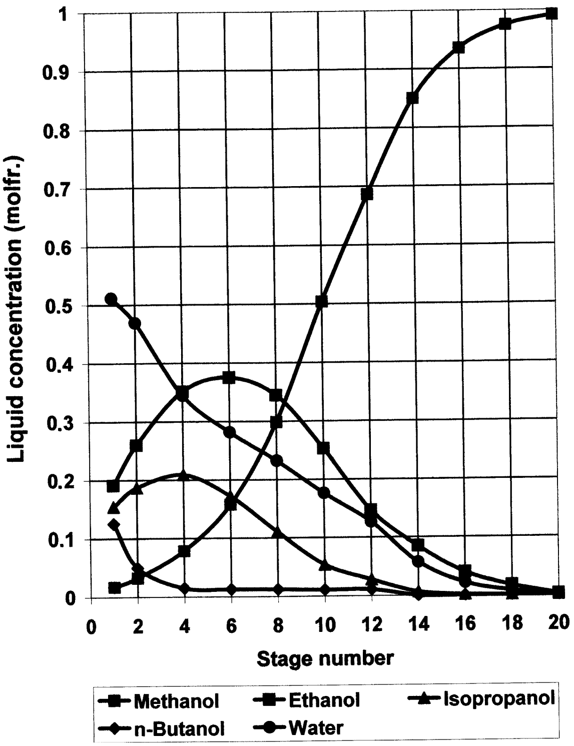
The flow rates and the compositions in the feed, distillate, and bottoms are given in Fig. 4.9.

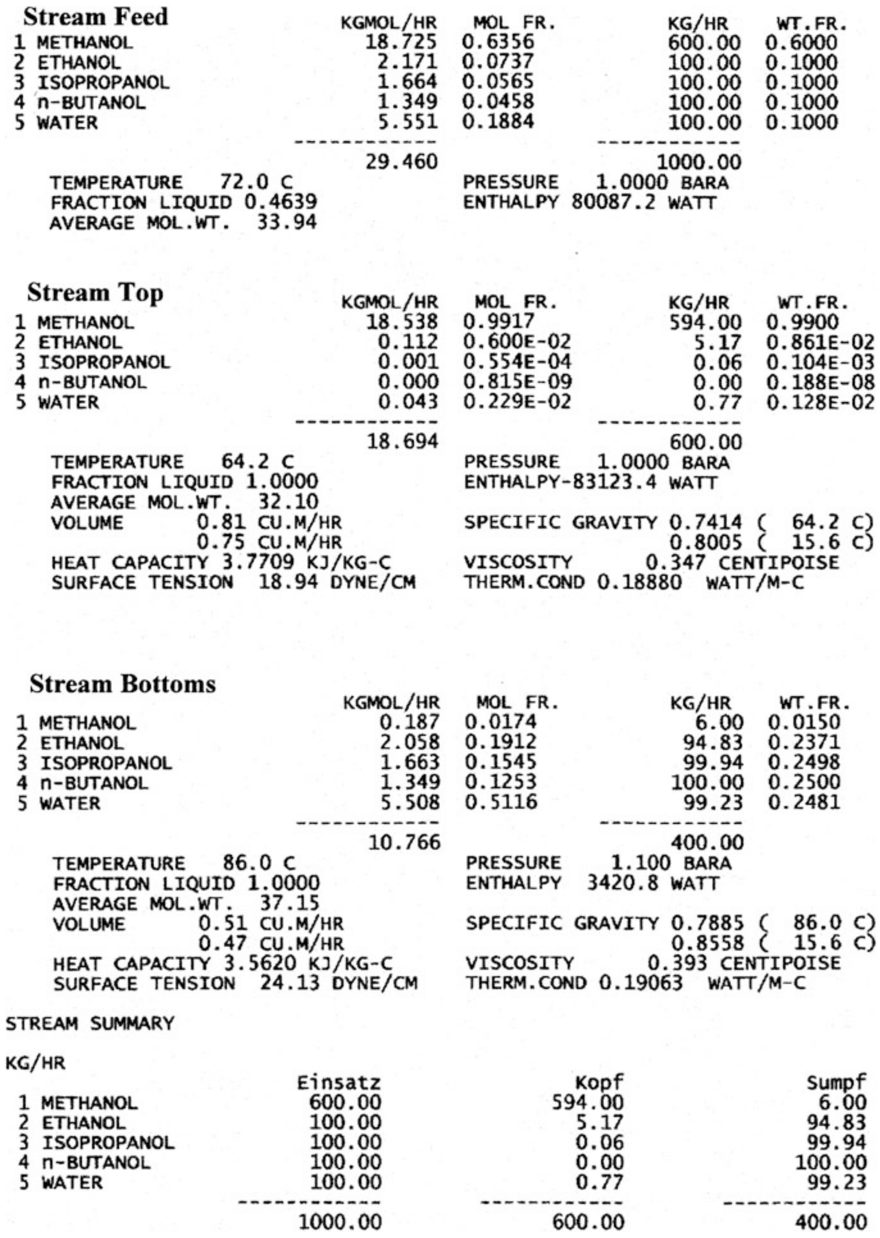
Figure 4.10 shows how the equilibrium constants K change from stage to stage in this non-ideal mixture.

The relative volatilities shown in Fig. 4.11 change less, making an estimation of the number of stages and reflux possible. This is shown in Example 4.5.2.

A great advantage of the simulation program is the output of the vapour and liquid loadings on the different trays in the column. This simplifies the choice of

Fig. 4.8 Liquid compositions of the components on the stages





```
Stream Feed                      KGMOL/HR   MOL  FR.          KG/HR    WT.FR.
1 METHANOL                         18.725   0.6356           600.00   0.6000
2 ETHANOL                           2.171   0.0737           100.00   0.1000
3 ISOPROPANOL                       1.664   0.0565           100.00   0.1000
4 n-BUTANOL                         1.349   0.0458           100.00   0.1000
5 WATER                             5.551   0.1884           100.00   0.1000
                               ------------              ------------
                                   29.460                   1000.00
   TEMPERATURE    72.0 C                PRESSURE    1.0000 BARA
   FRACTION LIQUID 0.4639               ENTHALPY  80087.2 WATT
   AVERAGE MOL.WT.   33.94


Stream Top
                                 KGMOL/HR   MOL  FR.          KG/HR    WT.FR.
1 METHANOL                         18.538   0.9917           594.00   0.9900
2 ETHANOL                           0.112   0.600E-02          5.17   0.861E-02
3 ISOPROPANOL                       0.001   0.554E-04          0.06   0.104E-03
4 n-BUTANOL                         0.000   0.815E-09          0.00   0.188E-08
5 WATER                             0.043   0.229E-02          0.77   0.128E-02
                               ------------              ------------
                                   18.694                    600.00
   TEMPERATURE    64.2 C                PRESSURE    1.0000 BARA
   FRACTION LIQUID 1.0000               ENTHALPY-83123.4 WATT
   AVERAGE MOL.WT.   32.10
   VOLUME          0.81 CU.M/HR         SPECIFIC GRAVITY 0.7414 (   64.2 C)
                   0.75 CU.M/HR                          0.8005 (   15.6 C)
   HEAT CAPACITY 3.7709 KJ/KG-C         VISCOSITY        0.347 CENTIPOISE
   SURFACE TENSION   18.94 DYNE/CM      THERM.COND 0.18880   WATT/M-C


Stream Bottoms
                                 KGMOL/HR   MOL  FR.          KG/HR    WT.FR.
1 METHANOL                          0.187   0.0174             6.00   0.0150
2 ETHANOL                           2.058   0.1912            94.83   0.2371
3 ISOPROPANOL                       1.663   0.1545            99.94   0.2498
4 n-BUTANOL                         1.349   0.1253           100.00   0.2500
5 WATER                             5.508   0.5116            99.23   0.2481
                               ------------              ------------
                                   10.766                    400.00
   TEMPERATURE    86.0 C                PRESSURE     1.100 BARA
   FRACTION LIQUID 1.0000               ENTHALPY   3420.8 WATT
   AVERAGE MOL.WT.   37.15
   VOLUME          0.51 CU.M/HR         SPECIFIC GRAVITY 0.7885 (   86.0 C)
                   0.47 CU.M/HR                          0.8558 (   15.6 C)
   HEAT CAPACITY 3.5620 KJ/KG-C         VISCOSITY        0.393 CENTIPOISE
   SURFACE TENSION   24.13 DYNE/CM      THERM.COND 0.19063   WATT/M-C

STREAM SUMMARY

KG/HR
                           Einsatz                  Kopf                  Sumpf
 1 METHANOL                 600.00                594.00                   6.00
 2 ETHANOL                  100.00                  5.17                  94.83
 3 ISOPROPANOL              100.00                  0.06                  99.94
 4 n-BUTANOL                100.00                  0.00                 100.00
 5 WATER                    100.00                  0.77                  99.23
                      ------------          ------------          ------------
                           1000.00                600.00                 400.00
```

Fig. 4.9 Mass balance with compositions for Example 4.5.1

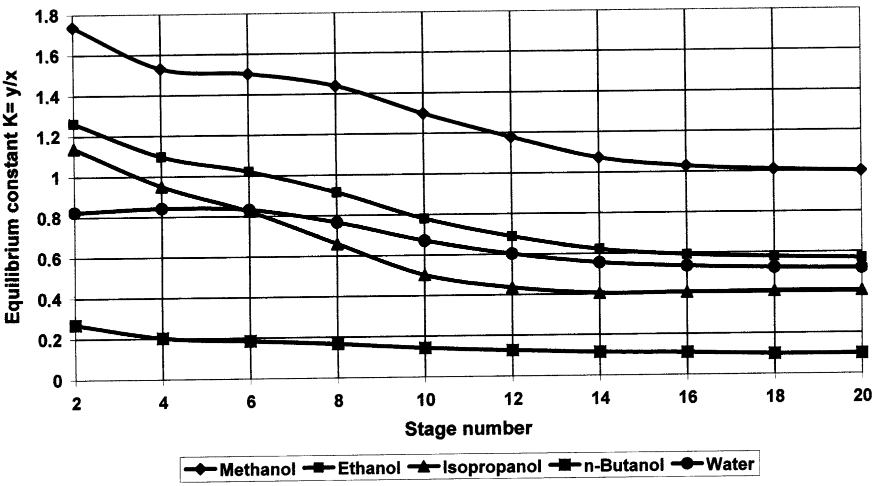


Fig. 4.10 Equilibrium constants of the components on different stages

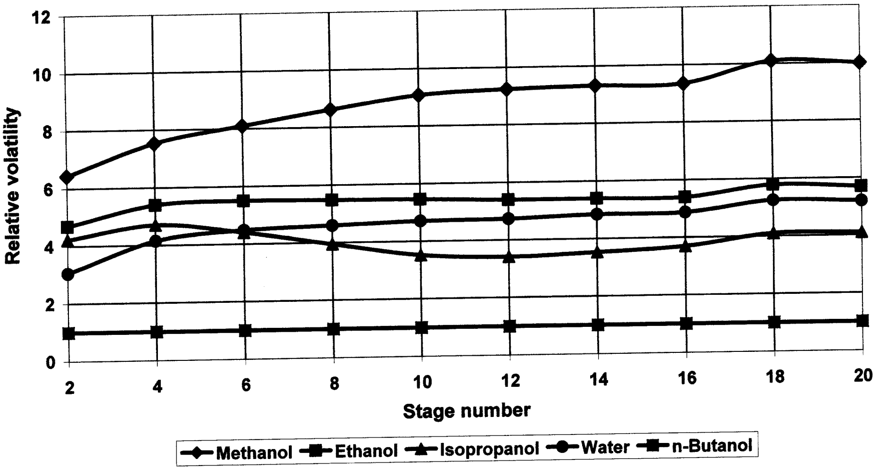


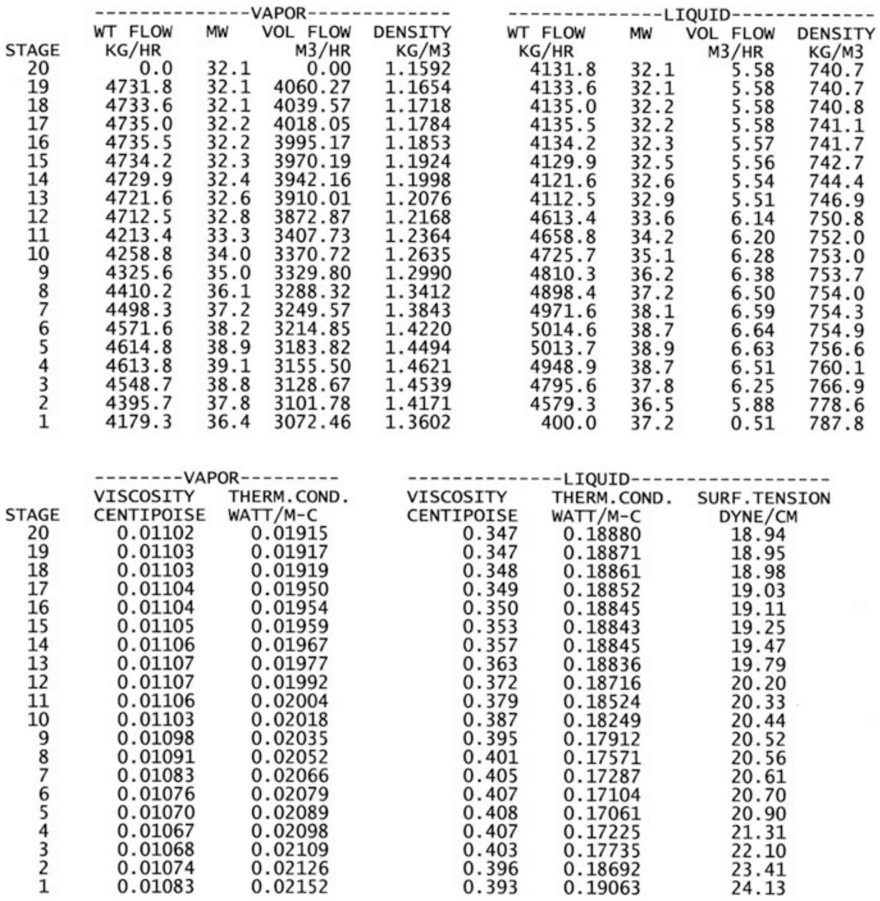
Fig. 4.11 Relative volatility of the components on different trays

suitable column internals and the fluid dynamic design of the trays, packings, or structured packings. In Fig. 4.12 the loadings for the methanol column in Example 4.5.1 are given.

If this exercise is calculated using the short-cut method for all five components one gets a similar result. However, the average relative volatilities of the individual components in the column must be known. If the calculation is performed as a binary mixture it is even simpler.

The separation between the components methanol and ethanol is calculated.

The heavier materials isopropanol, n-butanol, and water are added to ethanol.



```
       --------------VAPOR-------------     -------------LIQUID------------
        WT FLOW    MW   VOL FLOW  DENSITY    WT FLOW    MW   VOL FLOW  DENSITY
STAGE   KG/HR             M3/HR    KG/M3     KG/HR             M3/HR    KG/M3
 20       0.0     32.1     0.00   1.1592     4131.8    32.1     5.58    740.7
 19    4731.8     32.1  4060.27   1.1654     4133.6    32.1     5.58    740.7
 18    4733.6     32.1  4039.57   1.1718     4135.0    32.2     5.58    740.8
 17    4735.0     32.2  4018.05   1.1784     4135.5    32.2     5.58    741.1
 16    4735.5     32.2  3995.17   1.1853     4134.2    32.3     5.57    741.7
 15    4734.2     32.3  3970.19   1.1924     4129.9    32.5     5.56    742.7
 14    4729.9     32.4  3942.16   1.1998     4121.6    32.6     5.54    744.4
 13    4721.6     32.6  3910.01   1.2076     4112.5    32.9     5.51    746.9
 12    4712.5     32.8  3872.87   1.2168     4613.4    33.6     6.14    750.8
 11    4213.4     33.3  3407.73   1.2364     4658.8    34.2     6.20    752.0
 10    4258.8     34.0  3370.72   1.2635     4725.7    35.1     6.28    753.0
  9    4325.6     35.0  3329.80   1.2990     4810.3    36.2     6.38    753.7
  8    4410.2     36.1  3288.32   1.3412     4898.4    37.2     6.50    754.0
  7    4498.3     37.2  3249.57   1.3843     4971.6    38.1     6.59    754.3
  6    4571.6     38.2  3214.85   1.4220     5014.6    38.7     6.64    754.9
  5    4614.8     38.9  3183.82   1.4494     5013.7    38.9     6.63    756.6
  4    4613.8     39.1  3155.50   1.4621     4948.9    38.7     6.51    760.1
  3    4548.7     38.8  3128.67   1.4539     4795.6    37.8     6.25    766.9
  2    4395.7     37.8  3101.78   1.4171     4579.3    36.5     5.88    778.6
  1    4179.3     36.4  3072.46   1.3602      400.0    37.2     0.51    787.8
```

```
       --------VAPOR---------     -------------LIQUID-----------------
       VISCOSITY  THERM.COND.     VISCOSITY  THERM.COND.  SURF.TENSION
STAGE  CENTIPOISE WATT/M-C        CENTIPOISE WATT/M-C        DYNE/CM
 20      0.01102    0.01915          0.347    0.18880         18.94
 19      0.01103    0.01917          0.347    0.18871         18.95
 18      0.01103    0.01919          0.348    0.18861         18.98
 17      0.01104    0.01950          0.349    0.18852         19.03
 16      0.01104    0.01954          0.350    0.18845         19.11
 15      0.01105    0.01959          0.353    0.18843         19.25
 14      0.01106    0.01967          0.357    0.18845         19.47
 13      0.01107    0.01977          0.363    0.18836         19.79
 12      0.01107    0.01992          0.372    0.18716         20.20
 11      0.01106    0.02004          0.379    0.18524         20.33
 10      0.01103    0.02018          0.387    0.18249         20.44
  9      0.01098    0.02035          0.395    0.17912         20.52
  8      0.01091    0.02052          0.401    0.17571         20.56
  7      0.01083    0.02066          0.405    0.17287         20.61
  6      0.01076    0.02079          0.407    0.17104         20.70
  5      0.01070    0.02089          0.408    0.17061         20.90
  4      0.01067    0.02098          0.407    0.17225         21.31
  3      0.01068    0.02109          0.403    0.17735         22.10
  2      0.01074    0.02126          0.396    0.18692         23.41
  1      0.01083    0.02152          0.393    0.19063         24.13
```

Fig. 4.12 Vapour and liquid loadings for the methanol column in Example 4.5.1

Example 4.5.2: Short-cut calculation for Example *4.5.1*.

Component	Methanol	Ethanol
Feed composition (weight%)	60	40
Distillate composition (weight%)	99	1
Bottoms composition (weight%)	2	98

Using the average relative volatility $\alpha = 1.6$ for the separation of methanol/ethanol in the column the following results are obtained:

Minimum reflux ratio $R_{\min} = 2.52$.
Minimum number of trays $N_{\min} = 15.9$.

In order to convert to 20 theoretical stages, as in Example 4.5.1, a reflux ratio $R = 6.9$ is required. In addition, the mass balances are almost the same.

	Feed (kmol/h)	Distillate (kmol/h)	Bottoms (kmol/h)
Computer program	29.46	18.694	10.766
Short-cut method	29.5	18.7	10.8

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Chapter 5
Extractive and Azeotropic Distillation

5.1 Extractive Distillation [1, 2]

In boiling mixtures with an equilibrium curve close to the 45°-line one will need a high number of theoretical stages and a high reflux ratio with a correspondingly high-energy expense for normal distillation. A typical example is the separation of xylene isomers. For such separation tasks the extractive distillation shown in Fig. 5.1 is suitable.

By introducing the washing agent E in the rectification section the volatility of component *A* is increased so that the separation becomes simplified. In the first column the light boiling component *A* flows over the top and component *B* is washed out to the bottom using washing agent E. The mixture $B + \mathrm{E}$ is then separated in the second column. The washing agent E that flows out in the bottoms of the second column is then recycled into the rectification section of the first column. The extractive distillation is also quite suitable for the recovery of low-boiling alcohols and ketene which form an azeotrope with water. The commonly used azeoptropic distillations with light boiling "entrainers" have the disadvantage that the solvents get contaminated by the low-boiling entrainer.

Figure 5.2 shows an extractive distillation for the recovery of ethanol from an aqueous phase using propylene glycol as washing agent. Due to the extractive agent the activity coefficient of water is lowered and so yields water-free ethanol as a *distillate*. The azeotropic distillation shown in Fig. 5.9 yields ethanol however as a bottoms product. The extractive distillation is a secure process with respect to fluctuating water compositions in the feed because the sensible phase separation of the ternary top product is omitted.

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_5

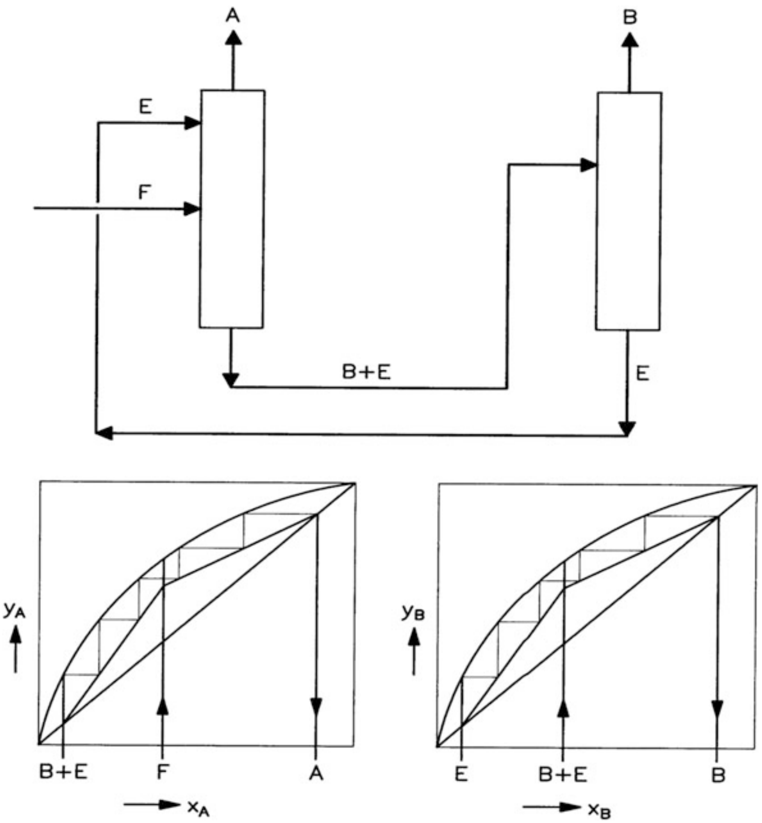


Fig. 5.1 Extractive distillation with the introduction of washing agent E

5.2 Azeotropic Distillation [3–8]

If the equilibrium curve crosses the 45°-line you have **homogeneous** or **heterogeneous** azeotropes.

Figure 5.3 shows the vapour–liquid equilibrium for *n*-butanol–water as an example of azeotropic equilibrium. At the point of intersection between the diagonal and the equilibrium curve sits the azeotropic composition. Above the azeotropic liquid composition the light boiling component *n*-butanol accumulates into the high-boiling component and the water accumulates in the vapour.

In azeotropic composition the boiling point of the mixtures is constant and the mixtures cannot be separated with simple distillation. The condensate of **heterogeneous** azeotropes have a mixture gap so that the distillate separates into two liquid phases with different compositions which can be separated by decantation. The process is shown in Fig. 5.5 with compositions from the Mcabe–Thiele diagram. Using the different liquid phase compositions in the decanter the azeotropic point can be bypassed.

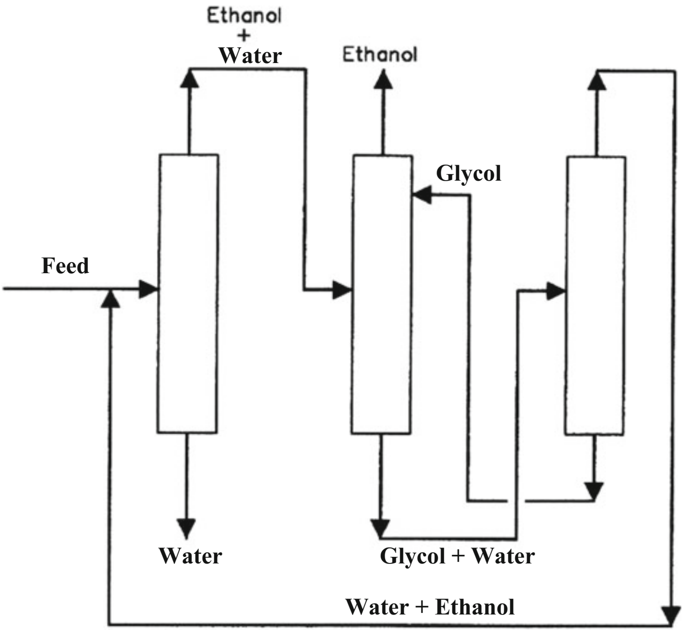


Fig. 5.2 Ethanol recovery by extractive distillation using propylene glycol

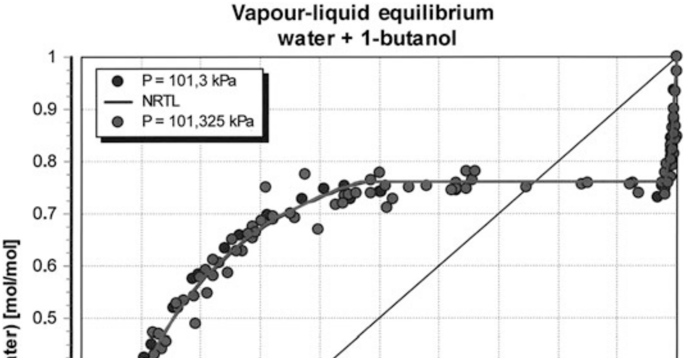


Fig. 5.3 Vapour–liquid equilibrium for *n*-butanol–water from Dortmund Data Bank Software Package (DDBST)

The **homogeneous** azeotropes yield a fully miscible liquid as a condensate. In such cases a separation can be achieved using **“fractionation with pervaporation”** or **“membrane permeation”** as shown in Fig. 5.4.

An alternative is the method of **entrainer distillation** shown in Fig. 5.9.

By introducing the entrainer the condensation of two liquids with different compositions can be achieved, which can then be separated by means of decantation. The homogeneous azeotropic distillation is thereby converted to a heterogeneous azeotropic distillation.

Further alternatives are pressure change or reactive distillation.

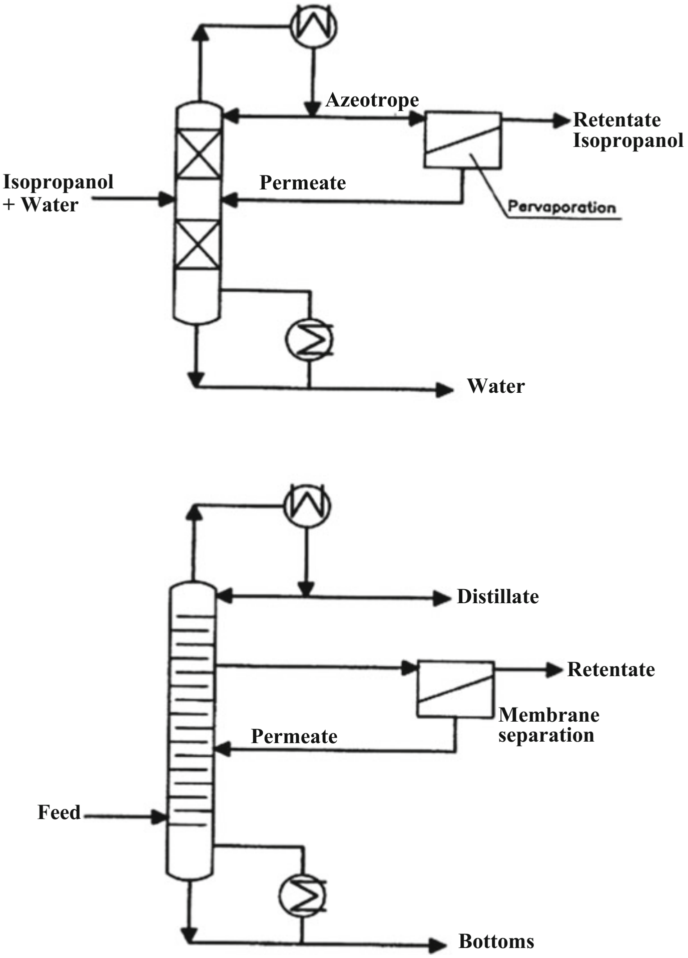


Fig. 5.4 Azeotropic fractionation with membrane permeation

5.2.1 Heteroazeotropic Distillation (Fig. 5.5)

The easiest separation is the separation of hetero-azeotropes, when the azeotropic mixture dissipates into two liquid phases with different compositions. Typical examples are butanol–water and butyl acetate–water separations. The butyl acetate–water azeotrope contains 27% water and in the butyl acetate phase of the condensed azeotrope only 1.3% of the water is miscible at 25 °C.

If the azeotrope water composition and the water solubility in the solvent are almost identical, and a phase separation is not possible, the conditions have to be changed. For instance in an Methyl ethyl ketone (MEK)–water mixture the composition of the azeotropic mixture is distilled off by changing the distillation pressure to such an extent that a phase separation in the decanter becomes possible. Figure 5.5 shows hetero-distillation for the separation of butanol from water.

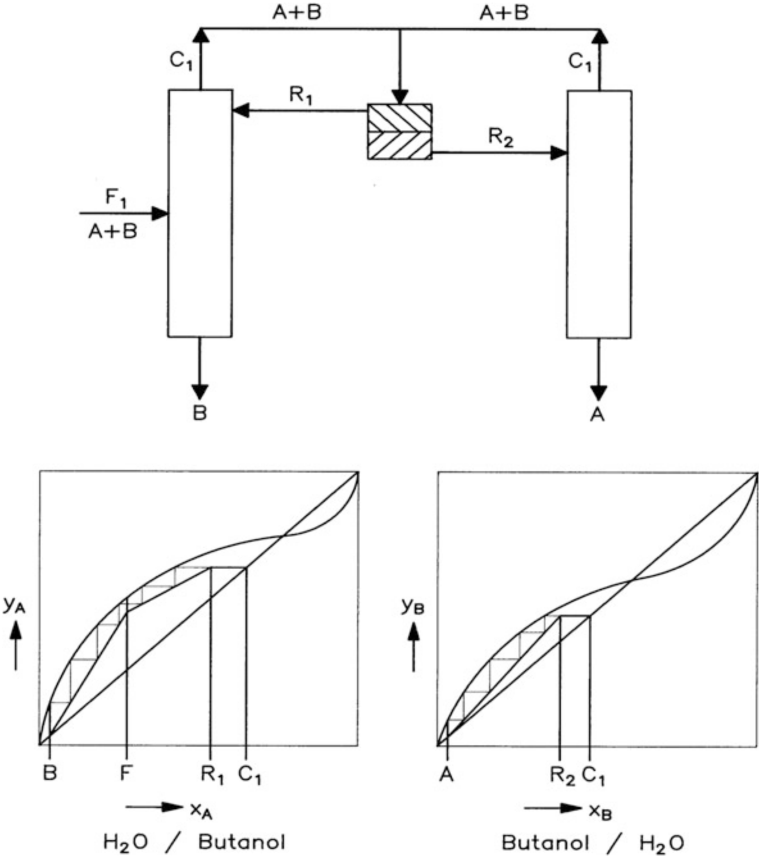


Fig. 5.5 Hetero-azeotropic distillation for the separation of butanol from water

Example 5.2.1.1 Mass balance for the separation of butanol/water

Feed flow rate F = 100 kmol/h x_{ein} = 0.4 = 40 mol% butanol.
Product composition in B = 99 mol% butanol ➔ x = 0.4.
Product composition in A = 0.1 mol% butanol in water ➔ x = 0.001.

$$B = \frac{100 * (0.4 - 0.001)}{0.99 - 0.001} = 40.3 \text{ kmol/h}$$
$$A = \frac{100 * (0.4 - 0.99)}{0.001 - 0.99} = 59.7 \text{ kmol/h}$$

For an inlet composition of 20 mol% butanol in the feed with x = 0.2:

$$B = \frac{100 * (0.2 - 0.001)}{0.001 - 0.99} = 20.1 \text{ kmol/h}$$
$$A = \frac{100 * (0.2 - 0.99)}{0.001 - 0.99} = 79.9 \text{ kmol/h}$$

The requirement is that the distillate composition in the hetero-distillation is dependent on the composition of the given reflux R_1 or R_2 [3] at the column top. The reflux composition R from the decanter is not equal to the top composition C.

Example 5.2.1.2 Separation of an i-butanol–water mixture

Feed: 1000 kg/h
Composition: 10 weight% *i*-Butanol, 90 weight% water
Water from the bottoms of the first column with 9 theoretical stages:
901.6 kg/h with 99.79 weight% water
i-butanol from the bottoms of the second column with 4 theoretical stages:
98.4 kg/h with 99.8 weight% *i*-butanol

The required equilibrium data are shown in Figs. 5.6 and 5.7. The results of a computer design are given in Fig. 5.8.

5.2.2 Entrainer Distillation (Fig. 5.9)

If the azeotropic mixture is homogeneous and does not dissipate into two phases, after condensation, a separation can be achieved by entrainer distillation as shown in Fig. 5.9. Thereby a third component, a so-called "*entrainer*", is added in order to form a **ternary heterogeneous Azeotrope with a miscible gap**. What this separation achieves is analogous to the hetero-azeotrope distillation. The azeotrope mixture dissipates into two liquid phases with different compositions and this is used for the separation. A typical example is the separation of the ethanol–water-mixture by entrainer distillation with toluene or cyclohexane as the entrainer.

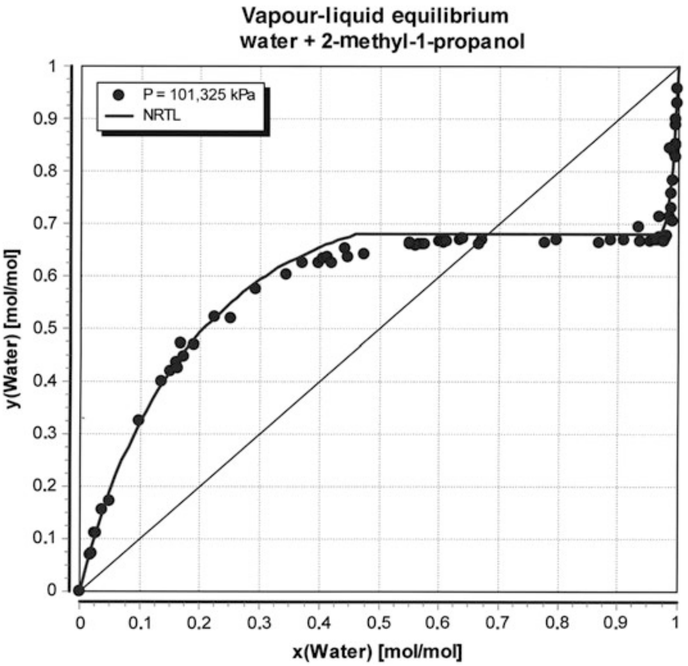


Fig. 5.6 Vapour–liquid equilibrium of *i*-butanol–water from DDBST

Figure 5.9 shows the process. Ethanol is component *A* and water is component *B*. First the ethanol–water azeotrope is separated from water in column K_1. The azeotrope distillate from column K_1 together with entrainer *C* is introduced to column K_2 from where ethanol is drawn from the bottoms.

Due to the entrainer a light boiling ternary azeotrope is formed which can be drawn from the top of K_2 as a distillate. After the condensation dissipates into two liquid phases they are separated in a decanter. The ethanol-rich phase R_1 goes as reflux back into column K_2. The aqueous phase R_2 is used in the stripper K_3 from which pure water is drawn from the bottoms. The ternary azeotrope goes out of the top of column K_3 and is recycled into the decanter.

The correct design of the decanter for the separation of the two liquid phases is very important especially when a phase reversal, by a little heating or cooling, is affected.

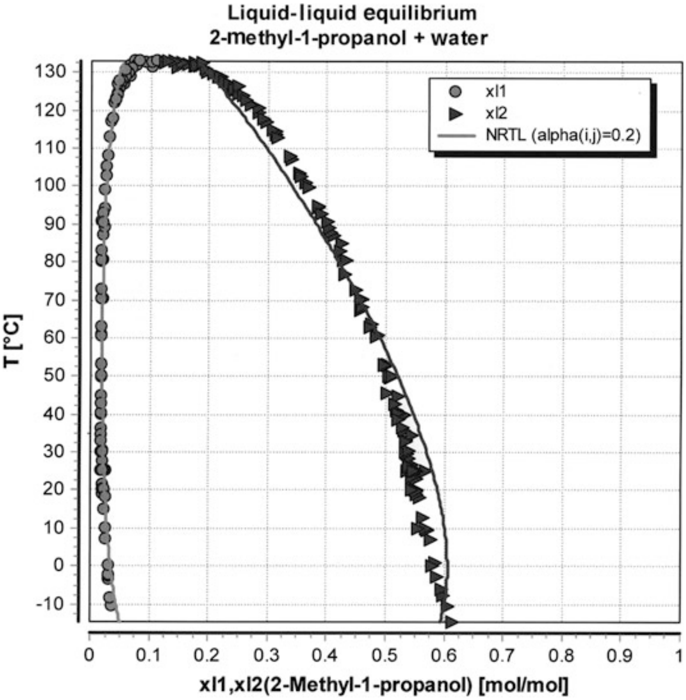
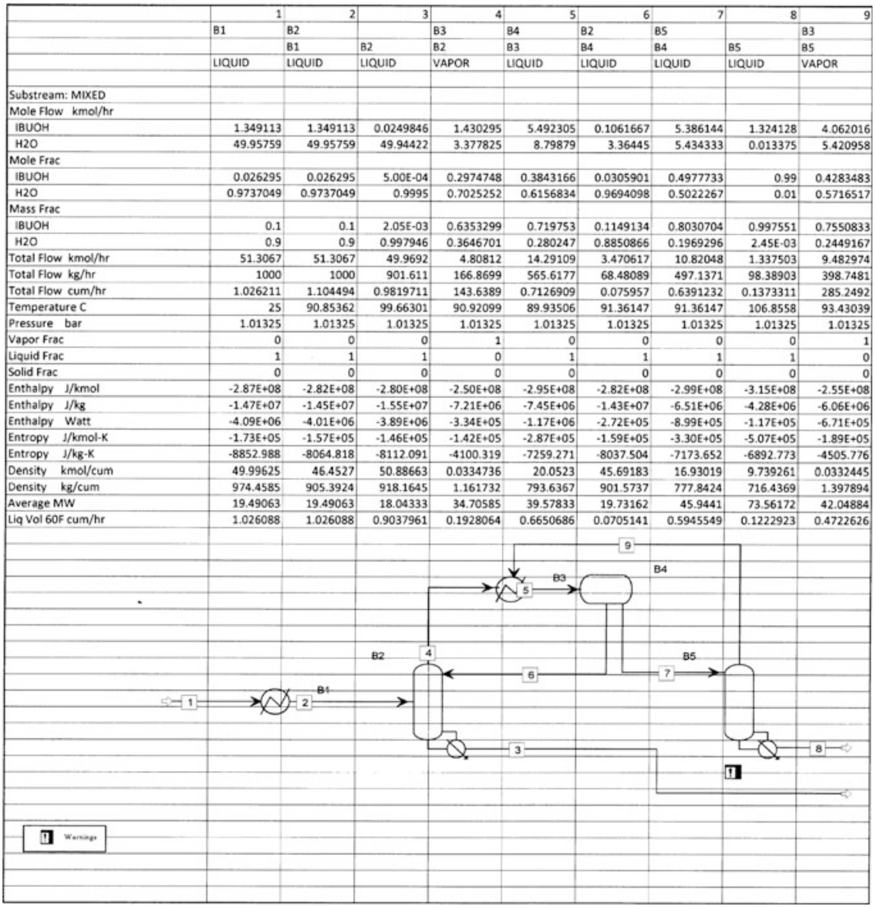


Fig. 5.7 Liquid–liquid equilibrium for *i*-butanol–water from DDBST



	1	2	3	4	5	6	7	8	9
	B1	B2		B3	B4	B2	B5		B3
		B1	B2	B2	B3	B4	B4	B5	B5
	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR
Substream: MIXED									
Mole Flow kmol/hr									
IBUOH	1.349113	1.349113	0.0249846	1.430295	5.492305	0.1061667	5.386144	1.324128	4.062016
H2O	49.95759	49.95759	49.94422	3.377825	8.79879	3.36445	5.434333	0.013375	5.420958
Mole Frac									
IBUOH	0.026295	0.026295	5.00E-04	0.2974748	0.3843166	0.0305901	0.4977733	0.99	0.4283483
H2O	0.9737049	0.9737049	0.9995	0.7025252	0.6156834	0.9694098	0.5022267	0.01	0.5716517
Mass Frac									
IBUOH	0.1	0.1	2.05E-03	0.6353299	0.719753	0.1149134	0.8030704	0.997551	0.7550833
H2O	0.9	0.9	0.997946	0.3646701	0.280247	0.8850866	0.1969296	2.45E-03	0.2449167
Total Flow kmol/hr	51.3067	51.3067	49.9692	4.80812	14.29109	3.470617	10.82048	1.337503	9.482974
Total Flow kg/hr	1000	1000	901.611	166.8699	565.6177	68.48089	497.1371	98.38903	398.7481
Total Flow cum/hr	1.026211	1.104494	0.9819711	143.6389	0.7126909	0.075957	0.6391232	0.1373311	285.2492
Temperature C	25	90.85362	99.66301	90.92099	89.93506	91.36147	91.36147	106.8558	93.43039
Pressure bar	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325	1.01325
Vapor Frac	0	0	0	1	0	0	0	0	1
Liquid Frac	1	1	1	0	1	1	1	1	0
Solid Frac	0	0	0	0	0	0	0	0	0
Enthalpy J/kmol	-2.87E+08	-2.82E+08	-2.80E+08	-2.50E+08	-2.95E+08	-2.82E+08	-2.99E+08	-3.15E+08	-2.55E+08
Enthalpy J/kg	-1.47E+07	-1.45E+07	-1.55E+07	-7.21E+06	-7.45E+06	-1.43E+07	-6.51E+06	-4.28E+06	-6.06E+06
Enthalpy Watt	-4.09E+06	-4.01E+06	-3.89E+06	-3.34E+05	-1.17E+06	-2.72E+05	-8.99E+05	-1.17E+05	-6.71E+05
Entropy J/kmol-K	-1.73E+05	-1.57E+05	-1.46E+05	-1.42E+05	-2.87E+05	-1.59E+05	-3.30E+05	-5.07E+05	-1.89E+05
Entropy J/kg-K	-8852.988	-8064.818	-8112.091	-4100.319	-7259.271	-8037.504	-7173.652	-6892.773	-4505.776
Density kmol/cum	49.99625	46.4527	50.88663	0.0334736	20.0523	45.69183	16.93019	9.739261	0.0332445
Density kg/cum	974.4585	905.3924	918.1645	1.161732	793.6367	901.5737	777.8424	716.4369	1.397894
Average MW	19.49063	19.49063	18.04333	34.70585	39.57833	19.73162	45.9441	73.56172	42.04884
Liq Vol 60F cum/hr	1.026088	1.026088	0.9037961	0.1928064	0.6650686	0.0705141	0.5945549	0.1222923	0.4722626

Fig. 5.8 Result of the simulation for the *i*-butanol–water separation

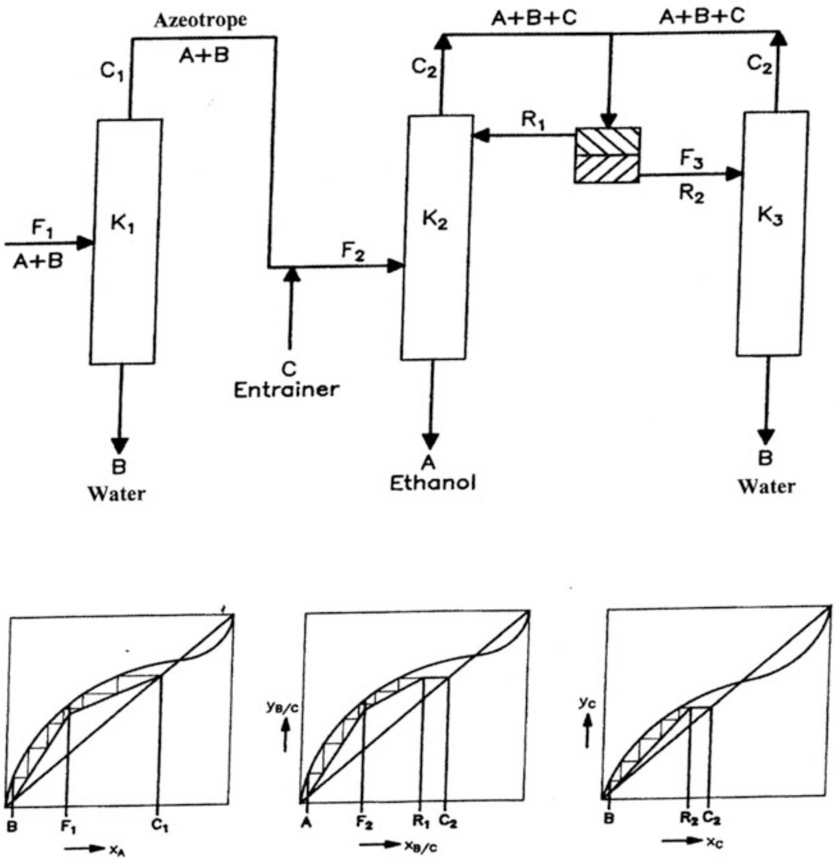
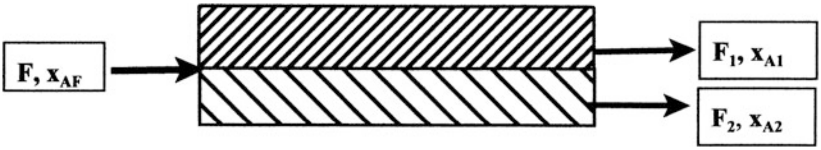


Fig. 5.9 Entrainer Distillation for homogeneous Azeotropes with Entrainer for the forming of ternary Azeotropes

5.2.3 Decanter Mass Balance

The dimensioning of decanters is covered in Chap. 7 (Fig. 5.10).

Decanter mass balance for a binary mixture:



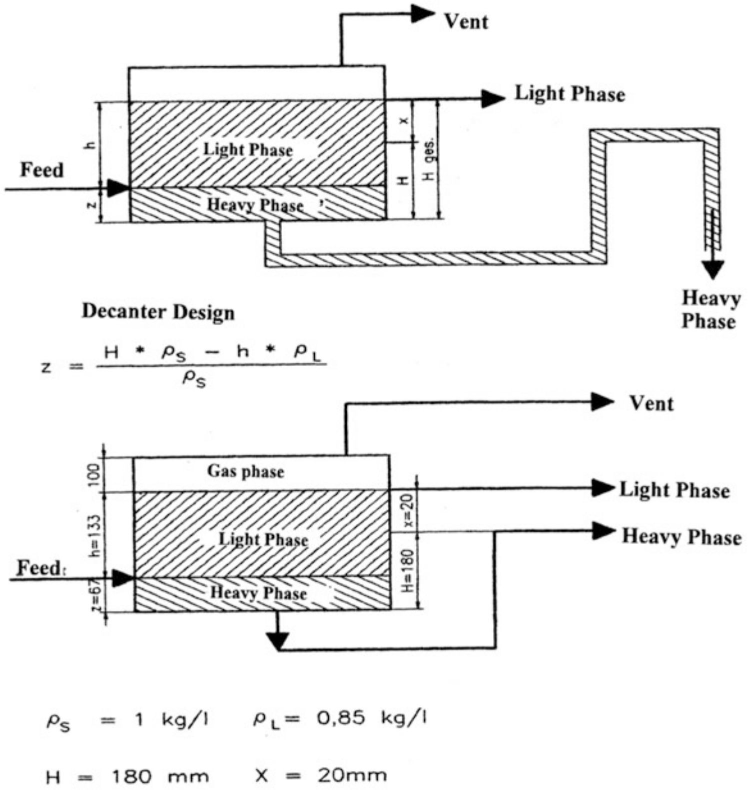


Fig. 5.10 Determination of the phase height in decanters

$$
\begin{aligned}
F &= F_1 + F_2 \ (\text{kg/h}) \\
F * x_{\text{AF}} &= x_{\text{A1}} * F_1 + x_{\text{A2}} * F_2 = x_{\text{A1}} * F_1 + x_{\text{A2}} * (F - F_1) \ (\text{kg/h}) \\
F_1 &= \frac{x_{\text{AF}} - x_{A2}}{x_{\text{A1}} - x_{\text{A2}}} * F \ (\text{kg/h}) \\
F_2 &= \frac{x_{\text{AF}} - x_{\text{A1}}}{x_{\text{A2}} - x_{\text{A1}}} * F \ (\text{kg/h})
\end{aligned}
$$

F = inlet flow rate (kg/h)
F_1 = light phase (kg/h)
F_2 = heavy phase (kg/h)
x_{AF} = input concentration of component A (weight fraction)
x_{A1} = concentration of component A in F_1 (weight fraction)
x_{A2} = concentration of component A in F_2 (weight fraction)

Example 5.3.1: Decanter mass balance

$$F = 695\,\text{kg/h} \quad \text{x}_{\text{AF}} = 0.58 = 58\,\text{weight}\% \quad \text{x}_{\text{A1}} = 0.78 \quad \text{x}_{\text{A2}} = 0.09$$

$$0.58 * 695 = 0.78 * F_1 + 0,09 * (695 - F_1)$$

$$403 = (0.78 - 0.09) * F_1 + 62.5$$

$$F_1 = \frac{340.5}{0.69} = 493.5\ \text{kg/h} \qquad F_2 = 695 - 493.5 = 201.5\ \text{kg/h}$$

$$F_1 = \frac{0.58 - 0.09}{0.78 - 0.09} * 695 = 493.5\ \text{kg/h}$$

$$F_2 = \frac{0.58 - 0.78}{0.09 - 0.78} * 695 = 201.5\ \text{kg/h}$$

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Chapter 6
Discontinuous Batch Distillation

In Fig. 6.1 the flowsheets of a batch distillation and a batch stripper are shown.

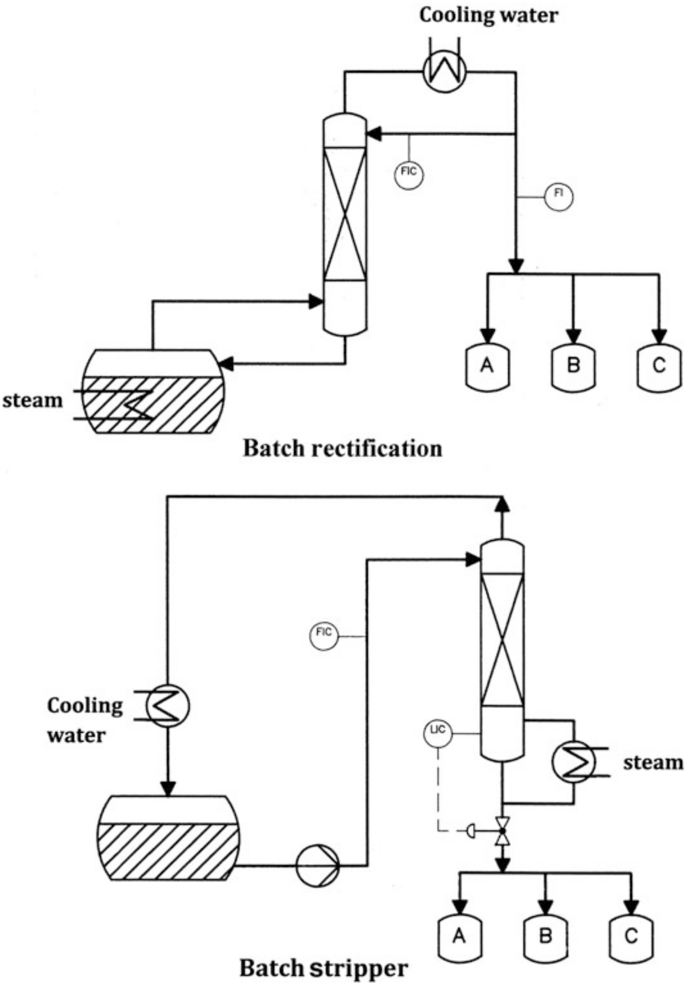


Fig. 6.1 Batch rectification and batch stripper

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_6

6.1 Differential Evaporation (Fig. 6.2)

The simplest form of discontinuous distillation is differential evaporation without a column and reflux, whereby the plant consists of (see Fig. 6.2) a vessel with a heating coil, a condenser, and several product drums. Large separations cannot be achieved with differential evaporation. The following equations are valid for an ideal equilibrium with constant volatility for mass separation:

$$\ln\frac{A_0}{A} = \alpha_{AB} * \ln\frac{B_0}{B} \tag{6.1a}$$

$$\ln\frac{A_0}{A} = \alpha_{AC} * \ln\frac{C_0}{C} \tag{6.1b}$$

$$\ln\frac{B_0}{B} = \alpha_{BC} * \ln\frac{C_0}{C} \tag{6.1c}$$

A_0 = liquid quantity of component A at the beginning.
A = rest quantity of component A in the batch.
B = rest quantitys of component B in the batch.
C = rest quantity of component C in the batch.
α_{AB} = volatility for components A/B.
α_{AC} = volatility for components A/C.
α_{BC} = volatility for components B/C.

Using the Eqs. (6.1a–c) the compositions of distillate and residue for four-component mixtures can be determined at any time so that it is possible to develop appropriate distillation curves.

Example 6.1.1: Mass balance of differential evaporation for three components

Batch filling: 300 kmol benzene (component A_0)
400 kmol toluene (component B_0)
300 kmol xylene (component C_0)

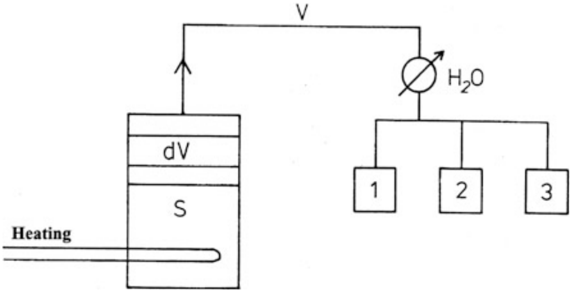


Fig. 6.2 Flow diagram for differential evaporation

Specification: 50% of the Benzene shall be distilled off! → $A = 150$ kmol

The distillate rate and the remaining rest rate of toluene in the batch is to be calculated.

Separation of benzene (A)/toluene (B) with volatility $\alpha_{AB} = 2.18$:

$$\ln\frac{A_0}{A} = \ln\frac{300}{150} = 2.18 * \ln\frac{400}{B}$$
$$0.318 = \ln\frac{400}{B} \quad 1.3743 = \frac{400}{B}$$
$$B = \frac{400}{1.3743} = 291\ \text{kmol}$$

It can be see that of the 400 kmol toluene there is a remaining rest of 291 kmol in the batch after distilling off 150 kmol of benzene.

Separation of benzene (A)/xylene (C) with volatility $\alpha_{AC} = 5.67$:

$$\ln\frac{A_0}{A} = \ln\frac{300}{150} = 5.67 * \ln\frac{300}{C}$$
$$C = \frac{300}{1.13} = 265.3\ \text{kmol}$$

It can be seen that of the 300 kmol xylene there is a remaining rest of 265.3 kmol in the batch after distilling off of 50% of the benzene.

Cross-check calculation with $\alpha_{BC} = 2.59$:

$$\ln\frac{B_0}{B} = \alpha_{BC} * \ln\frac{C_0}{C}$$
$$\ln\frac{400}{291} = 2.59 * \ln\frac{300}{265.3}$$
$$2.59 * 0.1229 = 0.318$$

Result of the calculations:

	Feed	Distillate	Residue
Benzene	300 kmol	150 kmol	150 kmol
Toluene	400 kmol	109 kmol	291 kmol
Xylene	300 kmol	34.7 kmol	265.3 kmol
Sum	1000 kmole	293.7 kmol	706.3 kmol

6.2 Batch Rectification [1–3]

A batch fractionation plant is shown in Fig. 6.3. It consists of a distillation batch with heating by a heating bundle or a falling film evaporator, a fractionation column for enriching the light boiling components, a top condenser for liquifying the rising vapour, and coolers for distillate and bottoms products. The condensate from the top condenser is partly recycled back to the column as reflux and partly drawn off as distillate.

The given batch rectification in Fig. 6.3 is advantageous for high, light boiling concentrations in the feed and for high-purity specification for light boiling components. The light boiling components are enriched in the rectification column and are taken off as distillate over the top. As a consequence of distilling off of the light components their concentration in the distilling batch decreases and therefore a constantly higher separation effort is necessary with increasing reduction of the light boiling components in order to maintain the required distillate composition. In order to keep the distillate composition constant the reflux ratio must therefore be increased if the light boiling components concentration in the batch decreases. The special advantage of batch distillations is their great **flexibility**. It is suitable for:

Different flow rates and compositions.
Physical or chemical pre-treatments.
Distillation at different pressures.
Dirty feed products (because only evaporated materials rise in the column).

The design of batch distillations with unsteady state conditions is extensively covered in the literature [4–8].

In discontinuous batch distillation there are two different modes of operation:

1. **Rectification with constant reflux and varying distillate compositions (see Fig.** 6.4):

   Distillate D1 with the distillate composition $x_{D1} = 0.9$ and bottoms composition $x_{S1} = 0.5$
   Distillate D2 with the distillate composition $x_{D2} = 0.7$ and bottoms composition $x_{S2} = 0.3$
   Distillate D3 with the distillate composition $x_{D3} = 0.5$ and bottoms composition $x_{S3} = 0.17$

The different fractions are stored in different storage tanks. The required final product is produced as a blend of individual distilled off fractions.

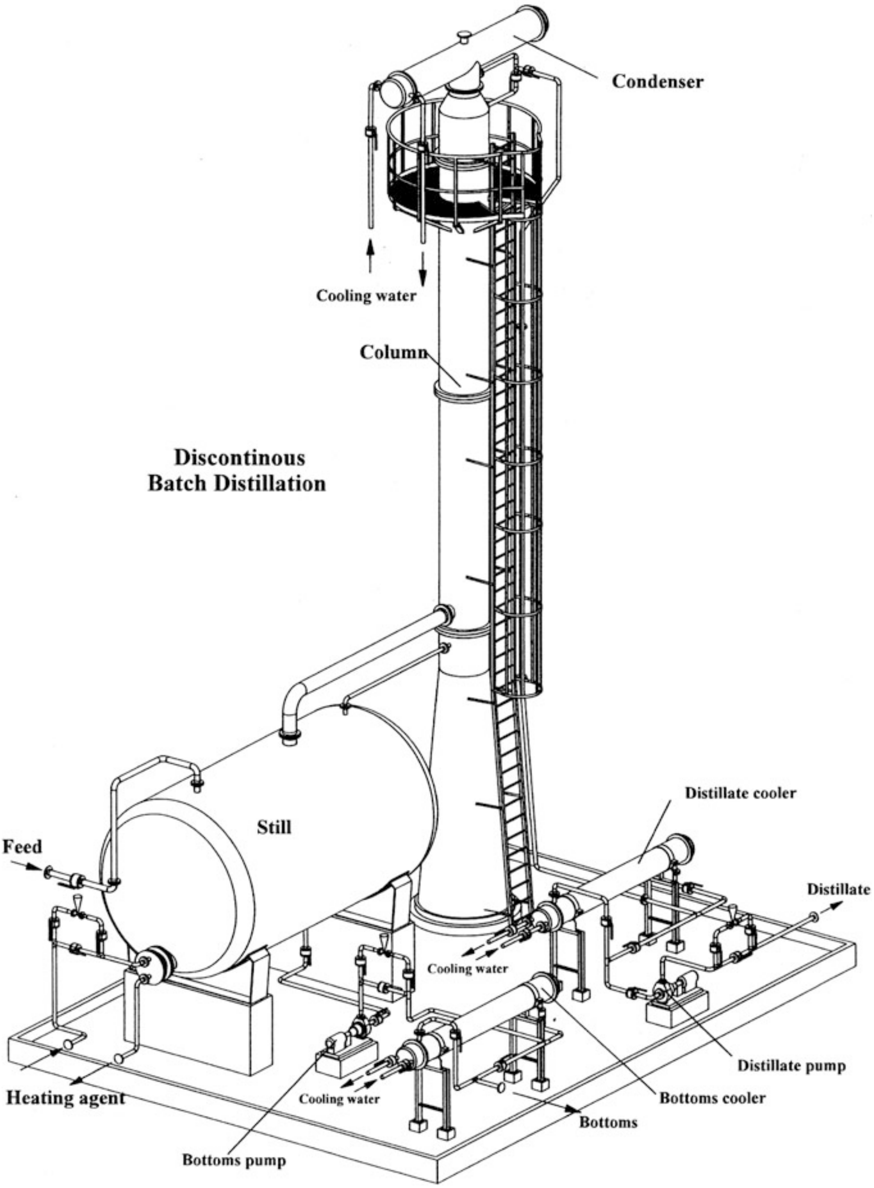


Fig. 6.3 Distillation batch with rectification column

Fig. 6.4 Batch distillation with constant reflux ratio and different distillate compositions D1, D2, and D3

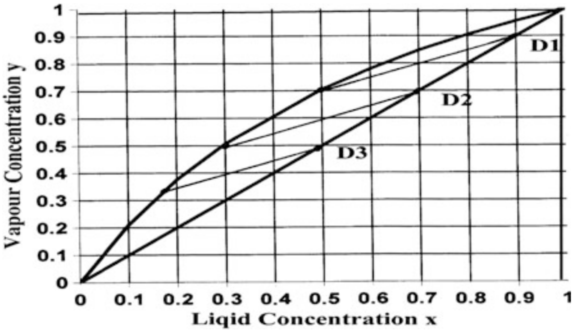
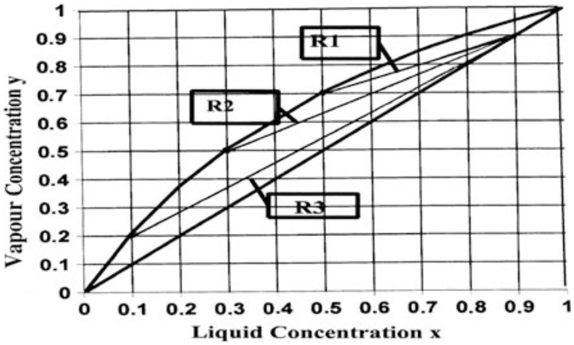


Fig. 6.5 Batch distillation with constant distillate compositions and different reflux ratios R1, R2, and R3



2. **Rectification with constant distillate composition x_D = 90 mol% and different reflux ratios (see Fig. 6.5)**:

   The reflux ratio is increased with decreasing concentration of the light boiling components in the distillate batch or increasing required separation effort up to an economically justifiable reflux highest value.

   With reflux ratio R1 = 1 a bottoms composition of $x_{S1} = 0.5$ is reached.
   With reflux ratio R2 = 1.94 a bottoms composition of $x_{S2} = 0.3$ is reached.
   With reflux ratio R3 = 7 a bottoms composition of $x_{S3} = 0.1$ is reached.
   Thereafter the fractions in between are produced which have to be re-distilled.

The optimization problem in the batch distillation is to minimize the intermediate fractions and to maximize the distillate yield.

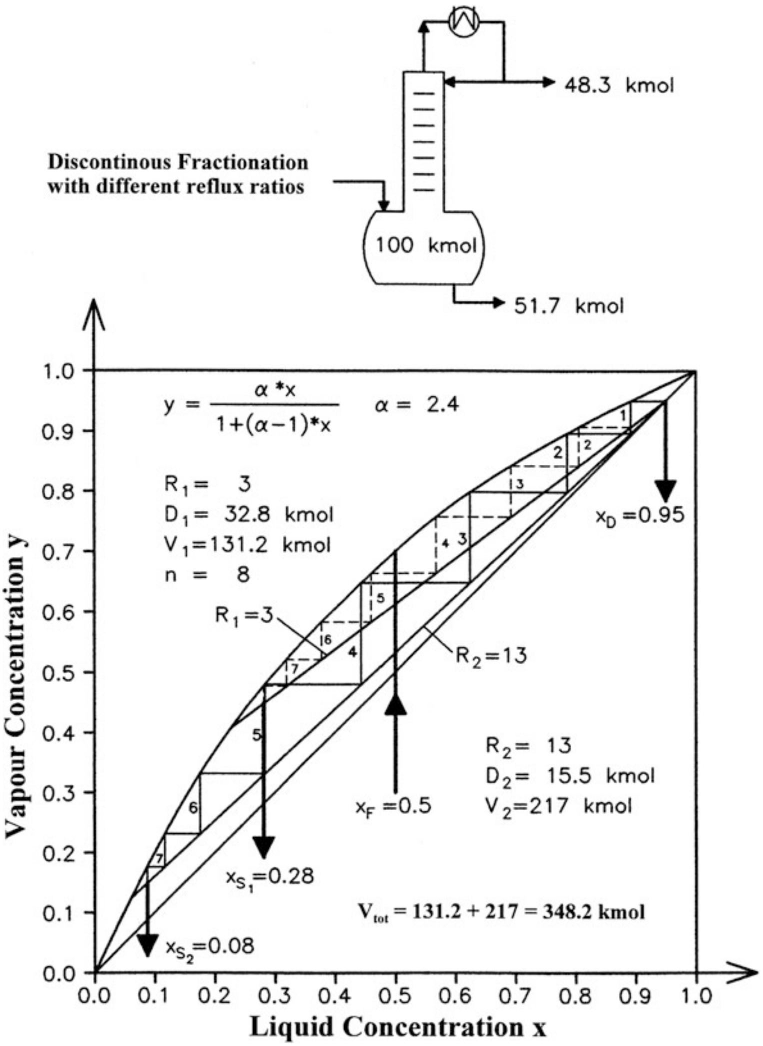


Fig. 6.6 Improvement of the distillate yield by increasing the reflux ratio

Example 6.2.1: Improvement of the distillate yield with a higher reflux

In Fig. 6.6 using the Mcabe–Thiele diagram it is shown that the distillate yield can be increased from 32.8 to 48.3 kmol by increasing the reflux ratio from $R = 3$ to $R = 13$.

Feed quantity = 100 kmol.

Light boiling feed composition $x_F = 0.5 = 50\ \text{mol\%}$.

Required distillate composition $x_D = 0.95 = 95\ \text{mol\%}$.

Number of theoretical stages = 8.

With a **reflux ratio R = 3** a bottoms concentration of $x_{S1} = 0.28$ can be achieved with eight stages, this means that the light boiling composition in the batch will be reduced from 50 to 28 mol%. This produces a distillate rate of **32.8 kmol**, with a concentration of 95 mol%.

In order to improve the distillate yield, and to decrease the bottoms concentration of the light boiling component further to $x_{S2} = 0.08 = 8$ mol%, the reflux ratio must be increased to **R = 13**.

The slope L/V of the operation line is thereby increased and the distance between the equilibrium curve and the operating line becomes larger.

With 8 stages a bottoms concentration of 8 mol% and a top composition of 95 mol% is achieved for light boilers.

Using the second distillation step with R = 13 an additional distillate rate of **15.5 kmol** is produced. Thereby, the total distillate amount increases to 48.3 kmol.

Below a light boiling component composition of 8 mol% in the batch a distillate composition of 95 mol% is no longer achievable with reasonable effort. In this case, the reflux ratio is reduced and an **intermediate run** is produced, which is re-distilled later.

L = liquid loading of the column (kmol/h).

V = vapours loading of the column (kmol/h).

The reflux ratio R is decisive for the energy requirement of batch distillation. The higher the reflux ratio the more vapours must be vaporized.

$$R = \frac{RM}{D} = \frac{\text{Reflux rate (kg/h)}}{\text{Distillate rate (kg/h)}}$$

$$\frac{R}{R+1} = \frac{L}{V} = \frac{\text{Liquid loading (kmol/h)}}{\text{Vapor loading (kmol/h)}}$$

$$R = \frac{L/V}{1 - L/V}$$

As a first estimate for the required reflux ratio R the so-called minimum ratio $(L/V)_{\text{min}}$, at an infinite number of stages, can be determined:

$$\left(\frac{L}{V}\right)_{\text{min}} = \frac{\Delta y}{\Delta x} = \frac{y_D - y_1}{x_D - x_1}$$

The real reflux ratio lies around a factor of 1.5–5 higher than the minimum reflux ratio.

A **mass balance for the batch distillation,** ignoring the column hold-up, is performed as follows:

$$D = S_0 * \frac{x_{S0} - x_{SE}}{x_D - x_{SE}}$$

$$S_E = S_0 * \frac{x_D - x_{S0}}{x_D - x_{SE}}$$

$$D = S_0 - S_E$$

D = distillate quantity.
S_0 = batch quantity at the beginning.
S_E = batch content at the end.
x_D = distillate composition of the light boiling component.
x_{S0} = feed composition of the light boiling component.
x_{SE} = final composition of the light boiling component in the batch.

Here, D is the distillate rate which is produced with the concentration x_D at a composition variation **x_{S0} - x_{SE} in the batch**. At the same discontinuous distillation step the batch rate is reduced from **S_0 to S_E**.

Example 6.2.2: Mass balance for a batch distillation

Feed quantity $S_0 = 40\,\text{t}$ with $x_{S0} = 50\%$.

Distillate composition $x_D = 95\%$.

From the MCabe–Thiele diagram it can be seen that with the existing number of trays, and the chosen reflux ratio, the composition of the light boiling component can be lowered to: x_{SE} = 25%.

$$D = 40 * \frac{50 - 25}{95 - 25} = 14.4\ \text{t}$$

$$S_E = 40 * \frac{95 - 50}{95 - 25} = 25.6\ \text{t}$$

As an alternative to the graphical determination of the number of trays, according to Mcabe-Thiele, one could use the calculation method described in Chap. 3 (i.e., from **tray to tray according to Mcabe-Thiele** the compositions on the trays below the condenser, up to the batch for a certain number of trays and a given reflux ratio, can be determined by calculation [see Example 6.2.3)].

Example 6.2.3: Concentration profile and distillate yield at different reflux ratios

Here we are required to calculate the achievable distillate yield in a rectification column with 10 trays at the refluxes R = 3 and R = 5.

$$S_0 = 1000\ \text{kmol} \quad x_{S0} = 0.6 \quad \alpha = 2.4$$

Light boiling component—liquid concentrations		
	$R = 3$	$R = 5$
Distillate	0.95	0.95
Condenser	0.8879	0.8879
Tray 1	0.7958	0.7862
Tray 2	0.6772	0.6450
Tray 3	0.5496	0.4881
Tray 4	0.4359	0.3512
Tray 5	0.3506	0.2550
Tray 6	0.2945	0.1972
Tray 7	0.2607	0.1656
Tray 8	0.2414	0.1493
Tray 9	0.2307	0.1411
Tray 10	0.2249	0.1370
Distillate quantity	517.3 kmol	569.5 kmol
Residue	482.7 kmol	430.5 kmol

By increasing the reflux ratio from $R = 3$ to $R = 5$ the concentration of the light boiling component in the batch can be lowered to $x = 0.137$ and the distillate rate can be increased to 569.5 kmol.

Alternatively, the number of the required rectification trays can be analytically calculated according to **Smoker** (Chap. 3) for the following conditions:

$$x_D = 0.95 \quad x_F = 0.2249 \quad \alpha = 2.4 \quad R = 3$$

Required number of trays n = 11.

The result according to Smoker is identical to the tray to tray calculation according to MCabe–Thiele. The required **distillation period** or the required **column diameter,** for the given distillation period and the required **energy input,** can be determined stepwise per discontinuous step, or by smoothly changing the reflux ratio by integration over different steps. The distillation period is strongly dependent on the reflux ratio and the column diameter. A higher reflux ratio requires larger reboilers and condensers and a larger column cross section. The equipment consequently becomes more expensive.

As part of the **total production time** the following times must be considered:

- Filling of the distillate batch.
- Unsteady state heating of the feed product to boiling temperature, for instance from 30 to 150 °C.
- Unsteady state cooling of the residue in the bottoms, for instance from 200 to 60 °C.
- Pumping out the residue from the distillate batch.

Figure 6.7 shows a typical flow diagram for batch distillation.

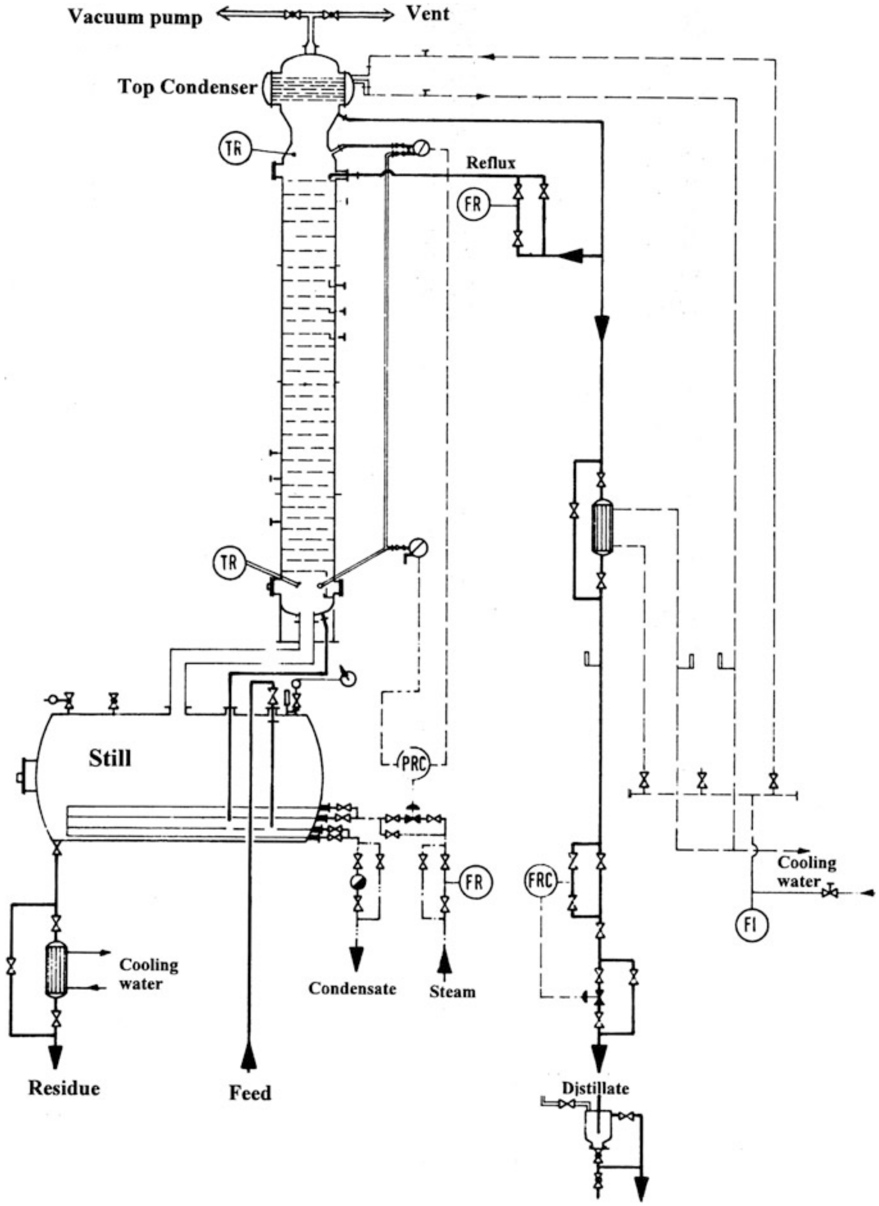


Fig. 6.7 Flow diagram for batch distillation with a fractionation column

6.3 Technical Equipment

Fractionation column with internals:

The column internals—trays or packings—are designed according to the problem definition: throughput, number of trays, efficiency, HETP-value or HTU-value, pressure loss, flexibility, and hold up (See Chaps. 9 and 10).

The "hold up" in the column influences the achievable degree of separation:

In the region of low reflux values and small numbers of trays the effect of the hold up on the degree of separation is insignificant.

At high reflux values, that means slow distillation, the column has more time to reach equilibrium and a higher hold up deteriorates the degree of separation. This is because the light boiling components are stored in the hold up and therefore the concentration of the light boiling components in the distillate batch reduces.

In principle batch distillation internals with lower hold up should be used, especially, if small single fractions must be separated.

Condensation:

Preferably **water-cooled or air-cooled top condensers, as shown in** Fig. 6.3, should be installed on the top of the column. The following advantages are thereby achieved.

- The hold up is much lower as with the condenser with reflux drum installed at the base.

The single fractions will not be "smeared" and a smaller flushing duration, for setting the required concentration in the accumulator, is required.

The required flushing period Δt is calculated using the following equation:

$$\Delta t = \frac{\mathrm{VS}}{D} \ln \frac{c_\mathrm{D} - c_1}{c_\mathrm{D} - c_\mathrm{P}} (\mathrm{h})$$

VS = accumulator volume (m^3).
c_D = distillate concentration (%).
c_P = required product concentration (%).
D = distillate rate (m^3/h).
c_1 = starting concentration in the accumulator (%).

Example 6.3.1
Flushing period calculation for a product concentration c_P = 99%.

$$\mathrm{VS} = 4\,\mathrm{m}^3 \quad D = 2\,\mathrm{m}^3/\mathrm{h} \quad c_\mathrm{D} = 99.5\% \quad c_1 = 90\% \quad c_\mathrm{P} = 99\%$$

$$\Delta t = \frac{4}{2} * \ln \frac{99.5 - 90}{99.5 - 99} = 5.9\ \mathrm{h}$$

For a top condenser with a **hold up of VS = 0.2 m^3** the **flushing period is reduced to 0.3 h**.

- The vapour line from the column top to the condenser installed below can be omitted and hence so can the pressure loss in the vapour line.
- No reflux pumps and distillate pumps are needed because sufficient pressure head is available. Problems in the condensation of freezing or sluggish products are avoided with the use of warm water or cooling by air circulation.

If in the condensation a two-phase mixture forms, a phase separator must be installed.

The right hydraulic dimensioning of the gravity driven reflux flow through a syphon back to the column, especially with vacuum distillation [9], is very important.

If the liquid feed height is insufficient, reflux variations occur and hence poor fractionation is achieved.

Heating and evaporation

The adequate selection of a heating system is important for the proper functioning of the batch distillation unit. For **heating coils, according to** Fig. 6.8, tall installation heights and pipe lengths are necessary. In steam heating the forming condensate blocks the heating area and dangerous steam shocks or condensation shocks can occur. Due to the large installation height of such heating coils the application range of the batch is limited because the heating pipes should always be covered with liquid. If this is not the case then the evaporator efficiency decreases and the vapour can be thermally damaged on the hot pipes.

Example 6.3.2

In a still with a 3 m diameter the following residue amounts form:

Heating coil pipe with 700 mm minimum filling height: remaining residue = 1254 l/m length.

Heating bundle with 350 mm minimum filling height: remaining residue = 460 l/m length.

Therefore, the **heating tube bundle** shown in Fig. 6.9 is preferred because it can be built very low and can easily be removed for cleaning. Particularly low installation heights are achieved using **finned tubes** and a configuration according to Fig. 6.10. Due to fin effectiveness, which considers the temperature drop at the fin,

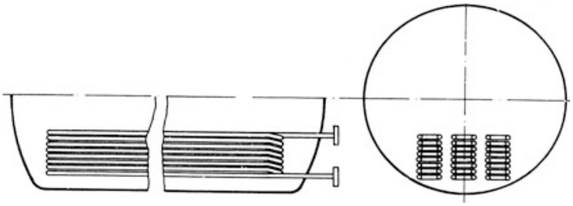


Fig. 6.8 Heatig coil

Fig. 6.9 Heating tube bundle

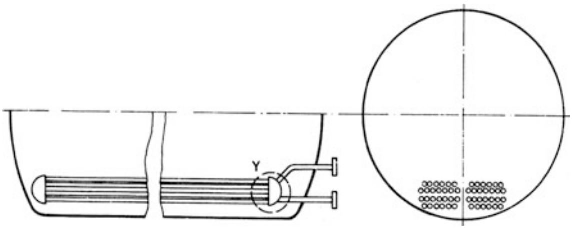
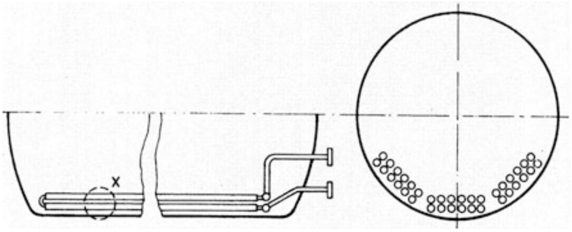


Fig. 6.10 Finned tubes



only tubes with low fin heights are used [9]. Due to the fin the outer area is increased by a factor of 2–3 and the heat duty per square meter of heating area is increased. This decreases the installation height of the fin heating tube bundle and increases the operation volume of the still. A danger of greater fouling of the fin tubes does not exist according anecdotal evidence.

A further alternative for increasing the operating capacity of the still is the configuration of a **thermosyphon or forced-flow reboiler** outside the batch. However, the specific problems of thermosyphon evaporators, and the required fluid-pumping rate for uniform evaporation, must be considered [9].

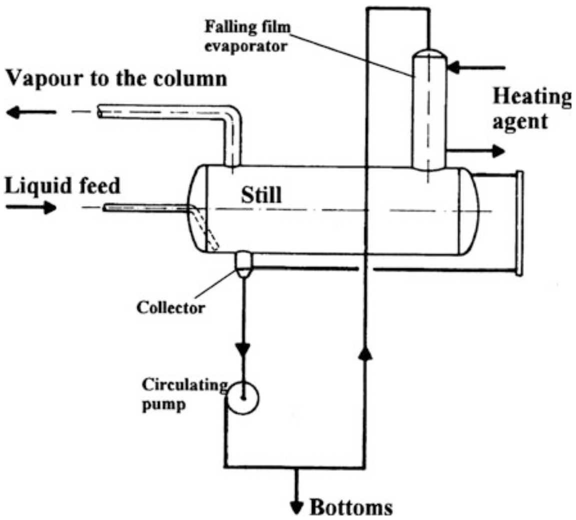
All the heating systems discussed so far have the disadvantage that the boiling temperature is raised by the hydrostatic pressure of the liquid above the heating area. This problem is predominant in vacuum distillation. For instance, in vacuum distillation it is not important to minimize the pressure loss of the column internals if in the still 2 m of liquid lies over the heating areas thus raising the boiling temperature.

That is why it is preferable, in vacuum distillation units, to use **falling film evaporators with circulating pumps** having low pressure drops (shown in Fig. 6.11). Sufficient circulation is important in order to avoid composition variations and a uniform and sufficient liquid feed on the tubes. In all cases a drying up of the evaporator has to be avoided. In addition, a minimum wetting rate must be kept [9]. The pump must circulate the product at high temperatures and has to be completely closed because of the dangers of explosions linked to air penetration. For example magnetic coupling pumps or canned motor pumps are adequate.

Due to the necessary NPSH value of the pump the batch has to be installed approximately 3 m above the pump suction nozzle.

If the batch distillation unit is also operated from time to time in continuous mode, the hold up of the distillation batch should be reduced in order to avoid thermal damage of the product by its long residence time in the hot bottoms. For

Fig. 6.11 Falling film evaporator



this reason the distillation batch is equipped with a small "receiver" from which the product is pumped through the falling film evaporator. In special cases batch heating can be effected with direct steam through a "steam spin", for instance with dirty feed products. Fouling of the heating area is avoided and thereby boiling point of the high boiling components is reduced.

Process control of the batch distillation

The **loading control** of batch distillation is simple (see flow diagram—Fig. 6.7). The heating medium feed is fed differentially or is bottoms pressure controlled. A differential pressure for the column is specified which is maintained by heating with steam or hot oil. Thereby, the temperature in the batch rises. This is different to the case in which for safety reasons, for instance with nitroparaffins, a maximum temperature may not be exceeded in order to avoid decomposition or explosion. In such cases the loading or the differential pressure of the column is controlled by the top pressure. Instead of raising the bottoms temperature the top pressure is lowered.

What is more difficult is **analytic control of the distillate composition** in which the concentration constantly changes and the optimum setting of the reflux ratio, in order to achieve the desired distillate composition and yield with a low-energy input. Therefore, the analyses must be performed constantly, manually, or with a process chromatograph in order to optimize the reflux ratio. In a stepwise increase of the reflux equilibrium disturbances in the column can occur. A uniform change of the reflux rate is recommended.

For two-component separations a constant concentration dependent control can relatively simply be achieved with a DVP controller. The top composition is thereby held constant and the reflux is increased permanently according to the additional separation task. Alternatively, the reflux ratio can be controlled depending on the batch temperature or the temperature difference between top and bottoms. The start-up of a batch distillation is such that the initial contents of the batch are heated to boiling temperature and then the equilibrium in the column is set at total reflux. Subsequently, distillate take-off begins.

Special problems

When dimensioning a batch distillate unit the ratio between **batch volume and hold up** of column and condenser is very important. If the still is underdesigned a reasonable separation or yield cannot be achieved. Therefore, it makes sense to choose a column with low hold up and a top condenser. If a still is too small only short distillation periods are allowed.

A case is known to the authors in which after the start-up the total batch charge was as hold up in the column and in the reflux drum under the condenser.

In addition, for **heating with a heating bundle in the batch,** a sufficiently large batch volume is required in order to avoid "dry line" on the top of the heating tubes shortly after start-up and continuous reduction of the evaporator surface.

The boiling point temperature rises with increasing operation time because the light boiling components are distilled-off. The **driving temperature gradient** for the evaporation is thereby reduced. A large hold up in the distillation plant, for instance a bubble cap tray column with a condenser on the base with an accumulator for the condensed distillate and a reflux pump and a reflux line to the column top, makes it particularly difficult to distill **small amounts of a component.**

The plant can be operated with total reflux in order to drive out parts of the polluting components and then quickly switch over to the **distillate draw** in order to remove the pollutants enriched in the distillate. Alternatively, it is possible to draw off the enriched polluting component **in its vapour** phase at a total reflux with reduced condensation in the vacuum. A third possibility is to install **catch trays** at different locations in the column.

First the polluting components are enriched in a certain region of the column at total reflux. Then the heating is turned off and the hold up of the column section, with enriched polluting components, flows into the installed catch tray below via a side draw. If there remains a small amount of light components to be evaporated, and there is insufficient vaporizing liquid available in the batch, a **higher boiling carrier** can be filled into the batch to transport the light boiling component into the column.

If **two liquid phases** exist in the batch then intermittent evaporation occurs. This must be avoided by introducing an azeotrope entrainer.

Strong foaming products or overfilling of the batch make the start-up difficult because evaporation is hindered by the **narrowed vapour outlet cross section.**

This disturbance can be identified in the fact that the temperature rises only slowly because the light components are not able to escape.

In batch evaporation **pollution residues** must always be expected. These can partly be removed only in a "mining fashion". This must be considered in the design:

- Man holes for access and dirt removal.
- Removable heating bundle on slides.
- Heating tube bundles with quadratic pitches.

6.4 Batch Stripper

The batch stripper shown in Fig. 6.12 is advantageous for small concentrations of light boiling components in the feed as well as high-purity specifications for the high boiling component or the stripper draw. From the batch the feed is fed to the column top as a liquid. The high boiling components run out in the bottoms and the light boiling components are evaporized with the help of the reboiler and boiled out from the high boiling component. The light boiling component vapour, which has

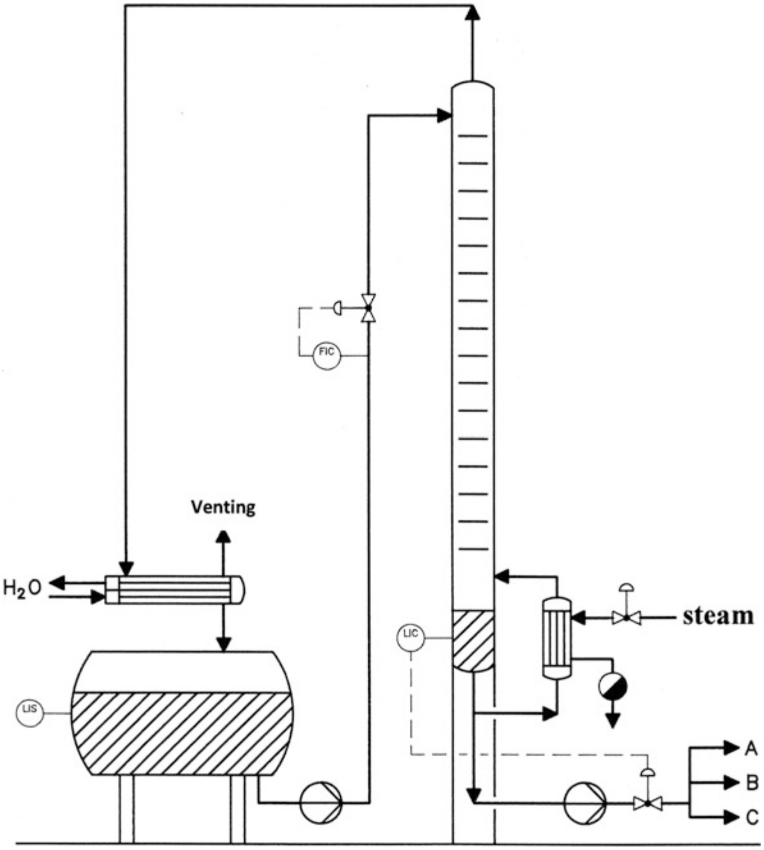


Fig. 6.12 A discontinuous batch stripper

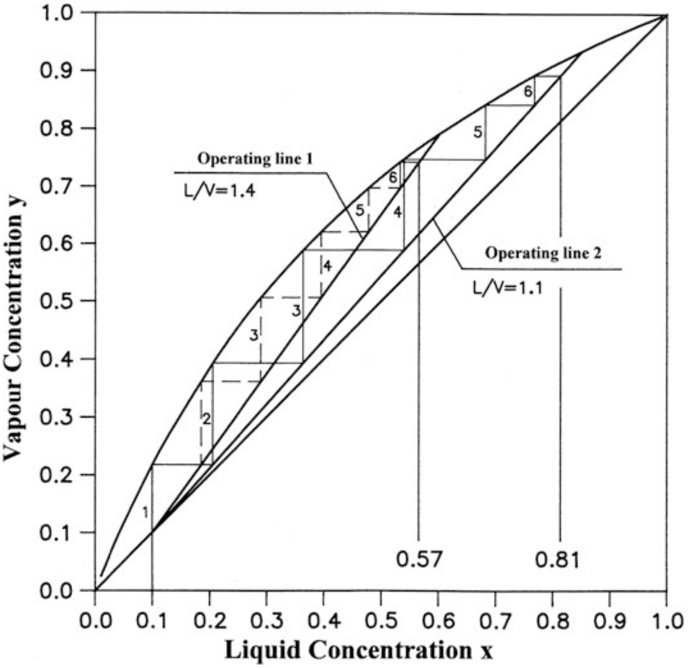


Fig. 6.13 Mcabe–Thiele diagram with two operating lines for a batch stripper

been driven out of the column, is liquidized in the condenser on the top of the batch and then run back into the batch itself. Thereby, the high boiling component composition in the batch is reduced, and a shallower slope L/V of the operating line is required in order to achieve the necessary concentration of the high boiling component, or the allowable light boiling component concentration in the stripper draw (see Fig. 6.13).

L = Liquid loading of the column (kmol/h).

V = Vapour loading of the column (kmol/h).

With a fixed evaporation load in the reboiler for the vapour rate V the ratio L/V can be reduced by reducing the feed rate *L* in order to lower the slope of the operating line (Fig. 6.13).

The light boiling component concentration is reduced with operating line 1 with L/V = 1.4 from $x = 0.57$ down to $x = 0.1$. Consequently the high boiling components are enriched from $x = 0.43$ to $x = 0.9$. With operating line 2 the light boiling component composition is reduced with L/V = 1.1 from $x = 0.81$ to $x = 0.1$. The high boiling components are then enriched from $x = 0.19$ to $x = 0.9$.

The particular **advantages of a batch stripper** are highlighted as follows:

- **The total batch contents do not need to be heated to the boiling temperature before the start of the distillation.**
- **The residence time in the hot section is much shorter, thus reducing thermal damage.**
- **Suitable for separation of a mixture with minimum azeotropes.**

The compositions on the stages above the reboiler, up to the feed tray, for a certain number of stages and a given evaporation load or vapour rate, can be determined using the described tray-to-tray calculation according to MCabe–Thiele (given in Chap. 3).

Example 6.7: Calculation of a batch stripper

The high boiling component yield that can be achieved in a batch stripper with 10 trays plus a reboiler at different evaporation loads from $V_A = 180$, 300, and 500 kmol/h, is calculated where the bottoms 60 kmol/h high boiling component, with $x_{SE} = 0.95$, is drawn.

$$S_0 = 1000\ \text{kmol} \quad x_{S0} = 0.6 \quad \alpha = 2.4$$

With an evaporation load $\mathbf{V_A}$ **= 180 kmol/h** the high boiling component concentration in the feed batch can be reduced from $x_{S0} = 0.6$ to $x_{SE} = 0.4062$ over 10 trays and the evaporator. From this results the high boiling component yield L = 356.4 kmol.

Mass balance for $V = 180$ kmol/h:

$$S_E = S_0 * \frac{x_D - x_{S0}}{x_D - x_{SE}} = 1000 * \frac{0.4062 - 0.6}{0.4062 - 0.95} = 356.4\ \text{kmol}$$

With an evaporated vapour rate of $\mathbf{V_A}$ **= 300 kmol/h**, a high boiling component concentration in the batch of $x = 0.2725$ and a high boiling component yield of $L = 483.4$ kmol, is reached.

Mass balance for 300 kmol/h:

$$S_E = S_0 * \frac{x_D - x_{S0}}{x_D - x_{SE}} = 1000 * \frac{0.2725 - 0.6}{0.2725 - 0.95} = 483.4\ \text{kmol}$$

Still better is the yield with an evaporation load of $\mathbf{V_A}$ **= 500 kmol/h**.

Mass balance for 500 kmol/h:

$$S_E = S_0 * \frac{x_D - x_{S0}}{x_D - x_{SE}} = 1000 * \frac{0.176 - 0.6}{0.176 - 0.95} = 547.8\ \text{kmol}$$

High boiling component concentration in the batch: $x = 0.176$. High boiling component yield L = 547.8 kmol.

	High boiling component liquid concentrations		
	V_A = 180	V_A = 300	V_A = 500 kmol/h
Tray 10	0.4062	0.2725	0.1760
Tray 9	0.4105	0.2759	0.1787
Tray 8	0.4186	0.2827	0.1846
Tray 7	0.4330	0.2963	0.1970
Tray 6	0.4584	0.3226	0.2226
Tray 5	0.5005	0.3708	0.2730
Tray 4	0.5644	0.4510	0.3628
Tray 3	0.6497	0.5650	0.4979
Tray 2	0.7454	0.6959	0.6568
Tray 1	0.8343	0.8135	0.7977
Reboiler	0.9034	0.8982	0.8945
Bottoms	0.95	0.95	0.95
High boiling component yield	356.4 kmol	483.4 kmol	547.8 kmol

Figure 6.14 shows the curve of the high boiling component composition over the theoretical number of trays.

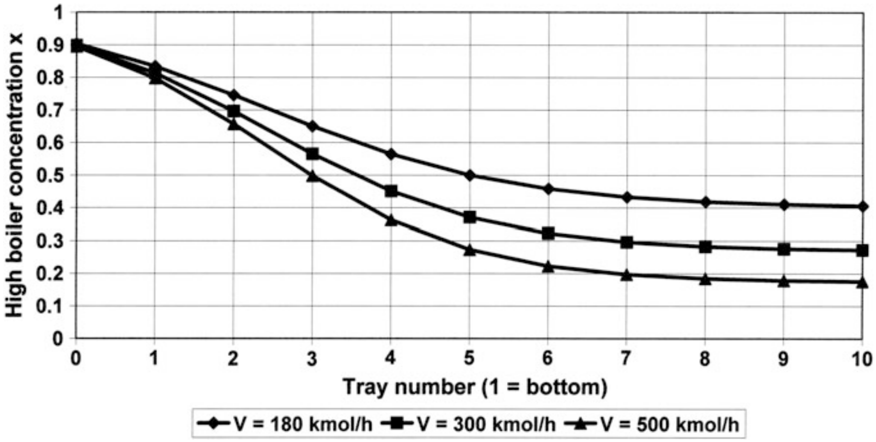


Fig. 6.14 High boiling concentration on the different trays at different evaporation rates

Fig. 6.15 Discontinuous waste water stripper

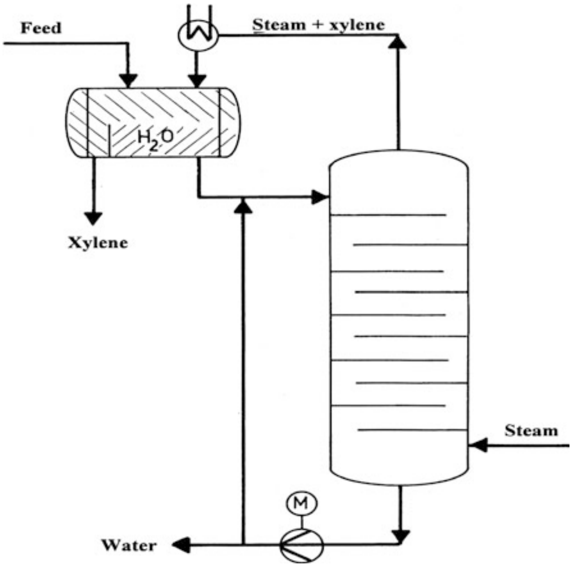


Figure 6.15 shows a batch stripper which might be used for the purification of waste water.

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Chapter 7
Steam Distillation

Steam distillation requires that the mixture is immiscible with water. In steam distillation the total vapour pressure in the system is the sum of the individual vapour pressures of water P_{0W} and the water immiscible organic component P_{0org} or the sum of the partial pressures $P_{org} + P_W$.

$$P_{tot} = P_{0org} + P_{0w} = P_{org} + P_W$$

Steam distillation is used in order to lower the boiling point of high boiling components using the water vapour pressure.

The organic high boiling component is distilled off with the water vapour acting as a carrier medium.

The Hausbrand diagram in Fig. 7.1 shows how the boiling point of a water immiscible solvent is lowered by steam. In steam distillation the boiling point of the organic component lies at the point of intersection between the vapour pressure curve of the component with the curve total pressure minus water vapour pressure $P_{tot} - P_{0w} = 1000 - P_W$.

As an example, the boiling point of toluene is lowered at $P_{tot} = 1000$ mbar from 110.7 to 84 °C in steam distillation.

Examples of applications of steam distillation:

- Vaporization of organic products by direct heating with steam, e.g., vaporization of high boiling turpentine oil or of gas oil.
- Stripping off solvents from residues containing solvents, e.g., synthetic resin and paint or colour from materials used in paper production.
- Stripping out of the light boiling components from organic high boiling components, e.g., gasoline from gas oil or benzene from lean oil.

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_7

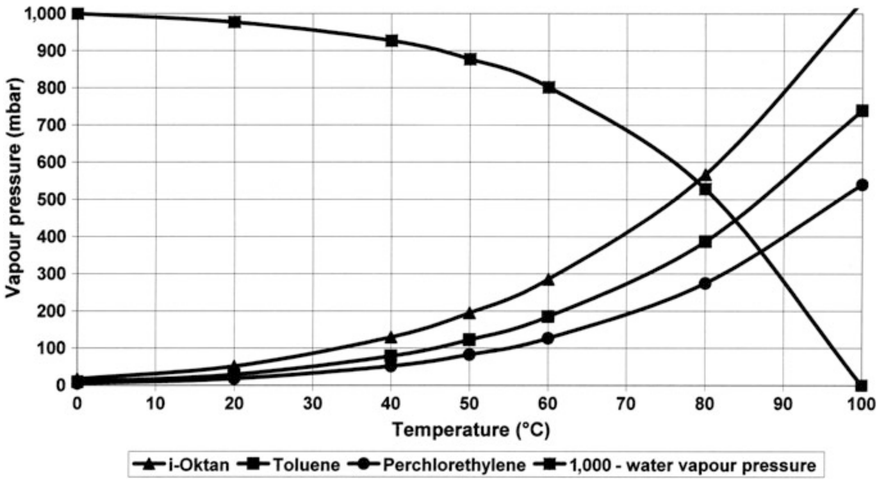


Fig. 7.1 Hausbrand diagram for steam distillation

7.1 Calculations of Steam Distillation [1]

One must differentiate between steam distillation **with water in its liquid phase**, i.e. two liquid phases, and steam distillation **without water** in its liquid phase.

Here, Gibb's phase rule applies: $F = 2 + C - P$

F = degrees of freedom.
C = number of components.
P = number of phases.

For two liquid phases (P = 2) and two components (C = 2) there is **one degree of freedom**.

$$F = 2 + 2 - 3 = 1$$

Only the **temperature** or **pressure** can be set.

For **one liquid phase** and two components there are **two degrees of freedom** result.

$$F = 2 + 2 - 2 = 2$$

Pressure and **temperature** can be chosen independently from each other.

If the organic component only contains a small fraction of non-volatile materials or is stripped out of solid residues the solubility of the organic light boiling component in the high boiling component or solid bottoms draw can be ignored. Stationary conditions apply.

Calculation equations for steam distillation:

$$\text{Vapor concentration} \quad y_{\text{org}} = \frac{P_{\text{org}}}{P_{\text{tot}}} \qquad\qquad y_{\text{W}} = \frac{P_{\text{W}}}{P_{\text{tot}}}$$

$$\text{Boiling point} \sum y = 1 = \frac{P_{\text{org}}}{P_{\text{tot}}} + \frac{P_{\text{W}}}{P_{\text{tot}}}$$

Required specific stripping steam rate :

$$\frac{n_{\text{W}}}{n_{\text{org}}} = \frac{P_{\text{W}}}{P_{\text{org}}} * \frac{1}{\eta} \left(\frac{\text{kmol}}{\text{kmol}}\right) \qquad\qquad \frac{m_{\text{W}}}{m_{\text{org}}} = \frac{M_{\text{W}}}{M_{\text{org}}} * \frac{P_{\text{W}}}{P_{\text{org}}} * \frac{1}{\eta} \left(\frac{\text{kg}}{\text{kg}}\right)$$

Calculation of the bubble point and dew point in steam distillation:

The **bubble point** is defined as the temperature at which the sum of the vapour pressures of water and hydrocarbon is equal to the total pressure of the system.

$$P_{\text{tot}} = P_{0\text{org}} + P_{0\text{W}}$$

The concentration of both components is not used in the calculation.

Example 7.1.1: Bubble point calculation of a toluene–water mixture at 1010 mbar

$$\text{Temperature}\, T = 84\,^{\circ}\text{C}.$$
$$P_{0\text{Tol}} = P_{\text{Tol}} = 444\,\text{mbar}.$$
$$P_{0\text{W}} = P_{\text{W}} = 566\,\text{mbar}.$$
$$P_{\text{tot}} = 444 + 566 = 1010\,\text{mbar}.$$

The bubble point for the water–toluene mixture is 84 °C.

In the **calculation of the dew point** the composition of the vapour mixture is important because the partial pressure of the components results from the molar composition y of the vapours.

$$P_{\text{org}} = y_{\text{org}} * P_{\text{ges}} \quad P_{\text{W}} = y_{\text{W}} * P_{\text{ges}}$$

The dew point is reached when the vapour pressure of the component falls below the partial pressure of the component.

$$P_{0\text{org}} < P_{\text{org}} \qquad P_{0\text{W}} < P_{\text{W}}$$

Example 7.1.2: Dew point calculation for a water–toluene vapour with 63 mol% water

Vapour compositon of water y_W = 0.63 molfr.
Total pressure P_{tot} = 1 bar.
Partial pressure of water P_{0W} = 0.63 * 1000 = 630 mbar.
Vapour pressure of water at 87.2 °C: P_{0W} = 630 mbar.
Water starts condensing at 87.2 °C.
The dew point is 87.2 °C.

7.2 Required Stripping Steam Rate

In the calculation of the required stripping steam rate it must be taken into account that there is a difference between steam distillation with one or two degrees of freedom.

7.2.1 Required Stripping Steam Rate for One Liquid Phase (Fig. 7.2)

Temperature and pressure can be set independently from each other according to Gibb's phase rule. This enables the optimization of the stripping process, i.e., a reduction of the required stripping vapour rate.

$$\frac{m_{org}}{m_W} = \frac{P_{org}}{P_{tot} - P_{org}} * \frac{M_{org}}{M_W} * \eta \left(\frac{\text{kg organ.Component}}{\text{kg steam}}\right)$$

$$P_{tot} = P_{org} + \left(P_{tot} - P_{org}\right)(\text{mbar})$$

Required stripping steam rate taking account of the stripping efficiency η:

$$n_W = n_{org} * \frac{P_{tot} - P_{org}}{P_{org}} * \frac{1}{\eta}\ (\text{kmol}) \qquad m_W = m_{org} * \frac{P_{tot} - P_{org}}{P_{org}} * \frac{M_W}{M_{org}} * \frac{1}{\eta}\ (\text{kg})$$

In case a light boiling organic component is to be stripped out of a large rate of high boiling components, for instance benzene from lean oil, the light boiling component concentration is lowered in the high boiling component oil during stripping, in a similar manner to differential distillation. The conditions are unsteady.

The partial pressure of the light boiling component decreases with increased stripping.

This has to be considered, for instance, by an average logarithmic partial pressure P_{ln}.

$$P_{\text{ln}} = \frac{P_{\text{org1}} - P_{\text{org2}}}{\ln \frac{P_{\text{org1}}}{P_{\text{org2}}}} \text{(mbar)}$$

P_{org1} = partial pressure of the organic component at the beginning (mbar).
P_{org2} = partial pressure of the organic component at the end (mbar).

The calculation of the required stripping steam rate is carried out using the average logarithmic partial pressure P_{ln}.

$$n_{\text{W}} = n_{\text{org}} * \frac{P_{\text{tot}} - P_{\text{ln}}}{P_{\text{ln}}} * \frac{1}{\eta} \text{(kmol)}$$

$$m_{\text{W}} = m_{\text{org}} * \frac{P_{\text{tot}} - P_{\text{ln}}}{P_{\text{ln}}} * \frac{M_{\text{W}}}{M_{\text{org}}} + \frac{1}{\eta} \text{(kg)}$$

An alternative calculation according to **Ellerbe** [1]:

$$n_{\text{W}} = \left(\frac{P_{\text{tot}}}{\eta * P_{0\text{org}}} - 1 \right) * (n_{\text{in}} - n_{\text{out}}) + n_{\text{org}} * \frac{P_{\text{tot}}}{\eta * P_{0\text{org}}} * \ln \frac{n_{\text{in}}}{n_{\text{out}}} \text{(kmol)}$$

Figure 7.2 shows a flow diagram for steam distillation without liquid water.

Steam distillation operates at temperatures above 100 °C or in a vacuum, so that no steam is condensed.

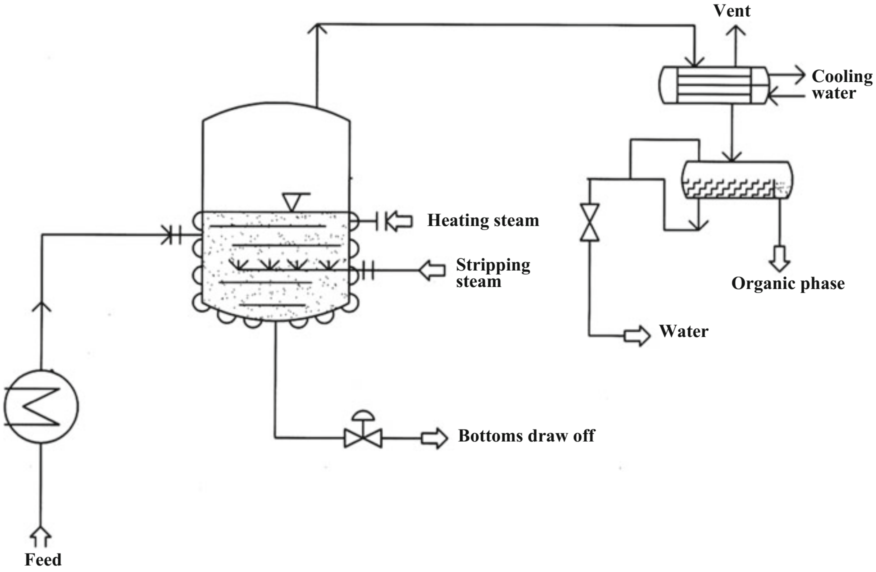


Fig. 7.2 Steam distillation without water in the liquid phase with two degrees of freedom

The feed product is indirectly heated to azeotrope boiling temperature.

The stripping steam is overheated and is introduced, evenly distributed across the total cross section, by means of a steam spider.

The vapours of the light organic component are stripped out, with the stripping steam a carrier, and liquified in the condenser.

The condensation starts at dew point and ends at bubble point.

In the decanter, the organic and the liquid phases are separated and drawn off.

The unit can either be operated continuously or discontinuously.

When organic products are evaporated from solid residues the residue is collected and then stripped.

Example 7.2.1.1: Steam distillation of toluene at 84.1 °C and 1013 mbar or 600 mbar

$$\mathrm{P_{0Tol}} = 444.2\,\mathrm{mbar\,at\,84.1^\circ C} \qquad \eta = 1 \qquad \mathrm{M_{Tol}} = 92.1 \qquad \mathrm{M_W} = 18$$

At atmospheric pressure P_{tot} = 1013 mbar:

$$\frac{m_{\mathrm{Toluol}}}{m_{\mathrm{W}}} = \frac{P_{\mathrm{Tol}}}{P_{\mathrm{tot}} - P_{\mathrm{Tol}}} * \frac{M_{\mathrm{Tol}}}{M_{\mathrm{W}}} = \frac{444.2}{1013 - 444.2} * \frac{92.1}{18} = 4\,\mathrm{kg\,Toluene/kg\,steam}$$

$$y_{\mathrm{Tol}} = \frac{P_{\mathrm{Tol}}}{P_{\mathrm{tot}}} = \frac{444.2}{1013} = 0.44 = 44\,\mathrm{mol\%}$$

$$y_{\mathrm{W}} = \frac{P_{\mathrm{W}}}{P_{\mathrm{tot}}} = \frac{1013 - 444.2}{1013} = 0.56 = 56\,\mathrm{mol\%}$$

In a vacuum at P_{ges} = 600 mbar:

$$\frac{m_{\mathrm{Tol}}}{m_{\mathrm{W}}} = \frac{444.2}{600 - 444.2} * \frac{92.1}{18} = 14.58\,\mathrm{kg\,toluene/kg\,steam}$$

$$y_{\mathrm{Tol}} = \frac{444.2}{600} = 0.74 = 74\,\mathrm{mol\%}$$

$$y_{\mathrm{W}} = \frac{600 - 444.2}{600} = 0.26 = 26\,\mathrm{mol\%}$$

In a vacuum the toluene yield rises from 4 to 14.58 kg toluene/kg steam.

The quantity of the organic component distilled off per kg stripping steam depends on the vapour pressure ratio and the molar weights.

In a vacuum the quotient ($P_{org}/P_{tot} - P_{org}$) rises and the stripping becomes more efficient.

The over-distilled organic product rate per kg of stripping steam increases.

Example 7.2.1.2: Steam distillation of *n*-nonane at 90 °C

$$\text{Vapour pressure of nonane } \mathrm{P_{0nonan}} = 144.5\,\text{mbar}.$$
$$\mathrm{M_{Nonan}} = 128.$$

At atmospheric pressure P_{tot} = 1000 mbar:

$$\frac{n_{\mathrm{Nonan}}}{n_{\mathrm{W}}} = \frac{144.5}{1000 - 144.5} = 0.169\,\text{kmol Nonane/kmol steam}$$
$$\frac{m_{\mathrm{Nonan}}}{m_{\mathrm{W}}} = 0.169 * \frac{128}{18} = 1.2\,\text{kg Nonane/kg steam}$$
$$y_{\mathrm{Nonan}} = \frac{144.5}{1000} = 0.144 \qquad y_{\mathrm{W}} = \frac{1000 - 144.5}{1000} = 0.856$$

In a vacuum at P_{tot} = 600 mbar:

$$\frac{n_{\mathrm{Nonan}}}{n_{\mathrm{W}}} = \frac{144.5}{600 - 144.5} = 0.317\,\text{kmol Nonan/kg steam}$$
$$\frac{m_{\mathrm{Nonan}}}{m_{\mathrm{W}}} = \frac{144.5}{600 - 144.5} * \frac{128}{18} = 2.25\,\text{kg Nonan/kg steam}$$
$$y_{\mathrm{Nonan}} = \frac{144.5}{600} = 0.24 \qquad y_{\mathrm{W}} = \frac{600 - 144.5}{600} = 0.76$$

In a vacuum the nonan yield increases from 1.2 to 2.25 kg per kg of stripping steam.

For **evaporation of high boiling oils** the boiling point can be reduced by injecting stripping steam.

Using the steam as a carrier the organic component is stripped out in the ratio of the partial pressures.

$$\frac{n_{\mathrm{org}}}{n_{\mathrm{W}}} = \frac{P_{\mathrm{org}}}{P_{\mathrm{tot}} - P_{\mathrm{org}}} \frac{\text{kmol organ. Component}}{\text{kmol steam}}$$

Example 7.2.1.3: Evaporation of a high boiling oil with stripping steam

Oil rate m_{oil} = 2000 kg = 10 kmol.
Molar weight of the oil $_{Moil}$ = 200.
Bubble point = 188 °C at 1 bar.
The bubble point is to be decreased to 170 °C.
Vapour pressure of the oil P_{0oil} = 650 mbar at 170 °C.
Required water vapour pressure P_W = 1000 − 650 = 350 mbar.

Bubble point check:

$$\sum y = \frac{650}{1000} + \frac{350}{1000} = 1$$

Required stripping steam rate for 2000 kg oil:

$$n_W = n_{oil} * \frac{P_{tot} - P_{oil}}{P_{oil}} = 10 * \frac{1000 - 650}{650} = 5.4\,\text{kmol steam}$$

$$m_W = 5.4 * 18 = 96.9\,\text{kg steam}$$

$$m_W = m_{oil} * \frac{P_{tot} - P_{oil}}{P_{oil}} * \frac{M_W}{M_{oil}} = 2000 * \frac{1000 - 650}{650} * \frac{18}{200} = 96.9\,\text{kg steam}$$

Example 7.2.1.4: Stripping benzene from a large lean oil rate at 177 °C

Feed: 10,000 kg lean oil (*M* = 220) with 10% benzene.
Required benzene rest content: 50 kg benzene = 0.64 kmol.
Benzene vapour pressure at 177 °C: $P_{0benz} = 9.443\,\text{mbar}$ $P_{tot} = 1013\,\text{mbar}$ $\eta = 0.9$

Feed mass balance:

	Rate		Rate	Composition	Vapour pressure	Partial pressure
Component	(kg)	M	(kmol)	(molfraction)	(mbar)	(mbar)
Benzene	1000	78	12.82	0.239	9443	2257
Lean oil	9000	220	40.9	0.761	–	

Required outlet mass balance for lean oil:

	Rate		Rate	Composition	Vapour pressure	Partial pressure
Component	(kg)	M	(kmol)	(molfraction)	(mbar)	(mbar)
Benzene	50	78	0.64	0.015	9443	141.6
Lean oil	9000	220	40.9	0.985		

At a lean oil temperature of 177 °C the partial pressure of benzene at 2257 mbar is higher than the total pressure of 1013 mbar.

Much of the benzene is vaporized until its partial pressure is reduced to 1013 mbar.

Calculation of the molar composition at P_{benz} = 1013 mbar:

$$x_{Ben} = \frac{P_{tot}}{P_{Benz}} = \frac{1013}{9443} = 0.107 \text{ Molfr.}$$

$$X_{Benz} = \frac{x}{1 - x} = \frac{0.107}{1 - 0.107} = 0.1198 \text{ kmol Benzene/kmol Oil}$$

Due to flash evaporation at 1013 mbar the benzene composition in the lean oil is reduced from 0.239 to 0.107 molfr.

The benzene partial pressure drops from 2257 to 1013 mbar.

Cross-check calculation:

$$P_{\text{Benz}} = 0.107 * 9.443 = 1.013\,\text{mbar}$$

Calculation of the amount of benzene remaining in the lean oil after flashing:

$$n_{\text{Benz}} = X * n_{\text{oil}} = 0.1198 * 40.9 = 4.9\,\text{kmol Benzol}$$

The remaining amount of benzene, 4.9 kmol, in the lean oil must be reduced to the required rest value of 0.64 kmol using steam stripping.

The benzene composition must be reduced from 0.107 molfr., at the beginning of the steam stripping process, to 0.015 molfr. in the lean oil.

During stripping the benzene partial pressure falls with dropping benzene concentration from 1013 to 141.6 mbar.

For the determination of the required stripping steam rate the average logarithmic partial pressure P_{ln} is needed.

$$P_{\text{ln}} = \frac{P_{\text{org1}} - P_{\text{org2}}}{\ln \frac{P_{\text{org1}}}{P_{\text{org2}}}} = \frac{1013 - 141.6}{\ln \frac{1013}{141.6}} = 442.8\ \text{mbar}$$

$$\frac{n_{\text{W}}}{n_{\text{Benz}}} = \frac{P_{\text{tot}} - P_{\text{ln}}}{\eta * P_{\text{ln}}} = \frac{1013 - 439.1}{0.9 * 439.1} = 1.452\,\text{kmol steam/kmol Benzene}$$

$$\frac{m_{\text{W}}}{m_{\text{Benz}}} = 1.452 * \frac{18}{78} = 0.335\ \text{kg steam/kg Benzene}$$

$$n_{\text{W}} = 1.452 * (4.9 - 0.64) = 6.18\ \text{kmol steam}$$

$$m_{\text{W}} = n_{\text{W}} * M_{\text{W}} = 6.18 * 18 = 111.3\ \text{kg steam}$$

Alternative calculation according to Ellerbe [1]:

$$n_{\text{W}} = \left(\frac{P_{\text{tot}}}{\eta * P_{0\text{org}}} - 1\right) * (n_{\text{in}} - n_{\text{out}}) + n_{\text{org}} * \frac{P_{\text{tot}}}{\eta * P_{0\text{org}}} * \ln \frac{n_{\text{in}}}{n_{\text{out}}}\ \ (\text{kmol})$$

$$n_{\text{W}} = \left(\frac{1013}{0.9 * 9443} - 1\right) * (4.9 - 0.64) + 40.9 * \frac{1013*}{0.9 * 9443} * \ln \frac{4.9}{0.64} = 6.17\ \text{kmol steam}$$

$$m_{\text{W}} = 6.17 * 18 = 111.1\ \text{kg steam}$$

7.2.2 *Required Stripping Steam Rate for Two Liquid Phases (Fig. 7.3)*

For two liquid phases the total vapour pressure of both components results from the sum of both of the individual vapour pressures.

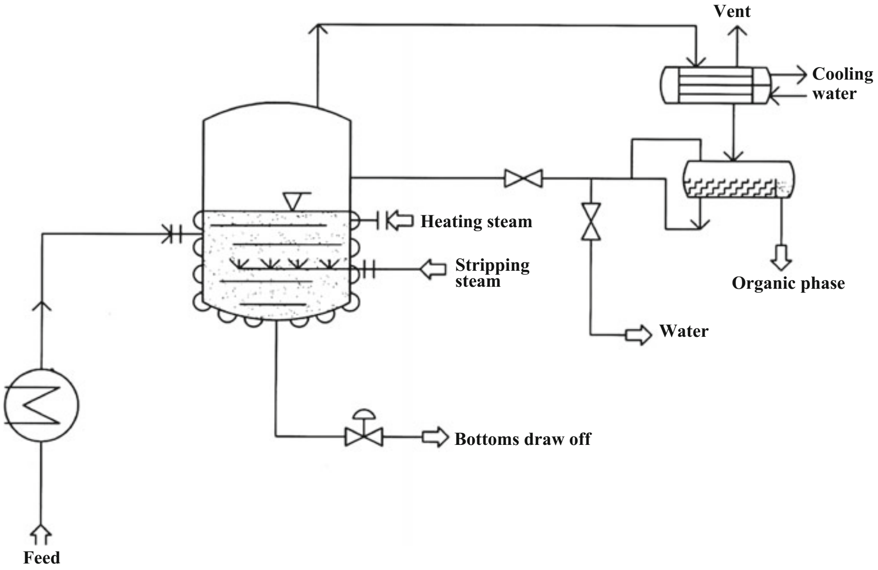


Fig. 7.3 Steam distillation with water in its liquid phase ($F = 1$)

$$P_{\text{tot}} = P_{0\text{org}} + P_{0\text{W}} \ (\text{mbar})$$

Only one degree of freedom F exists.

The pressure is also fixed with the temperature.

Required stripping steam rate considering the stripping efficiency η:

$$n_{\text{W}} = n_{\text{org}} * \frac{P_{0\text{W}}}{P_{0\text{org}}} * \frac{1}{\eta} \ (\text{kmol}) \qquad m_{\text{W}} = m_{\text{org}} * \frac{P_{0\text{W}}}{P_{0\text{org}}} * \frac{M_{\text{W}}}{M_{\text{org}}} * \frac{1}{\eta} \ (\text{kg})$$

$$\frac{m_{\text{org}}}{m_{\text{W}}} = \frac{P_{0\text{org}}}{P_{0\text{W}}} * \frac{M_{\text{org}}}{M_{\text{W}}} * \eta = \frac{P_{0\text{org}}}{P_{\text{tot}} - P_{0\text{org}}} * \frac{M_{\text{org}}}{M_{\text{W}}} * \eta \ (\text{kg/kg})$$

Figure 7.3 shows the flow diagram of steam distillation with water in its liquid phase.

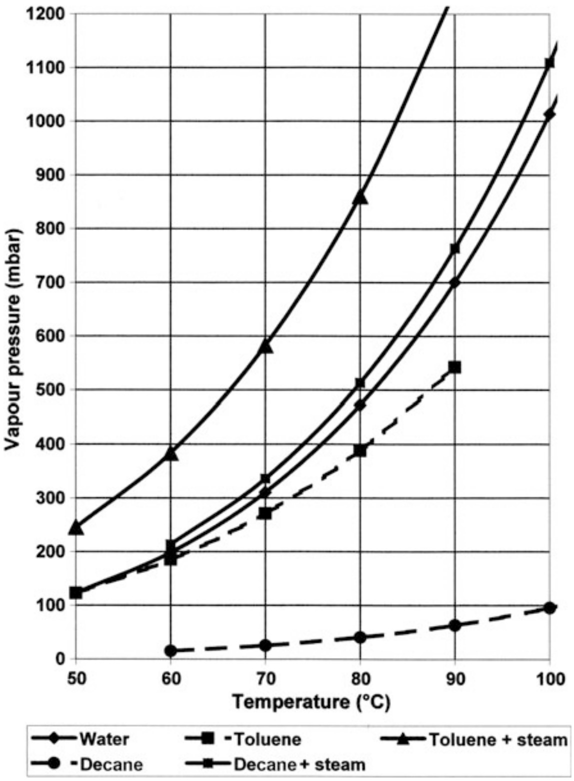
The plant can be operated continuously or batch-wise.

The light organic component is drawn off together with the stripping steam and is liquified in the condenser. The decanted water in the separator is either moved back into the evaporator or drawn off.

Heating to the azeotrope boiling point can occur directly with stripping steam or by indirect heating through the vessel wall or a built-in heating coil.

The choice of temperature determines the pressure, which is the sum of the vapour pressures of the components.

Fig. 7.4 Vapour pressures of toluene and decane in steam distillation



$$P_{\text{tot}} = P_{0\text{org}} + P_{0\text{W}}\ (\text{mbar})$$

This relationship for the steam distillation of toluene and decane is shown in Fig. 7.4.

Example 7.2.2.1: Calculation of the steam distillation of toluene at different temperatures

Temperature (°C)	$P_{0\text{W}}$	$P_{0\text{Tol}}$	P_{tot}	$m_{\text{Tol}}/m_{\text{w}}$	y_{Tol}
	(mbar)	(mbar)	(mbar)	(kg/kg)	(molfr.)
60	198.7	185.3	383.9	4.77	0.48
70	310.9	271.2	582.6	4.46	0.47
80	472.7	388.3	861	4.2	0.45
90	700.4	542.3	1242.7	3.96	0.44

With increasing temperature the toluene yield drops.

Example 7.2.2.2: Steam distillation of turpentine oil at atmospheric pressure and in vacuum

Total pressure P_{tot} = 1010 mbar at 95.5 °C:

Vapour pressure of turpentine $P_{0Turp} = 151$ mbar.
Steam pressure $P_{0W} = 859$ mbar.
Mole weight of turpentine $M_{turp} = 136$.

$$\frac{w_{Turp}}{w_W} = \frac{151}{859} * \frac{136}{18} = 1.33 \text{ kg Turpentine/kg steam}$$

Total pressure P_{tot} = 400 mbar at 72 °C:

$P_{0Turp} = 59.85$ mbar.
$P_{0W} = 339.15$ mbar.

$$\frac{w_{Turp}}{w_W} = \frac{P_{Terp}}{P_W} * \frac{M_{Turp}}{M_W} = \frac{59.85 * 136}{339.15 * 18} = 1.33 \text{ kg Turpentine/kg steam}$$

With water in its liquid phase no turpentine yield advantage is achievable in a vacuum.

Legends:

M_{org} = mole weight of organic component.
M_W = mole weight of water.
m_{org} = molar stream of organic component (kg/h).
m_W = molar stream of water (kg/h).
n_{org} = molar stream of organic component (kmol/h).
n_W = molar stream of water (kmol/h).
n_{in} = molar inlet of organic component (kmol).
n_{out} = molar outlet of organic component (kmol).
P_{tot} = total pressure (mbar).
P_{01} = vapour pressure of component 1 (mbar).
P_{0org} = vapour pressure of organic component (mbar).
P_{0W} = vapour pressure of water (mbar).
P_{org} = partial pressure of organic component (mbar).
P_W = partial pressure of water (mbar).
y_{org} = vapour composition of organic component (molfraction).
y_W = steam composition (molfraction).
η = stripping efficiency ($\eta = 0.7-0.9$).

7.3 Design of the Decanter for the Separation of Two Liquid Phases [2–4]

For the dimensioning of a decanter the settling and the rising velocities of the droplets in the continuous phase, as well as the required resident times for the separation of the two different heavy liquids, are needed.

7.3.1 *Calculation of the Droplet Settling Velocities*

The settling or rising velocity w_S is calculated according to Stokes:

$$w_S = \frac{9.81}{18} * d^2 * \frac{\rho_S - \rho_L}{\eta} \,(\text{m/s})$$

For a droplet size of 0.1 mm = 100 µ:

$$w_S = 5.45 * 10^{-9} * \frac{\rho_S - \rho_L}{\eta} \,(\text{m/s})$$

$$w_S = 327 * 10^{-6} * \frac{\rho_S - \rho_L}{\eta} \,(\text{mm/min})$$

Maximum falling velocity = **250 mm/min**

d = droplet diameter (m).
w_S = falling or rising velocity (m/s or mm/min).
ρ_S = density of the heavy liquid (kg/m^3).
ρ_L = density of the light liquid (kg/m^3).
η = viscosity of the continuous phase (Pa).

Example 7.3.1: Calculation of the falling and rising velocities for 100-µ droplets

$$\rho_S = 986\ \text{kg/m}^3 \quad \eta_S = 0.5\ \text{mPa} \quad \rho_L = 867\ \text{kg/m}^3 \quad \eta_L = 1\ \text{mPa}$$

$$\text{Settling velocity } w_S = 327 * 10^{-6} * \frac{986 - 867}{1 * 10^{-3}} = 38.9\ \text{mm/min}$$

$$\text{Rising velocity } w_S = 327 * 10^{-6} * \frac{986 - 867}{0.5 * 10^{-3}} = 77.8\ \text{mm/min}$$

7.3.2 Dimensioning of the Decanter

For a given phase height h the required settling or rising time t_{ris} of the droplets can be determined:

$$t_{ris} = \frac{h\,(\text{mm})}{w_S\,(\text{mm/min})}\ (\text{min})$$

The residence time t_{res} results from the flow rates F and the settler volume V_S:

$$t_{res} = \frac{V_S\,(\text{m}^3)}{F\,(\text{m}^3/\text{min})} = \frac{A\,(\text{m}^2) * L\,(\text{m})}{F\,(\text{m}^3/\text{min})}\ (\text{min})$$

A = cross sectional area of a phase in the separator (m^2).
F = throughput of a phase (m^3/min).
L = settler length (m).

The resident time should be twice the rising time.

$$t_{res} = 2 * t_{ris}\ (\text{min})$$

The maximum allowable settling height is h_{max}:

$$h_{max} = \frac{A * L * w_S}{2 * F}\ (\text{mm})$$

The required decanter length L for a desired residence time t_{res} results as follows:

$$L = \frac{F(\text{m}^3/\text{min}) * t_{res}}{A}\ (\text{m})$$

The rule of thumb for the first estimation of the decanter diameter D:

A separator's diameter for an estimated residence time t_{res} is determined.
A good estimate for the residence time t_{res} = 10 min.

$$D = \left(\frac{4}{\pi} * \frac{t_{res} * F_1}{r * y}\right)^{1/3}\ (\text{m})$$

F_1 = throughput rate of the larger phase (m^3/min).
$r = L/D$ = quotient from length and diameter of the decanter, mostly $r = 3.4$.
$y = F_1/F_{tot}$ = quotient from the larger phase/total rate.

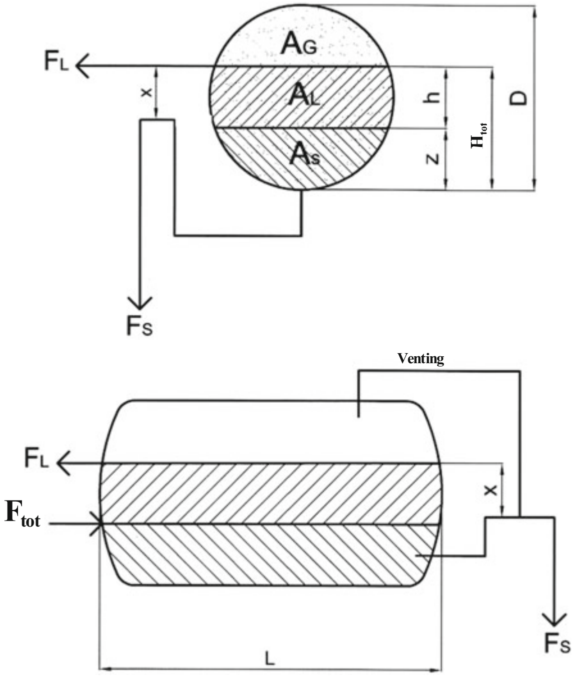


Fig. 7.5 Decanter with designations

A_G = circle area for the gas (m^2).
A_L = circle area for the light phase (m^2).
A_S = circle area for the heavy phase (m^2).
D = diameter of the horizontal decanter (m).
F_{tot} = total feed rate of both phases (m^3/min).
F_L = throughput rate of the light phase (m^3/min).
F_S = throughput rate of the heavy phase (m^3/min).
H_{tot} = total liquid height in the decanter (mm).
h = layer height of the light liquid (mm).
L = separator length (m).
x = height difference between the nozzles for both phases (mm).
z = layer height of the heavy liquid (mm).

Example 7.3.2.1: Estimation of the decanter dimensions (Fig. 7.5)

$$F_L = 21.56\,\mathrm{m^3/h} \qquad F_L = F_1 \qquad r = 3.4 \qquad t_{res} = 10\,\mathrm{min}$$

$$F_S = 8.15\,\mathrm{m^3/h}$$

$$F_{tot} = 30.41\,\mathrm{m^3/h}$$

$$y = \frac{21.56}{30.41} = 0.7$$

$$D = \left(1.27 * \frac{t_{\text{res}} * F_1}{r * y}\right)^{1/3} = \left(1.27 * \frac{10 * 21.56/60}{3.4 * 0.7}\right)^{!/3} = 1.24\,\text{m}$$

$$L = r * D = 3.4 * 1.24 = 4.21\,\text{m}$$

Example 7.3.2.2: Decanter design

$$w_{\text{settle}} = 38.9\,\text{mm/min} \qquad w_{\text{rising}} = 77.8\,\text{mm/min} \qquad \text{Estimate}: t_{\text{res}} = 15\,\text{min}$$

$$F_{\text{L}} = 1\,\text{m}^3/\text{h} \qquad F_{\text{S}} = 2\,\text{m}^3/\text{h} \qquad F_{\text{tot}} = 3\,\text{m}^3/\text{h} \qquad \text{y} = 0.666$$

$$\text{Estimate of diameter}\, D = \left(1.27 * \frac{15 * 2/60}{3.4 * 0.666}\right)^{1/3} = 0.65\,\text{m}$$

Chosen separator diameter $D = 0.8\,\text{m}$

Light phase $F_{\text{L}} = 1\,\text{m}^3/\text{h} = 0.0166\,\text{m}^3/\text{min}$ $\quad S_{\text{H}}/D = 0.8$ $\quad S_{\text{H}} =$ segmental height

$S_{\text{H}} = 0.8 * 0.8 = 0.64\,\text{m}$ $\quad A_{\text{L}} = 0.18\,\text{m}^2$

Heavy phase $F_{\text{S}} = 2\ \text{m}^3/\text{h} = 0.0333\ \text{m}^3/\text{min}$ $\quad S_{\text{H}}/D = 0.5$

$S_{\text{H}} = 0.5 * 0.8 = 0.4\ \text{m}$ $\quad A_{\text{S}} = 0.25\,\text{m}^2$

Calculation of the settling and rising times:

$$t_{\text{settl}} = \frac{640 - 400}{38.9} = 6.17\,\text{min} \qquad t_{\text{rising}} = \frac{400}{77.8} = 5.14\,\text{min}$$

Required **residence time**:

t_{res} = 12 min for the light phase.
t_{res} = 10 min for the heavy phase.

Calculation of the required **decanter length *L*** for t_{res} = 12 min or 10 min:

$$L_{\text{L}} = \frac{t_{\text{res}} * F}{A} = \frac{12 * 0.0166}{0.18} = 1.1\,\text{m} \qquad L_{\text{S}} = \frac{10 * 0.0333}{0.25} = 1.3\,\text{m}$$

Cross-check calculation for the chosen length L = 1.5 m:

$$t_{\text{res}} = \frac{A_{\text{L}} * L}{F_{\text{L}}} = \frac{0.18 * 1.5}{0.0166} = 16\,\text{min} \qquad h_{\max} = \frac{0.18 * 1.5 * 38.9}{2 * 0.0166} = 316\,\text{mm} > 240\,\text{mm}\ \text{for settling}$$

$$t_{\text{res}} = \frac{A_S * L}{F_{\text{S}}} = \frac{0.25 * 1.5}{0.0333} = 11.3\,\text{min} \qquad h_{\max} = \frac{0.25 * 1.5 * 77.8}{2 * 0.0333} = 438\,\text{mm} > 400\,\text{mm}\ \text{for rising}$$

The following table can be used for quick determination of the circle diameter areas A_L, A_S, and A_G depending on the quotient: segmental height S_H/diameter D.

Circle section area $A = C * D^2$

S_H/D	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
C	0.0409	0.1118	0.1982	0.2934	0.393	0.492	0.587	0.674	0.745

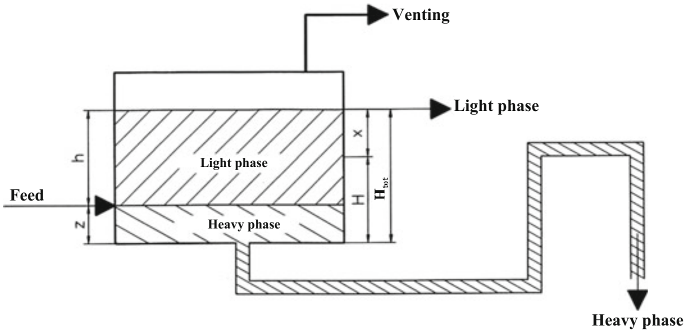
Example 7.3.2.3: Calculation of the cross sectional areas in the decanter for D = 0.8 m

$$S_H/D = 0.5 \quad A_{0.5} = A_S = C * D^2 = 0.393 * 0.8^2 = 0.25\ \text{m}^2$$

$$S_H/D = 0.8 \quad A_{0.8} = C * D^2 = 0.674 * 0.8^2 = 0.43\ \text{m}^2$$

$$A_L = A_{0.8} - A_S = 0.43 - 0.25 = 0.18\ \text{m}^2$$

7.3.3 *Setting of the Phase Height in the Decanter*



The height of the **light phase *h*** and the **heavy phase *z*** in the decanter is set with the difference of the draw heights x for the light and the heavy liquid, or with the **draw height *H* of the heavy phase.**

Calculations:

$$\text{Layer height of the light phase } h = \frac{x}{1 - \frac{\rho_L}{\rho_S}}\ (\text{mm})$$

$$\text{Difference of the draw heights } x = h * \left(1 - \frac{\rho_L}{\rho_S}\right)\ (\text{mm})$$

$$\text{Layer height of the heavy phase } z = \frac{H * \rho_S - h * \rho_L}{\rho_S}\ (\text{mm})$$

$$\text{Draw height of the heavy phase}\, H = \frac{h * (\rho_L - \rho_S) + H_{tot} * \rho_S}{\rho_S}$$

$$\text{Draw height of the heavy phase}\, H = h * \frac{\rho_L}{\rho_S} + z\ (\text{mm})$$

$$H_{tot} = H + x = h + z\ (\text{mm})$$

Example 7.3.3.1: Calculation of the draw height *H* for *h* = 240 mm and *z* = 400 mm

$$H_{tot} = 240 + 400 = 640\,\text{mm} \qquad \rho_S = 986\,\text{kg/m}^3 \qquad \rho_L = 867\ \text{kg/m}^3$$

$$H = \frac{240 * (867 - 986) + 640 * 986}{986} = 611\ \text{mm}$$

$$H = 240 * \frac{867}{986} + 400 = 611\ \text{mm}$$

$$x = 240 * \left(1 - \frac{867}{986}\right) = 29\ \text{mm}$$

$$H_{tos} = H + x = 611 + 29 = 640 = h + z = 240 + 400 = 640\,\text{mm}$$

$$h = \frac{29}{1 - \frac{867}{986}} = 240\,\text{mm}$$

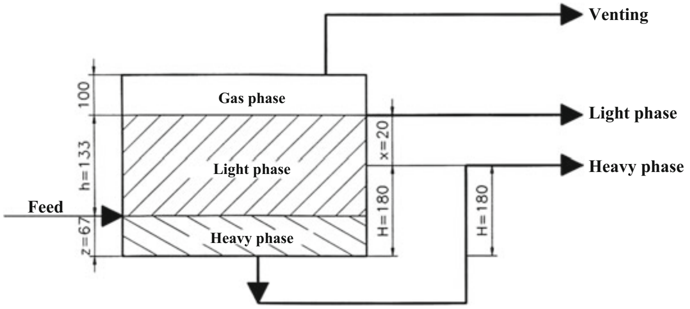
$$z = \frac{611 * 986 - 240 * 867}{986} = 400\,\text{mm}$$

Example 7.3.3.2: Calculation of the layer heights *h* and *z* and the total height H_{tot}

$$H = 180\,\text{mm} \qquad x = 20\,\text{mm} \qquad \rho_S = 1000\,\text{kg/m}^3 \qquad \rho_L = 850\,\text{kg/m}^3$$

$$h = \frac{20}{1 - \frac{850}{1000}} = 133\,\text{mm} \qquad z = \frac{180 * 1000 - 133 * 850}{1000} = 67\ \text{mm}$$

$$H_{tot} = H + x = 180 + 20 = 200 = z + h = 67 + 133 = 200\,\text{mm}$$



7.4 Stripping Steam Distributor Design [5]

A distributor for stripping steam or stripping gas must be designed for compressible flow, i.e. using the flow function ψ.

The following calculation equations are valid [6]:

$$\text{Throughput rate } G = \alpha * \psi * A * \sqrt{2 * P_1 * \rho_1}\ (\text{kg/s})$$

$$\text{Adiabatic flow function } \psi = \sqrt{\frac{\kappa}{\kappa - 1} * \left[\left(\frac{P_2}{P_1}\right)^{2/\kappa} - \left(\frac{P_2}{P_1}\right)^{\frac{\kappa+1}{\kappa}}\right]}$$

$$\text{Required cross section area } A = \frac{G}{\alpha * \psi * \sqrt{2 * P_1 * \rho_1}}\ (\text{m}^2)$$

$$\text{Hole diameter } d = 1000 * \sqrt{\frac{4 * A}{n * \pi}}\ (\text{mm})$$

A = flow cross sectional area (m^2).
G = throughput rate (kg/s).
n = number of holes.
P_1 = static inlet pressure in the distributor (Pa).
P_2 = static pressure outlet (Pa).
α = resistance coefficient of the hole = 0.61.
κ = isentropic exponent.
ρ_1 = inlet density in the distributor (kg/m^3).

For a reasonably uniform gas or steam distribution over the total cross section it is important that the static pressure P_1 in the distributor pipe, before the holes, is kept unchanged as much as possible. With decreasing pressure P_1 the gas or steam throughput decreases at equal hole diameters.

The static pressure in the distributor pipe changes because of the pressure drop in the pipe and the variation of the dynamic pressure due to the velocity reduction.

$$P_1 = P_{\text{in}} - \Delta P_{\text{frict}} - \Delta p_{\text{dyn}}\ (\text{Pa})$$

P_{in} = inlet pressure in the distributor pipe (Pa).
ΔP_{frict} = friction pressure loss in the distributor pipe (Pa).
Δp_{dyn} = variation of the dynamic pressure with decreasing flow velocity (Pa).

By choosing a larger distributor pipe diameter with a low flow velocity the inlet pressure P_1 can widely be held constant.

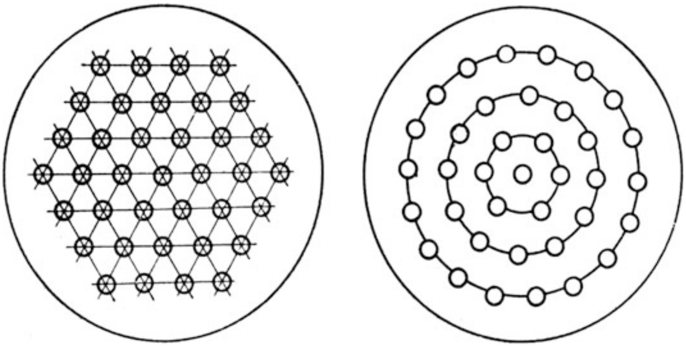


Fig. 7.6 Sieve trays with hexagonal and concentric pitches

Upon reaching the critical pressure ratio P_2/P_1 the sound velocity persists in the holes and the adiabatic flow function ψ reaches its maximum.

$$\kappa = 1.4 \quad P_2/P_{1\text{krit}} = 0.528 \; \psi_{\max} = 0.484$$
$$\kappa = 1.3 \quad P_2/P_{1\text{krit}} = 0.546 \; \psi_{\max} = 0.473$$

The stripping steam should be distributed over the cross section of the evaporator as evenly as possible, for instance using a circular ring or an Archimedes spiral or sieve tray.

The holes can be arranged as a hexagon or as circular rings (Fig. 7.6).

For the calculation of the pitch T and the total number of holes n the following equations apply:

Hexagonal pattern:

$$T = \frac{R_n}{\sqrt{\frac{n}{3}+0.25}-0.5}\ (\text{mm}) \quad n = 3 * \frac{R_n^2}{T^2}$$
$$R_\text{n} = \text{net radius without border flange (mm)}$$

Circular pattern:

$$T = \sqrt{\frac{3.63 * R_n^2}{n}}\ (\text{mm}) \qquad n = 3.63 * \frac{R_n^2}{T^2}$$

With the circular pattern 21% more holes can be accommodated.

Example 7.4.1: Calculation of the pitch and number of holes

Radius $R = 0.4\,\text{m}$ Border flange $S = 10\,\text{mm}$ $R_n = 400 - 10 = 390\,\text{mm}$ $n = 100$

Circular pattern:

$$T = \sqrt{\frac{3.63 * 390^2}{100}} = 74.3\,\text{mm} \qquad n = \frac{3.63 * 390^2}{74.3^2} = 100$$

Example 7.4.2: Stripping air distributor design

$P_2 = 1\,\text{bar} \qquad \alpha = 0.61$

Air density $\rho_1 = 1.428\ \text{kg/m}^3$ at 20 °C and 1.2 bar $\qquad \kappa = 1.4$

Gas rate : $100\,\text{m}^3/\text{h} = 142.8\,\text{kg/h} \quad G = 0.03967\,\text{kg/s} \qquad \text{Holes}\,n = 10$

(a) $\boldsymbol{P_1 = 1.2\,\text{bar} \qquad \rho_1 = 1.428\,\text{kg/m}^3}$

$$\psi = \sqrt{\frac{1.4}{1.4-1} * \left[\left(\frac{1}{1.2}\right)^{2/1.4} - \left(\frac{1}{1.2}\right)^{2.4/1.4}\right]} = 0.37$$

$$A = \frac{0.03967}{0.61 * 0.37 * \sqrt{2 * 1.2 * 10^5 * 1.428}} = 0.0003\,\text{m}^2$$

$$d = 1000 * \sqrt{\frac{4 * 0.0003}{10 * \pi}} = 6.18\ \text{mm}$$

(b) $\boldsymbol{P_1 = 1.5\,\text{bar} \qquad \rho_1 = 1.785\,\text{kg/m}^3}$

$$\psi = \sqrt{\frac{1.4}{1.4-1} * \left[\left(\frac{1}{1.5}\right)^{2/1.4} - \left(\frac{1}{1.5}\right)^{2.4/1.4}\right]} = 0.463$$

$$A = \frac{0.03967}{0.61 * 0.463 * \sqrt{2 * 1.5 * 10^5 * 1.785}} = 0.000192\,\text{m}^2$$

$$d = 1000 * \sqrt{\frac{4 * 0.000192}{10 * \pi}} = 4.94\ \text{mm}$$

c) $\boldsymbol{P_1 = 2\,\text{bar} \qquad \rho_1 = 2.38\,\text{kg/m}^3}$

$$\psi = \sqrt{\frac{1.4}{1.4-1} * \left[\left(\frac{1}{2}\right)^{2/1.4} - \left(\frac{1}{2}\right)^{2.4/1.4}\right]} = 0.484$$

$$A = \frac{0.03967}{0.61 * 0.484 * \sqrt{2 * 2 * 10^5 * 2.38}} = 0.000138\,\mathrm{m}^2$$

$$d = 1000 * \sqrt{\frac{4 * 0.000138}{10 * \pi}} = 4.19\,\mathrm{mm}$$

The required hole diameter for a specific air rate changes with the variation of the inlet pressure P_1.

7.5 Design Example

Steam distillation for dirty toluene at 84 °C:

Vapour pressure of toluene $P_{0\mathrm{Tol}} = 444\,\mathrm{mbar}$ $M_{\mathrm{Tol}} = 92.1$ $m_{\mathrm{Tol}} = 450\,\mathrm{kg}$

$$P_{\mathrm{W}} = 566\,\mathrm{mbar} \qquad P_{\mathrm{tot}} = 444 + 566 = 1.010\,\mathrm{mbar} \qquad \eta = 0.75$$

Boiling point check:

$$\sum y = \frac{444}{1010} + \frac{566}{1010} = 1$$

7.5.1 *Required Stripping Steam Rate with Efficiency η = 0.75*

$$m_{\mathrm{W}} = m_{\mathrm{Tol}} * \frac{P_{\mathrm{W}} * M_{\mathrm{W}}}{P_{\mathrm{Tol}} * M_{\mathrm{Tol}}} * \frac{1}{\eta} = 450 * \frac{566 * 18}{444 * 92.1} * \frac{1}{0.75} = 149.5 \text{ kg steam}$$

Chosen steam rate: 150 kg.

Distillate mass balance:

	Quantity (kg/h)	Weight%	mol%
Toluene	450	75	37
Steam	150	25	63
Total	600	100	100

Average mole weight of the vapour $M_{\mathrm{m}} = 0.37 * 92.1 + 0.63 * 18 = 45.4$.

$$\text{Vapor density } \rho_{\mathrm{D}} = \frac{45.4}{22.4} * \frac{1010}{1013} * \frac{273}{273 + 84} = 1.54\,\mathrm{kg/m^3}$$

$$\text{Vapor volume } V_{\mathrm{D}} = \frac{600}{1.54} = 390\,\mathrm{m^3/h}$$

7.5.2 Required Steam for Heating from 24 to 84°C and Evaporating the Toluene

Specific heat capacity $c_{\mathrm{Tol}} = 0.58\,\mathrm{Wh/kg\,K}$ Toluene rate $m_{\mathrm{Tol}} = 450\,\mathrm{kg/h}$

Latent heat $r_{\mathrm{Tol}} = 100.9\,\mathrm{Wh/kg}$

$Q_{\mathrm{tot}} = Q_{\mathrm{heating}} + Q_{\mathrm{evapor}} = m_{\mathrm{Tol}} * (c * \Delta t + r) = 450 * (0.58 * 60 + 100.9) = 61{,}065\ \mathrm{W}$

$\mathrm{Q}_{\mathrm{heating}} = 15.660\ \mathrm{W}$ $\mathrm{Q}_{\mathrm{evapor}} = 45.405\ \mathrm{W}$

Heating steam : 4 bar, 143.6 °C Latent heat $r_{\mathrm{W}} = 592.5\,\mathrm{Wh/kg}$

Vapour enthalpy $i_{\mathrm{WD}} = 760.5\,\mathrm{Wh/kg}$

Required steam rate for indirect heating and evaporating over the vessel wall:

$$m_{\mathrm{steam}} = \frac{61{,}065}{592.5} = 103\,\mathrm{kg\ steam}$$

Theoretically, the sensible heat of the stripping steam that is fed with the 150 kg stripping steam can be subtracted from the heating steam requirement.

In the adiabatic flash from 4 bar to 1 bar the steam is cooled from 143.6 to 130 °C.

Sensible heat introduced with the stripping steam:

$$\mathrm{Q}_{\mathrm{sens\ steam}} = 150 * 0.545 * (130 - 84) = 3760\,\mathrm{W}$$

$$\text{Saving of steam } \Delta m_{\mathrm{Wsteam}} = \frac{3760}{592.5} = 6.3\,\mathrm{kg\ steam}$$

Total steam requirement $m_{\mathrm{steam}} = 103 - 6.3 = 96.7$ kg steam

Required steam rate for direct heating with condensing steam:

$$m_{\mathrm{steam}} = \frac{Q_{\mathrm{tot}}}{i_{\mathrm{steam}} - i_{\mathrm{Water}}} = \frac{61{,}065}{760.5 - 97.4} = 92.1\,\mathrm{kg\ steam}$$

Heating with direct steam requires a little less steam because the condensate is subcooled to 84°C.

Due to the problems with water in the residue (i.e., an additional separator and waste water treatment being required) indirect heating should be adopted.

7.5.3 Evaporator Design

Required heating area A for an overall heat transfer coefficient of $U = 250\ \mathrm{W/m^2K}$.

Due to fouling, a small overall heat transfer coefficient is chosen.

$$A = \frac{Q_{\mathrm{tot}}}{U * \mathrm{LMTD}} = \frac{61{,}065}{250 * 85.34} = 2.86\,\mathrm{m}^2$$

Chosen: vessel with a nominal content of 1 m^3, D = 1.2 m, H = 1.55 m, heating height H_{H} = 0.5 m.

Heating area at the shell F_{M} = 1.87 m^2
Heating area at the bottom F_{B} = 1.3 m^2
Total heating area A = 1.87 + 1.3 = 3.17 m^2

7.5.4 Check on the Entrainment of Droplets

Flow velocity w of the vapour for D = 1.2 m:

$$w = \frac{390}{3600 * 1.2^2 * 0.785} = 0.096\,\mathrm{m/s}$$

Allowable flow velocity w_{allow} in a vertical droplet separator:

$$w_{\mathrm{allow}} = 0.04 * \sqrt{\frac{\rho_{\mathrm{FL}}}{\rho_{\mathrm{D}}} - 1} = 0.04 * \sqrt{\frac{813}{1.54} - 1} = 0.92\,\mathrm{m/s}$$

Conclusion: the determining factor for deciding on the evaporator diameter is the required heating area.

Chosen: D = 1.2 m.

7.5.5 Condenser Design for 450 Kg/H Toluene and 150 Kg/H Stripping Steam

Heat load:

$$Q_{\mathrm{con}} = 450 * 100.9 + 150 * (760.5 - 97.4) = 144{,}870\,\mathrm{W}$$

Dew point T_{T} = 87.5°C
Bubble point T_{S} = 84°C
LMTD = 54.5°C
Overall heat transfer coefficient U = 1000 $\mathrm{W/m^2K}$
Cooling water 25–35 °C

Calculation of the required heat exchanger area A:

$$A = \frac{Q_{\text{cond}}}{U * \text{LMTD}} = \frac{144{,}870}{1000 * 54.5} = 2.7\,\text{m}^2$$

Chosen: A = 3.7 m^2 with 12 tubes 25 × 2, 4 m long, in triangular pitch 32 mm, shell DN 150

Required cooling water rate:

$$G_{\text{W}} = \frac{Q_{\text{con}}}{c_{\text{W}} * (35 - 25)} = \frac{144{,}870}{1.16 * 10} = 12{,}488\,\text{kg/h}$$

7.5.6 Decanter Design

$F_{\text{L}} = 450\,\text{kg/h} = 0.554\,\text{m}^3/\text{h} = 0.0092\,\text{m}^3/\text{min}$ toluene $\rho_{\text{L}} = 813\,\text{kg/m}^3$ $\eta = 0.207\,\text{mPa}$

$F_{\text{S}} = 150\,\text{kg/h} = 0.152\,\text{m}^3/\text{h} = 0.0025\,\text{m}^3/\text{min}$ water $\rho_{\text{S}} = 986\,\text{kg/m}^3$ $\eta = 0.325\,\text{mPa}$

Calculation of the settling velocity of the water droplets in toluene:

$$w_{\text{settl}} = 327 * \frac{986 - 813}{0.207 * 10^{-3}} = 273\,\text{mm/min}$$

Calculation of the rising velocity of toluene droplets in the water phase:

$$w_{\text{ris}} = 327 * \frac{986 - 813}{0.325 * 10^{-3}} = 174\,\text{mm/min}$$

Chosen: w_{ris} = 250 mm/min

Estimate of the decanter dimensions:

$$D = \left(1.27 * \frac{10 * 0.0092}{3.4 * 0.786}\right)^{1/3} = 0.35\,\text{m} \qquad L = 3.4 * 0.35 = 1.2\,\text{m}$$

Chosen:

L = 1 m
D = 400 mm

Calculation of the layer heights in the decanter:

Chosen draw height of the heavy liquid H = 300 mm, x = 30 mm

$$h = \frac{x}{1 - \frac{\rho_L}{\rho_S}} = \frac{30}{1 - \frac{813}{986}} = 171\,\text{mm}$$

$$H_{\text{tot}} = H + x = 300 + 30 = 330\,\text{mm}$$

$$z = \frac{H * \rho_S - h * \rho_L}{\rho_S} = \frac{300 * 986 - 171 * 813}{986} = 159\,\text{mm}$$

$$H_{\text{tot}} = h + z = 171 + 159 = 330\,\text{mm}$$

Calculation of the circular sectional areas A_S and A_L:

$$\frac{z}{D} = \frac{159}{400} = 0.4 \qquad C = 0.2934 \qquad A_S = 0.2934 * 0.4^2 = 0.0469\,\text{m}^2$$

$$\frac{H_{\text{tot}}}{D} = \frac{330}{400} = 0.8 \quad C = 0.674 \qquad A_L = (0.674 - 0.2934) * 0.4^2 = 0.0609\,\text{m}^2$$

Cross-check of the residence times t_{res} and the settling or rising times t_{settl} and t_{ris}:

$$\text{Water}: t_{\text{res}} = \frac{A_S * L}{F_S} = \frac{0.0469 * 1.0}{0.0025} = 18.8\,\text{min} \qquad t_{\text{settls}} = \frac{h}{w_{\text{settl}}} = \frac{171}{273} = 0.62\,\text{min}$$

$$\text{Toluene}: t_{\text{res}} = \frac{A_L * L}{F_L} = \frac{0.0609 * 1.0}{0.0092} = 6.6\,\text{min} \qquad t_{\text{ris}} = \frac{z}{w_{\text{ris}}} = \frac{159}{250} = 0.6\,\text{min}$$

7.5.7 Stripping Steam Distributor Design

Steam condition : 4 bar, 143.6 °C Steam density $\rho = 2.16\,\text{kg/m}^3$ $\kappa = 1.3$
$G = 150\,\text{kg/h} = 0.0417\,\text{kg/s}$ $P_1 = 4\,\text{bar}$ $P_2 = 1\,\text{bar}$ $n = 20\,\text{holes}$
$P_2/P_1 = 1/4 = 0.25 \rightarrow$ super critical pressure ratio with $\psi_{\max} = 0.473$

$$A = \frac{150/3600}{0.61 * 0.473 * \sqrt{2 * 4 * 10^5 * 2.16}} = 0.00011\,\text{m}^2$$

$$d = 1000 * \sqrt{\frac{4 * 0.00011}{20 * \pi}} = 2.6\,\text{mm}$$

Chosen: 20 holes each being 4 mm diameter ➔ $A = 0.00251\ \text{m}^2$
Calculation of the maximum possible throughput $G_{\max}$:

$$G_{\max} = 0.61 * 0.473 * 0.000251 * \sqrt{2 * 4 * 10^5 * 2.16} = 0.0952\,\text{kg/s} = 342.7\,\text{kg/h}$$

Construction: distributor ring DN 50 with 1 m diameter and length L = 3.14 m
Having 20 holes each with a 4 mm diameter; pitch distance = 157 mm
The steam rate is measured and control fed to the evaporator.

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Chapter 8
Absorption and Stripping Columns

8.1 Equilibria for the Design of Absorption and Desorption Columns

In absorption and desorption the potential for the mass transfer is determined by the deviation from the phase equilibrium (Figs. 8.1 and 8.2).

Knowledge of the solution equilibrium in the physical absorption and the chemical equilibrium in chemical washing is a prerequisite for the design of technical absorption and desorption plants.

8.1.1 Physical Equilibrium [1–3]

In the following it is shown how to calculate the equilibrium between the vapour or gas concentration of a component y_i and the liquid composition x_i.

In the **absorption, the composition y_i of a component in the gas stream is to be reduced.**

$$y_i = \frac{H}{P_{\text{tot}}} * x_i = \frac{\gamma * p_{0\text{i}} * x_i}{P_{\text{tot}}} = \frac{p_i}{P_{\text{tot}}} = K * x_i \tag{8.1}$$

H = Henry-coefficient
γ = activity coefficient
x_i = gas composition in the washing liquid (molfraction)
y_i = gas composition in the gas mixture to be cleaned (molfraction)
P_{tot} = total pressure (bar)
$p_{0\text{i}}$ = vapour pressure of the component to be absorbed (bar)
p_i = partial pressure of the component to be absorbed (bar)
K = equilibrium constant = y/x

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_8

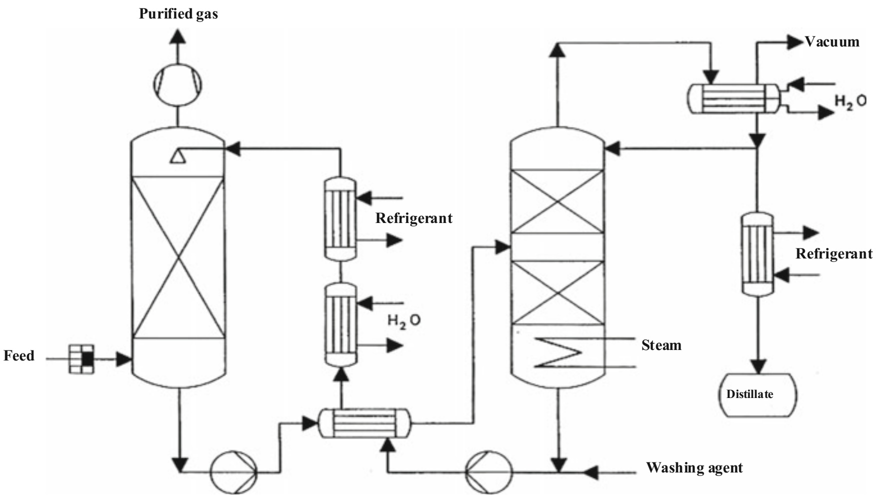


Fig. 8.1 Flow diagram of an absorption–desorption plant

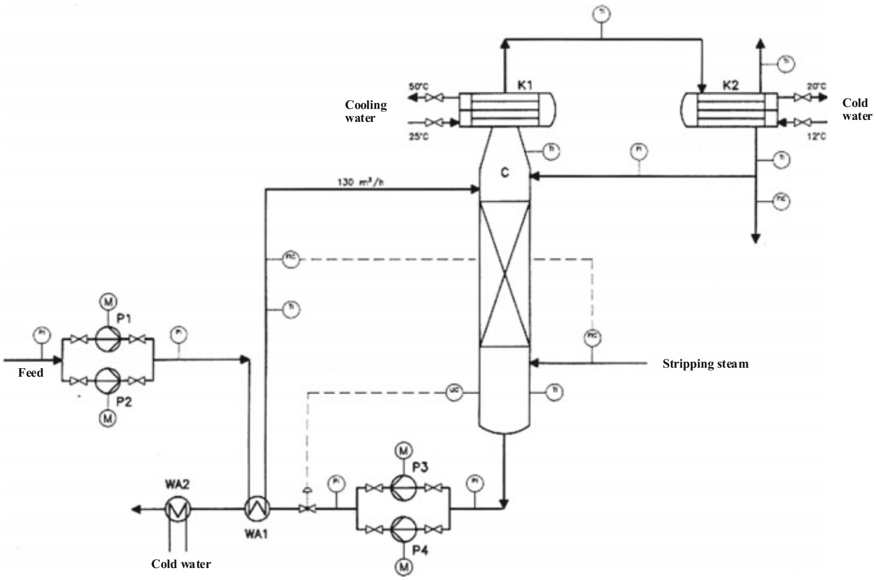


Fig. 8.2 Flow diagram of an SO_2–stripper

From Eq. (8.1) it can be derived that the outlet loading y_i reduces after an absorption:

with low values of H and γ: ➔ selection of the washing agent and the washing temperature

at low liquid concentrations x_i: ➔ good desorption of the absorbent and high washing fluid rates

with increasing total pressure P_{tot}: ➔ absorption at high pressure

with low vapour pressures $p_{0\text{i}}$ ➔ low absorbent temperature

The absorptive is only absorbed by the washing liquid if the partial pressure in the gas is larger than the partial pressure in the washing liquid.

$$y_i * P_{\text{tot}} > H * x_i \text{ or } > \gamma * p_{0\text{i}} * x_i$$

In desorption the liquid composition x_i of a component in the liquid is to be reduced.

$$x_i = \frac{y_i * P_{\text{tot}}}{H} = \frac{y_i * P_{\text{tot}}}{\gamma * p_{0\text{i}}}$$

y_i = composition y_i of the component in the stripping gas (molfraction)

The desorption becomes greater and the rest loading x_i in the liquid becomes smaller:

with greater values for H and γ: ➔ absorption media and high temperature in stripping

at low y_i values in the stripping gas: ➔ stripping gas cleaning and high flow rate

with decreasing total pressure P_{tot}: ➔ desorption in vacuum

with increasing vapour pressure $p_{0\text{i}}$: ➔ higher temperatures with stripping.

In exhaust air purification based on the values given in the Technical Guidelines, i.e., TA Luft in Germany, the concentration x_i in the washing fluid should be reduced to approximately 50% of the equilibrium value of the permitted outlet concentration.

In boiling washing fluids, for instance water, the good end purification to low x_i values by distillation is no problem. However, with high boiling organic wash media which are not boiling, the absorbed light boiling components must be stripped out with steam or nitrogen (Fig. 8.3).

This creates new problems: contamination of the solvent or emissions within the stripping gas.

Requirements of absorbents:

High capacity and selectivity: ➔ low γ and mole weight M.

Low vapour pressure and low viscosity (<5 mPas).

No problem with regards to corrosion, ex-protection, and MAK-value.

Easy to regenerate, i.e., to desorb.

For absorption the Henry coefficient *H*, or the activity coefficient γ, should be small.

For desorption the Henry coefficient *H*, or the activity coefficient γ, should be large.

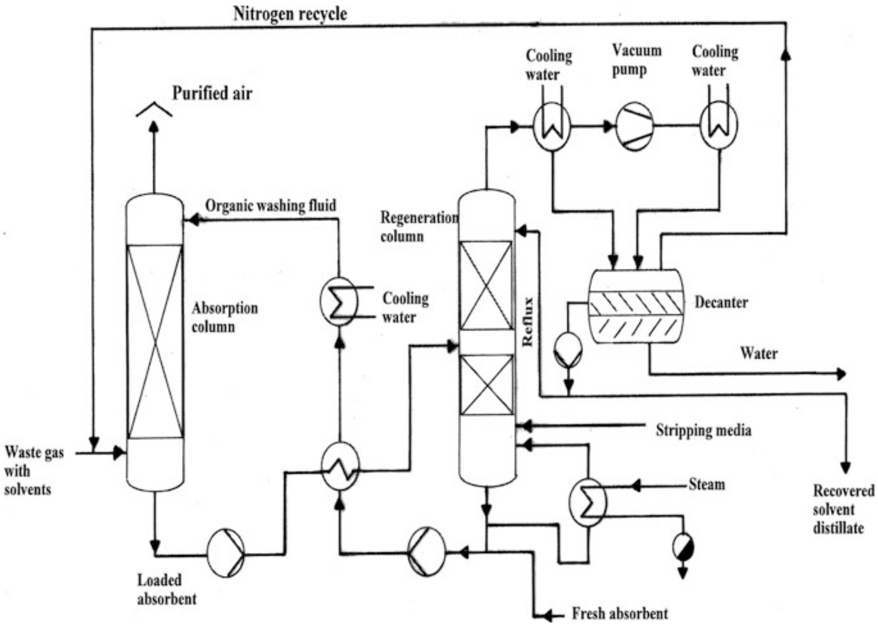


Fig. 8.3 Absorption of solvents with high boiling organic absorbents

8.1.1.1 Equilibrium Calculation with the Henry Coefficient H for Super-Critical Gases

The Henry coefficient is dependent on the material system and on the temperature and can be found in data tables.

Henry's law should only be used in diluted solutions with $x_i < 0.02$ applications.

Equilibrium calculation using the Henry coefficient (Table 8.1):

Table 8.1 Henry constants for different gases in water

T	N_2	CO_2	H_2S	SO_2	NH_3
(°C)	(bar)	(bar)	(bar)	(bar)	(bar)
10	64,700	1090	370	15.5	0.45
20	75,500	1440	496	24.4	0.77
30	87,100	1860	652	37.5	1.27
40	99,600	2360	843	56	2

$$y_i = \frac{x_i * H_i}{P_{\text{tot}}} = K * x_i \qquad K = \frac{y_i}{x_i} = \frac{H_i}{P_{\text{tot}}} = \frac{\gamma_\infty * p_{0i}}{P_{\text{tot}}}$$

Example 8.1.1: Equilibrium of CO_2 in water at 25 °C and P_{tot} = 1 bar

$$H = 1650\,\text{bar} \qquad x_{\text{CO2}} = 0.586 * 10^{-4}\text{molfr.}\,\text{CO}_2$$

$$y_{\text{CO2}} = 1650 * 0.586 * 10^{-4} = 0.0967\,\text{molfr.}\,\text{CO}_2 = 9.67\,\text{vol\%}\,\text{CO}_2$$

For the calculation of the equilibrium line several values of y_i and x_i are necessary.

$$y_i = K_i * x_i = \frac{H_i}{P_{\text{tot}}} * x_i = \frac{1650}{1} * x_i = 1650 * x_i$$

x_i	0.1*10^{-4}	0.2*10^{-4}	0.3*10^{-4}	0.4*10^{-4}	0.5*10^{-4}
y_i	0.0165	0.033	0.049	0.066	0.0825

8.1.1.2 Equilibrium Calculation for Ideal Condensable Vapour with γ = 1

In this case Raoult's law is valid.

$$y_i = \frac{x_i * P_{0\text{i}}}{P_{\text{tot}}} = K * x_i \qquad K = \frac{y_i}{x_i} = \frac{p_{0\text{i}}}{P_{\text{tot}}}$$

Example 8.1.2: Oil wash for dichloromethane at 50 °C and P_{tot} = 1 bar and at P_{tot} = 5 bar

$$\text{Vapour pressure of dichloromethane at } 50\,^\circ\text{C}: \quad p_{0i} = 1417\,\text{mbar}$$

$$M_{\text{DC}} = 84.9 \quad M_{\text{Ö}}\text{L} = 360 \quad M_{\text{Luft}} = 29 \quad x_{\text{DC}} = 0.08\,\text{molfr.}$$

Equilibrium at a total pressure of P_{tot} = 1 bar:

$$K = \frac{p_{0\text{i}}}{P_{\text{tot}}} = \frac{1417}{1000} = 1.4 \qquad y_i = 1.4 * x_i$$

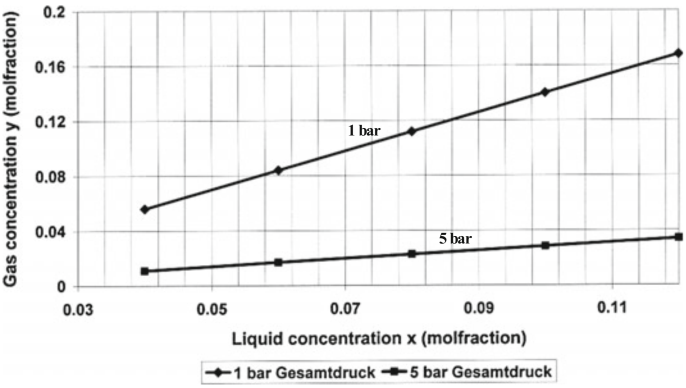


Fig. 8.4 Equilibrium lines for dichloromethane in wash oil at 1 bar and at 5 bar

x_i	0.04	0.06	0.08	0.1	0.12
y_i	0.056	0.084	0.112	0.14	0.168

Equilibrium at a total pressure of P_{tot} = 5 bar:

$$K = \frac{p_{0i}}{P_{tot}} = \frac{1417}{5 * 1000} = 0.283$$

Calculated equilibria at 5 bar:

x_i	0.04	0.06	0.08	0.1	0.12
y_i	0.011	0.017	0.0226	0.0283	0.034

In Fig. 8.4 both of the equilibrium lines at 1 and 5 bar are given.

It can be clearly seen that using a pressure wash at 5 bar the dichloromethane concentration in the gas phase is more strongly reduced than by absorption at 1 bar.

However, it must also be considered that under pressure a lot of inert gas is dissolved in the wash oil. After flashing at 5 bar in the washing column to 1 bar in the oil tank the inert gas flashes off and escapes as an emission into the atmosphere.

Example 8.1.3: Hexane washing for the absorption of butane at 6 bar and 25 °C

Dissolved nitrogen quantity at 6 bar: $2.54 * 10^{-3}\,\mathrm{kg\,N_2/kg\,hexane}$

Dissolved nitrogen quantity at 1 bar: $0.34 * 10^{-3}\,\mathrm{kg\,N_2/kg\,hexane}$

Released nitrogen rate: $2.2 * 10^{-3}\,\mathrm{kg\,N_2/kg\,hexane} = 2.2\,\mathrm{kg\,N_2/t\,hexane}$

Hexane emission at saturation: 1.7 kg hexane/t of hexane wash

At a hexane wash rate of 5 t/h there will be 8.5 kg/h butane emitted from the hexane tank.

Conclusion:

Absorption under pressure produces new emissions due to the escaping inert gas that is released from the washing liquid and is loaded with organic vapour.

8.1.1.3 Equilibrium Calculation for Non-ideal Condensable Vapours with $\gamma \neq 1$

For non-ideal mixtures, for instance acetone/water, methanol/water, or ethanol/water, the activity coefficient γ is necessary, which is dependent on temperature and composition.

Generally, in absorption an activity coefficient $\gamma\infty$ at infinite dilution is chosen.

The calculation of the activity coefficient γ follows according to the calculation models of Wilson or NRTL (see Chap. 2). For vapour–liquid equilibrium the following is valid:

$$y_i = \frac{\gamma_\infty * p_{0\mathrm{i}} * x_i}{P_{\mathrm{tot}}} = K * x_i \qquad K = \frac{\gamma_\infty * p_{0\mathrm{i}}}{P_{\mathrm{tot}}}$$

Example 8.1.4: Water washing for acetone vapour in the air at 20 °C with P_{tot} = 1 bar.

$$\text{Vapour pressure of acetone at } 20\,^\circ\mathrm{C}: p_{0\mathrm{Ac}} = 304.6\,\mathrm{mbar}$$
$$\text{Activity coefficient } \gamma = 6.7$$

$$K = \frac{6.7 * 304.6}{1000} = 2.04 \qquad y_i = 2.04 * x_i$$

Calculated equilibria:

x_i	0.004	0.006	0.008	0.01	0.012
y_i	0.008	0.0122	0.0163	0.02	0.0245

8.1.1.4 Equilibrium Calculation Using Solubility Tables with Partial Pressure

These solubility tables are used, for instance, for the design of water washes for NH_3, HCl, SO_2, and also for acetone.

Example 8.1.5: Water wash for acetone at 30 °C with P_{tot} = 1 bar Tabulated value: partial pressure P_i = 14.1 mbar for 2 kg acetone in 100 kg water (2 weight%)

$$\text{Gas concentration } y_i = \frac{P_i}{P_{\text{tot}}} = \frac{14.1}{1000} = 0.014 \text{ Molfr. aceton}$$

$$\text{Molar loading } X = B * \frac{M_W}{M_G} = \frac{2}{100} * \frac{18}{58.1} = 0.00619 \text{ kmol aceton/kmol water}$$

$$\text{Liquid concentration } x_i = \frac{0.00619}{1 + 0.00619} = 0.006158 \text{ Molfr. aceton}$$

$$\text{Equilibrium constant } K = \frac{y_i}{x_i} = \frac{0.014}{0.006158} = 2.27$$

Example 8.1.6: Water washing for NH_3 from air at 30 °C and P_{tot} = 1.013 bar Tabulated value: partial pressure P_i = 25.7 mbar for 2 kg NH_3 in 100 kg water (B = 0.02 kg/kg)

$$\text{Gas concentration } y_i = \frac{P_i}{P_{\text{ges}}} = \frac{25.7}{1013} = 0.0254 \text{ NH}_3$$

$$\text{Molar loading } X = B * \frac{M_W}{M_G} = 0.02 * \frac{18}{17} = 0.02118 \text{ kmol NH}_3\text{/kmol Water}$$

$$\text{Liquid concentration } x_i = \frac{X}{1 + X} = \frac{0.02118}{1.02118} = 0.0207 \text{ Molfr. NH}_3$$

$$\text{Equilibrium constant } K = \frac{y_i}{x_i} = \frac{0.0254}{0.0207} = 1.224$$

8.1.1.5 Calculation of the Gas Solubility in a Liquid Using the Henry Constant H

The Henry constant H is not constant but is a temperature dependent physical property.

The Henry value rises with increasing temperature.

$$x_G = \frac{P_{\text{tot}} - P_V}{H} \text{ (Molfr. Gas in Water)}$$

$$W = \frac{x_G * M_G}{M_{\text{Fl}} * (1 - x_G)} \text{ (kg Gas/kg Liquid)}$$

$$S = \frac{\rho_{\text{Fl}}}{\rho_G} * W \text{ (m}^3\text{ Gas/m}^3\text{ Liquid)}$$

x_G = molfraction of the gas in the liquid
P_{tot} = total pressure (bar)
P_V = vapour pressure of the liquid (bar)
M_G = mole weight of the gas
M_{fl} = mole weight of the liquid
W = gas loading of the liquid (kg gas/kg liquid)
S = gas solubility (m^3 gas/m^3 liquid)

Example 8.1.7: Calculation of gas solubility for CO_2, H_2S, and Cl_2 in water at 25 °C

$$\mathbf{CO_2}: \quad P_{\text{ges}} = 1\,\text{bar.} \qquad \text{Water vapour pressure}\, P_V = 0.032\,\text{bar.}$$
$$\text{Henry constant}\, H = 1.650\,\text{bar.}$$

$$x_G = \frac{1 - 0.032}{1650} = 0.586 * 10^{-3}\,\text{Molfr.} \qquad W = 1.43\,g\,\text{CO}_2/\text{kg Water}$$

$$\mathbf{H_2S}: \quad P_{\text{ges}} = 1\,\text{bar.} \quad \text{Water vapour pressure}\, P_V = 0.032\,\text{bar.}$$
$$H = 552\,\text{bar.}$$

$$x_G = \frac{1 - 0.032}{552} = 1.75 * 10^{-3}\,\text{Molfr. H}_2\text{S} \qquad W = 3.32\,g\,\text{H}_2\text{S}/\text{kg Water}$$

$$\mathbf{Cl_2}: \quad P_{\text{ges}} = 1\,\text{bar.} \quad \text{Water vapour pressure}\, P_V = 0.032\,\text{bar.}$$
$$H = 605\,\text{bar.}$$

$$x_G = \frac{1 - 0.032}{605} = 1.6 * 10^{-3}\,\text{Molfr. Cl}_2 \qquad W = 6.2\,g\,\text{Cl}_2/\text{kg Water}$$

8.1.2 Chemical Equilibrium [4, 5]

In chemical washes absorption is improved compared with physical washes because the gas in the washing fluid to be absorbed is chemically bound, for instance by hydrolysis or chemical reaction (Fig. 8.5).

The chemical equilibrium of a reaction is described by the mass efficiency law (MWG) and the equilibrium constant K. A high K-value means that the forward reaction dominates and the equilibrium is shifted to the product's side.

Example: Dissociation of hydrochloric acid in water.

$HCl \rightarrow H^+ + Cl^-$

$$K = \frac{[H^+] * [Cl^-]}{[HCl]} = 10^7$$

The K-value is very high. This means that HCl is nearly completely dissociated.

Since the vapour pressure of the ions is practically zero an absorption of HCl with pure water is principally possible. However, this is only valid for low HCL compositions in water.

The possible improvement by a chemical reaction depends on:

the chemical reaction: irreversible or reversible;
the reaction velocity k_1 and the reaction level;
the composition of the reactants and the pH value;

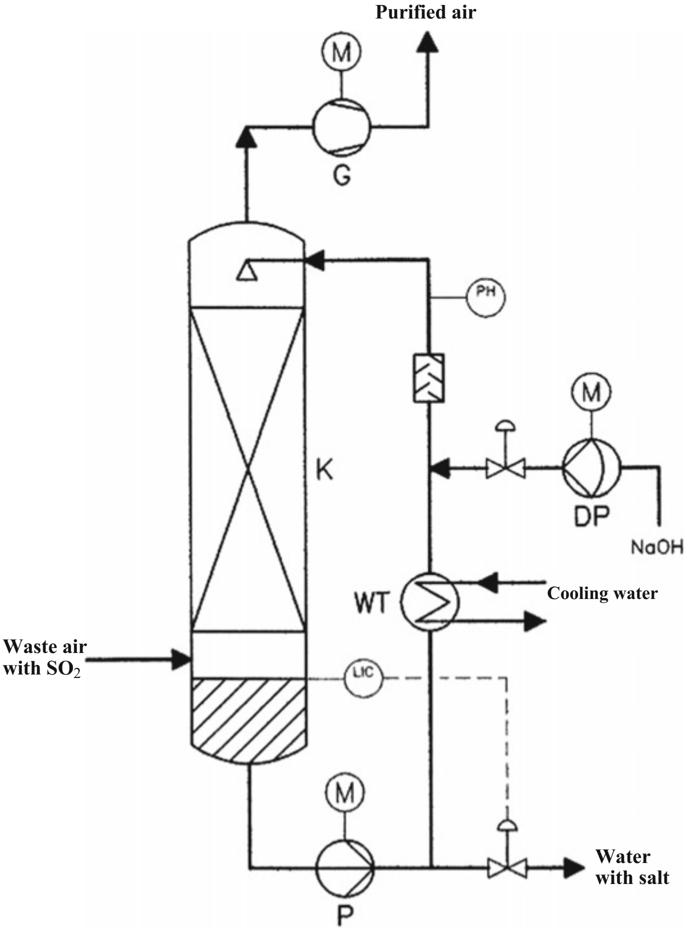


Fig. 8.5 Caustic wash for exhaust air containing SO_2

the diffusion coefficient in the liquid phase D_A;
the mass transfer coefficient in the liquid phase k_L; and
the composition c_{A0} in the liquid stream.

The mass transfer N_A for an irreversible reaction to first order is calculated as follows:

$$N_A = k_L * c_{\mathrm{Ai}} - \left[\frac{c_{\mathrm{A0}}}{\cosh\sqrt{M}}\right] * \frac{\sqrt{M}}{\tanh\sqrt{M}} \quad (\mathrm{kmol/m^2s})$$

$$M = \frac{D_A * k_1}{k_L^2}$$

$$Ha = \sqrt{M} = \sqrt{\frac{D_A * k_1}{k_L^2}}$$

The Hatta number Ha is defined as the ratio of the maximum reaction rate in the film to the diffusion stream of the material component.

The improvement of the material transfer by the reaction is given by the enhancement factor E.

$$E = \frac{Ha}{\tanh\ Ha}$$

Example 8.1.8: Calculation of the enhancement factor E for Cl_2, SO_2, and CO_2 in water at 20 °C
Cl_2 in water: $HOCl \leftrightarrow OCl^- + H^+$

$$k_1 = 11\,\mathrm{s^{-1}} \quad k_L = 10^{-4}\,\mathrm{m/s} \quad D_A = 10^{-9}\,\mathrm{m^2/s}$$

$$M = \frac{D_A * k_1}{k_L^2} = \frac{10^{-9} * 11}{(10^{-4})^2} = 1.1 \qquad \sqrt{1.1} = 1.05$$

$$E = \frac{\sqrt{M}}{\tanh\sqrt{M}} = \frac{1.05}{0.78} = 1.34$$

Due to the dissociation of HOCl the absorption is ca. 34% better than with a pure physical wash.

SO_2 in water: $H_2SO_3 \leftrightarrow HSO_3$- + H^+

$$k_1 = 3.4 * 10^6\,\mathrm{s^{-1}} \quad k_L = 10^{-4}\,\mathrm{m/s} \quad D_A = 10^{-9}\,\mathrm{m^2/s}$$

$$M = \frac{10^{-9} * 3.4 * 10^6}{(10^{-4})^2} = 340000 \qquad E = \sqrt{340000} = 583$$

Due to hydrolysis the absorption in the liquid phase is strongly accelerated and the gas side resistance becomes the limiting factor.

CO_2 in water: $H_2CO_3 \leftrightarrow HCO_3$- + H+

$$k_l = 0.02\,s^{-1} \quad k_L = 10^{-4}\,m/s \quad D_A = 10^{-9}\,m^2/s$$

$$M = \frac{10^{-9} * 0.02}{(10^{-4})^2} = 0.002 \qquad \sqrt{M} = \sqrt{0.002} = 0.0447$$

$$E = \frac{0.0447}{\tanh 0.0447} = \frac{0.0447}{0.04467} = 1.001$$

Due to the low reaction velocity no improvement exists.

The resistance for **the mass transfer** lies **in the gas phase** if, during the physical absorption, the gas is very soluble with a low K-value, or, as part of the chemical wash, the reaction is fast and irreversible:

$$NH_3\,\text{in}\,H_2O \quad SO_2\text{in}\,H_2O \quad SO_2\text{in Alkali} \quad HCl\,\text{in}\,H_2O \quad H_2S\,\text{in}\,H_2O$$

For poorly soluble gases with large *K*-values or slowly reversible reactions the **main resistance lies in the liquid phase**:

$$CO_2\,\text{in}\,H_2O \quad CO_2\,\text{in NaOH} \quad Cl_2\,\text{in}\,H_2O \quad O_2\text{in}\,H_2O \quad H_2\,\text{in}\,H_2O$$

Under conditions where the composition of the dissolved gas is nearly zero, because only ions are present which have no vapour pressure, very high *K*-values in chemical washes result.

$$K = \frac{y_i}{x_i} \approx 1 * 10^6$$

In a design using chemical equilibrium for the given mass balance it is important to check how much non-ionised gas is dissolved in the liquid.

The partial pressure of the free gas is then determined from the concentration of the free gas in the liquid and the Henry coefficient.

Example 8.1.9: NH_3 wash with aqueous nitric acid at 25 °C. y_{ein} = 0.005 molfraction NH_3 The following equilibrium holds:

$$[NH_3] = 5.75 * 10^{-10} * \frac{[NH_4^+]}{[H^+]}$$

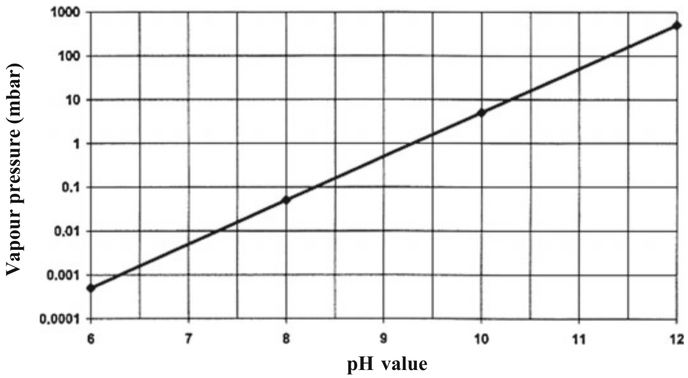


Fig. 8.6 Vapour pressure of ammonia at 25 °C as a function of the pH value

From the mass balance it follows:

$$[NH_4^+] = 0.0438\ \text{gmol/l}$$
$$[H^+] = 0.0304\ \text{gmol/l}$$
$$[NH_3] = 5.75 * 10^{-10} * \frac{0.0438}{0.0304} = 8.28 * 10^{-10}\ \text{gmol/l}$$

After dividing by the molar density the composition in the liquid phase is:

$$x_{NH3} = \frac{8.28 * 10^{-10}}{55.1} = 15 * 10^{-12}\ \text{Molfr. NH}_3$$

From the concentration x and the Henry coefficient H of NH_3 the partial pressure of the free NH_3 is calculated:

$$p_i = x_{NH3} * H_{NH3} = 15 * 10^{-12} * 1.27 = 19.09 * 10^{-12}\ \text{bar}$$

This value is negligible.

Additionally, the equilibrium constant K can be determined:

$$K = \frac{y_{ein}}{x_{NH3}} = \frac{0.005}{15 * 10^{-12}} = 333 * 10^6$$

In some mixtures the pH value has a large influence on the dissociation or the partial pressure.

Figure 8.6 gives the partial pressure of ammonia in water, for an NH_{4+} concentration of 0.05 gmol/l as a function of the pH value.

Remark Due to the reaction heat large heat tone can occur in the chemical wash. The temperature rise should always be checked.

8.2 Calculation of the Required Mass Transfer Units, NTU_{OG} and NTU_{OL}, Using the Slope m of the Equilibrium Line

In the region of low concentration the absorption and desorption equilibrium line is straight, and the following calculation method holds for a linear equilibrium and balance lines with a constant gas/liquid ratio in the column [6–9].

Determination of required transfer units NTU_{OG} for the gas side mass transfer in absorption:

$$NTU_{\mathrm{OG}} = \frac{\ln\left[(1-S)*\left(\frac{y_{\mathrm{in}}-m*x_{\mathrm{in}}}{y_{\mathrm{out}}-m*x_{\mathrm{out}}}\right)+S\right]}{1-S}$$

Determination of the liquid side mass transfer units NTU_{OL} for desorption:

$$NTU_{\mathrm{OL}} = \frac{\ln\left[\left(1-\frac{1}{S}\right)*\left(\frac{x_{\mathrm{in}}-\frac{y_{\mathrm{in}}}{m}}{y_{\mathrm{out}}-\frac{y_{\mathrm{in}}}{m}}\right)+\frac{1}{S}\right]}{1-\frac{1}{S}}$$

S = Strippingfaktor = $m*\frac{G}{L}$
G = Gas loading (kmol/h)
L = Liquid loading (kmol/h)
m = Slope of the equilibrium line = $\Delta y/\Delta x$
y_{in} = Gas inlet concentration (molfraction)
y_{out} = Gas outlet concentration (molfraction)
x_{in} = Liquid inlet concentration (molfraction)
x_{out} = Liquid outlet concentration (molfraction)

If the equilibrium line is a straight line, and goes through the origin, the slope of the equilibrium line m equals the equilibrium factor K.

In most of the cases in the diluted region K = m.

Example 8.2.1: Calculation of the required gas side mass transfer units NTU_{OG} for absorption. Gas inlet concentration $y_{\mathrm{in}} = 0.217$

Required gas outlet composition $y_{\mathrm{out}} = 0.0105$
Washing fluid inlet composition $x_{\mathrm{in}} = 0$
Slope of the equilibrium line $m = 2$

Gas–liquid equilibrium: $y = m * x = 2 * x$

$$\text{Inlet gas rate G} = 15.75\,\text{kmol/h} \qquad \text{Washing liquid rate L} = 167\,\text{kmol/h}$$

$$\text{Stripping faktor S} = m * \frac{G}{L} = 2 * \frac{15.75}{167} = 0.188$$

$$\text{NTU}_{\text{OG}} = \frac{\ln\left[(1 - 0.188) * \left(\frac{0.217-0}{0.0105-0}\right) + 0.188\right]}{1 - 0.188} = 3.48$$

Example 8.2.2: Calculation of the required liquid side mass transfer units $\mathbf{NTU_{OL}}$ for desorption Liquid inlet concentration $x_{\text{in}} = 0.0218$
Required liquid outlet concentration $x_{\text{out}} = 0.529 * 10^{-4}$
Stripping gas inlet concentration $y_{\text{in}} = 0$

$$m = 13 \quad G = 24.4\,\text{kmol/h} \quad L = 222.5\,\text{kmol/h}$$

$$\text{Stripping faktor } S = m * \frac{G}{L} = 13 * \frac{24.4}{222.5} = 1.4256 \qquad \frac{1}{S} = 0.7$$

$$\text{NTU}_{\text{OL}} = \frac{\ln\left[(1 - 0.7) * \left(\frac{0.0218-0}{0.529*10^{-4}}\right) + 0.7\right]}{1 - 0.7} = 16.1$$

8.3 Calculation of the Required Mass Transfer Units $\mathbf{NTU_{OG}}$ or $\mathbf{NTU_{OL}}$ Using the Logarithmic Partial Pressure or Concentration Difference

8.3.1 Required Gas Side Mass Transfer Units NTU_{OG} for Absorption

$$\text{NTU}_{\text{OG}} = \frac{y_{\text{in}} - y_{\text{out}}}{\Delta y_{\ln}} = \frac{P_{\text{in}} - P_{\text{out}}}{\Delta P_{\ln}}$$

Calculation of the logarithmic partial pressure difference $\Delta P_{\ln}$:

$$\Delta P_{\ln} = \frac{\left(P_{\text{in}} - P^*_{\text{in}}\right) - \left(P_{\text{out}} - P^*_{\text{out}}\right)}{\ln\left(\frac{\left(P_{\text{in}} - P^*_{\text{in}}\right)}{\left(P_{\text{out}} - P^*_{\text{out}}\right)}\right)}$$

P_{in} = inlet partial pressure = $y_{\text{in}} * P_{\text{tot}}$
P_{out} = outlet partial pressure = $y_{\text{out}} * P_{\text{tot}}$
$P^*_{\text{in}} = y^*_{\text{in}} * P_{\text{tot}}$
$P^*_{\text{out}} = y^*_{\text{out}} * P_{\text{tot}}$

Calculation of the logarithmic concentration difference Δy_{ln}:

$$\Delta y_{\mathrm{ln}} = \frac{\left(y_{\mathrm{in}} - y*_{\mathrm{in}}\right) - \left(y_{\mathrm{out}} - y^*_{\mathrm{out}}\right)}{\ln\left[\frac{y_{\mathrm{in}} - y^*_{\mathrm{in}}}{y_{\mathrm{out}} - y^*_{\mathrm{out}}}\right]}$$

$$y^*_{\mathrm{in}} = m * x_{\mathrm{out}} + b \qquad y^*_{\mathrm{out}} = m * x_{\mathrm{in}} + b$$

y^*_{in} = gas equilibrium composition to the liquid inlet concentration x_{out} = m^* x_{out}
y^*_{out} = gas equilibrium composition to the liquid outlet concentration x_{in} = m^* x_{in}
y_{out} = gas outlet concentration (molfraction)

Calculation of the liquid outlet concentration x_{out}:

$$x_{\mathrm{out}} = \frac{G}{L} * \left(y_{\mathrm{in}} - y_{\mathrm{out}}\right) + x_{\mathrm{in}}$$

Example 8.3.1.1: Calculation of $\mathrm{NTU_{OG}}$ using the logarithmic concentration gradient Gas inlet concentration y_{in} = 0.217

Required gas outlet concentration y_{out} = 0.0105

$$G = 15.75\,\mathrm{kmol/h} \quad L = 167\,\mathrm{kmol/h} \quad m = 2 \quad x_{\mathrm{in}} = 0$$

$$x_{\mathrm{out}} = \frac{G}{L} * \left(y_{\mathrm{in}} - y_{\mathrm{out}}\right) + x_{\mathrm{in}} = \frac{15.75}{167} * (0.217 - 0.0105) + 0 = 0.019475 \text{ molfr.}$$

$$y^*_{\mathrm{in}} = m * x_{\mathrm{out}} = 2 * 0.019475 = 0.03895\,\mathrm{molfr.}$$
$$y^*_{\mathrm{out}} = m * x_{\mathrm{in}} = 2 * 0 = 0\,\mathrm{molfr.}$$

$$\Delta y_{\mathrm{ln}} = \frac{(0.217 - 0.03895) - (0.0105 - 0)}{\ln\left[\frac{0.217 - 0.03895}{0.0105}\right]} = 0.05919$$

$$\mathrm{NTU_{OG}} = \frac{0.217 - 0.0105}{0.05919} = 3.48$$

Example 8.3.1.2: Calculation of $\mathrm{NTU_{OG}}$ using the logarithmic partial pressure gradient

$$P_{\mathrm{in}} = 0.217 * 1000 = 217\,\mathrm{mbar} \qquad P_{\mathrm{out}} = 0.0105 * 1000 = 10.5\,\mathrm{mbar}$$
$$P^*_{\mathrm{in}} = 0.03895 * 1000 = 38.95\,\mathrm{mbar}$$

$$\Delta P_{\mathrm{ln}} = \frac{(217 - 38.95) - (10.5 - 0)}{\ln \frac{217 - 38.95}{10.5 - 0}} = 59.19$$

$$\mathrm{NTU_{OG}} = \frac{217 - 10.5}{59.19} = 3.48$$

The results of Examples 8.3.1.1 and 8.3.1.2 are identical to the result of Example 8.2.1.

8.3.2 Calculation of the Liquid Side Mass Tranfer NTU_{OL} for Desorption

Calculation of the $\mathrm{NTU}_{\mathrm{OL}}$ using the logarithmic concentration difference:

$$\mathrm{NTU}_{\mathrm{OL}} = \frac{x_{\mathrm{in}} - x_{\mathrm{out}}}{\Delta x_{\mathrm{ln}}}$$

Calculation of the logarithmic concentration difference:

$$\Delta x_{\mathrm{ln}} = \frac{\left(x_{\mathrm{in}} - x_{\mathrm{in}}^*\right) - \left(x_{\mathrm{out}} - x_{\mathrm{out}}^*\right)}{\ln \frac{x_{\mathrm{in}} - x_{\mathrm{in}}^*}{x_{\mathrm{out}} - x_{\mathrm{out}}^*}}$$

$$x_{\mathrm{in}}^* = \frac{y_{\mathrm{out}} - b}{m} \qquad x_{\mathrm{out}}^* = \frac{y_{\mathrm{in}} - b}{m}$$

Stripping gas outlet concentration y_{out}:

$$y_{\mathrm{out}} = \frac{L}{G} * \left(x_{\mathrm{in}} - x_{\mathrm{out}}\right) + y_{\mathrm{in}}$$

Example 8.3.2.1: Calculation of $\mathrm{NTU}_{\mathrm{OL}}$ using the logarithmic concentration gradient

Liquid rate $L = 222.5\,\mathrm{kmol/h}$ Liquid inlet concentration $x_{\mathrm{in}} = 0.0218$ molfr.
Stripping gas rate $G = 24.4\,\mathrm{kmol/h}$ Stripping gas inlet concentration $y_{\mathrm{in}} = 0$
Required liquid outlet composition $x_{\mathrm{out}} = 0.529 * 10^{-4}$molfr.
Equilibrium factor $m = 13$

$$y_{\mathrm{out}} = \frac{222.5}{24.4} * \left(0.0218 - 0.529 * 10^{-4}\right) = 0.1983 \text{ molfr.}$$

$$x*_{\mathrm{in}} = \frac{y_{\mathrm{out}}}{m} = \frac{0.1983}{13} = 0.015255 \text{ molfr.}$$

$$\Delta x_{\mathrm{ln}} = \frac{(0.0218 - 0.15255) - (0.529 * 10^{-4} - 0)}{\ln\left[\frac{0.0218 - 0.15255}{0.529 * 10^{-4}}\right]} = 0.001348 \text{ molfr.}$$

$$\mathrm{NTU}_{\mathrm{OL}} = \frac{0.0218 - 0.529 * 10^{-4}}{0.001348} = 16.1$$

The result is consistent with the result from Example 8.2.2.

8.4 Calculation of the Required Theoretical Stages NT for Absorption and Desorption

The calculation method is valid for **linear equilibrium and operation lines** with a constant stripping factor. The required theoretical trays NT for absorption or desorption tasks are calculated in the following text.

8.4.1 Determination of the Theoretical Stages NT for Absorption [9, 10]

The required number of theoretical trays NT for absorption is determined as follows:

$$\mathrm{NT}_{\mathrm{Abs}} = \frac{\lg\left[(1-S) * M + S\right]}{\lg \frac{1}{S}}$$

$$\text{Strippingfaktor } S = m * \frac{G}{L} \qquad M = \frac{y_{\mathrm{in}} - m * x_{\mathrm{in}}}{y_{\mathrm{out}} - m * x_{\mathrm{in}}}$$

Example 8.4.1: Calculation of the required theoretical stages for absorption

Gas inlet rate $G = 15.75\ \mathrm{kmol/h}$ Gas inlet concentration $y_{\mathrm{in}} = 0.217$ molfr.
Absorbent inlet rate $L = 167\ \mathrm{kmol/h}$ Washing liquid loading $x_{\mathrm{in}} = 0$ molfr.
Equilibrium constant $m = 2$
Required gas outlet concentration $y_{\mathrm{out}} = 0.0105$ molfr.

$$S = 2 * \frac{15.75}{167} = 0.188 \qquad M = \frac{0.217 - 0}{0.0105 - 0} = 20.66$$

$$\mathrm{NT} = \frac{\lg\left[(1-0.188) * 20.66 + 0.188\right]}{\lg \frac{1}{0.188}} = 1.69$$

Washing fluid outlet concentration:

$$x_{\mathrm{out}} = \frac{G}{L} * (y_{\mathrm{in}} - y_{\mathrm{out}}) + x_{\mathrm{ein}} = \frac{15.75}{167} * (0.217 - 0.0105) + 0 = 0.019475 \text{ molfr.}$$

8.4.2 Calculation of the Theoretical Stages NT for Desorption

The required theoretical stages for desorption are determined as follows:

$$\mathrm{NT}_{\mathrm{Des}} = \frac{\lg\,[(1-1/S)*M+1/S]}{\lg S}$$

$$S = m*\frac{G}{L} \qquad M = \frac{x_{\mathrm{in}} - y_{\mathrm{in}}/m}{x_{\mathrm{out}} - y_{\mathrm{in}}/m}$$

Example 8.4.2: Calculation of the theoretical stages for a stripper

Liquid inlet rate L = 222.5 kmol/h	Liquid inlet concentration x_{ein} = 0.0218 molfr.
Stripping gas rate G = 24.4 kmol/h	Stripping gas inlet concentration y_{ein} = 0
Slope of the equilibrium line m = 13	
Required liquid outlet concentration x_{out} = 0.529 * 10^{-4} molfr.	

$$S = m*\frac{G}{L} = 13*\frac{24.4}{222.5} = 1.4256 \qquad \frac{1}{S} = 0.701$$

$$M = \frac{0.0218-0}{0.529*10^{-4}-0} = 412$$

$$\mathrm{NT} = \frac{\lg\,[(1-0.701)*412+0.701]}{\lg\;1.4256} = 13.6$$

8.5 Conversion of the Required Mass Transfer Units $\mathrm{NTU}_{\mathrm{OG}}$ and $\mathrm{NTU}_{\mathrm{OL}}$ to the Required Number of Theoretical Trays NT, and Vice Versa

The following is valid for the conversion from $\mathrm{NTU}_{\mathrm{OG}}$ for absorption:

$$R_{\mathrm{OG}} = \frac{\mathrm{NTU}_{\mathrm{OG}}}{\mathrm{NT}} = \frac{\ln\,S}{S-1}$$

$$\mathrm{NTU}_{\mathrm{OG}} = R_{\mathrm{OG}}*\mathrm{NT} = \frac{\ln S}{S-1}*\mathrm{NT} \qquad \mathrm{NT} = \mathrm{NTU}_{\mathrm{OG}}*\frac{S-1}{\ln S}$$

Example 8.5.1: Conversion from $\mathrm{NTU_{OG}}$ to NT

$$\mathrm{S} = 0.188 \quad \mathrm{NTU_{OG}} = 3.5$$

$$R_{\mathrm{OG}} = \frac{\ln 0.188}{0.188 - 1} = 2.05$$

$$\mathrm{NT} = \frac{\mathrm{NTU_{OG}}}{R_{\mathrm{OG}}} = \frac{3.5}{2.05} = 1.7 = \mathrm{NTU_{OG}} * \frac{S-1}{\ln S} = 3.5 * \frac{0.188 - 1}{\ln 0.188} = 1.7$$

The conversion from $\mathrm{NTU_{OL}}$ for desorption holds:

$$R_{\mathrm{OL}} = \frac{\mathrm{NTU_{OL}}}{\mathrm{NT}} = \frac{S * \ln S}{S-1}$$

$$\mathrm{NTU_{OL}} = R_{\mathrm{OL}} * \mathrm{NT} = \frac{S * \ln S}{S-1} \qquad \mathrm{NT} = \mathrm{NTU_{OL}} * \frac{S-1}{S * \ln S}$$

Example 8.5.2: Conversion from NT to $\mathrm{NTU_{OL}}$

$$\mathrm{S} = 1.4 \quad \mathrm{NT} = 13.6$$

$$R_{\mathrm{OL}} = \frac{S * \ln S}{S-1} = \frac{1.4 * \ln 1.4}{1.4 - 1} = 1.177$$

$$\mathrm{NTU_{OL}} = \mathrm{NT} * \frac{S * \ln S}{S-1} = 13.6 * \frac{1.4 * \ln 1.4}{1.4 - 1} = 16 = R_{\mathrm{OL}} * \mathrm{NT} = 1.177 * 13.6 = 16$$

8.6 Determination of the Required Packing Height $\mathrm{H_{Pack}}$

The required packing height for absorption or desorption tasks results from the product of the required mass transfer units NTU with the NTU required packing height HTU, or from the product of the required theoretical stages NT and the required packing height HETP for a theoretical stage.

$$\mathrm{H_{Pack}} = \mathrm{NT} * \mathrm{HETP} \qquad \mathrm{H_{Pack}} = \mathrm{NTU_{OG}} * \mathrm{HTU_{OG}} \qquad \mathrm{H_{Pack}} = \mathrm{NTU_{OL}} * \mathrm{HTU_{OL}}$$

First of all, the total packing heights $\mathrm{HTU_{OG}}$ or $\mathrm{HTU_{OL}}$ for the gas side and the liquid side mass transfer have to be determined along with HETP values.

$$\mathrm{HTU_{OG}} = \mathrm{HTU}_G + S * \mathrm{HTU}_L \qquad \mathrm{HETP} = \frac{\ln S}{S-1} * \mathrm{HTU_{OG}}$$

$$\mathrm{HTU_{OL}} = \mathrm{HTU}_L + \frac{\mathrm{HTU}_G}{S} \qquad \mathrm{HETP} = \frac{S * \ln S}{S-1} * \mathrm{HTU_{OL}}$$

HETP = required packing height for a theoretical stage (m packing height/NT)
HTU_G = required packing height for a gas side mass transfer unit NTU_{OG}
HTU_L = required packing height for a liquid side mass transfer unit NTU_{OL}

Calculation of the required HTU and HETP values is shown in Chap. 10.

Example 8.6.1: Determination of the required packing height

$$\begin{array}{llll} \mathrm{NTU_{OG}} = 3.5 & \mathrm{NT} = 1.7 & \mathrm{NTU_{OL}} = 0.66 & \mathrm{S} = 0.188 \\ \mathrm{HTU_G} = 0.375\,\mathrm{m} & \mathrm{HTU_L} = 0.71\,\mathrm{m} & \mathrm{HETP} = 1.05\,\mathrm{m} & \end{array}$$

$$HTU_{OG} = HTU_G + S * HTU_L = 0.375 + 0.188 * 0.71 = 0.508\ \mathrm{m}$$

$$HTU_{OL} = HTU_L + \frac{1}{S} * HTU_G = 0.71 + \frac{1}{0.188} * 0.375 = 2.7\ \mathrm{m}$$

$$HETP = \frac{\ln S}{S-1} * HTU_{OG} = \frac{\ln 0.188}{0.188 - 1} * 0.508 = 1.05\ \mathrm{m}$$

$$HETP = \frac{S * \ln S}{S-1} * HTU_{OL} = \frac{0.188 * \ln 0.188}{0.188 - 1} * 2.7 = 1.05\ \mathrm{m}$$

$$H_{Füll} = NTU_{OG} * HTU_{OG} = 3.5 * 0.508 = 1.78\ \mathrm{m}$$

$$H_{Füll} = NT * HETP = 1.7 * 1.08 = 1.78\ \mathrm{m}$$

$$H_{Füll} = NTU_{OL} * HTU_{OL} = 0.66 * 2.7 = 1.78\ \mathrm{m}$$

8.7 Calculation of the Packing Height Using the Mass Transfer Number K_{Ga}

In chemical washes in packing columns using caustic solutions, acids, amines, or water the required bed height is often determined using the empirical mass transfer number k_{Ga}.

$$H_{\mathrm{Pack}} = \frac{G(\mathrm{kmol/h})}{A(\mathrm{m}^2) * \Delta P_{\ln} * k_{\mathrm{Ga}}}\ (\mathrm{m}) = \frac{G_M(\mathrm{kmol/h\,m^2})}{\Delta P_{\ln} * k_{\mathrm{Ga}}}\ (\mathrm{m})$$

G = absorptive rate (kmol/h)
G_M = absorptive loading (kmol/h m^2)
A = column cross sectional area (m^2)
$\Delta P_{\ln}$ = logarithmic partial pressure gradients (bar)
k_{Ga}= mass transfer number (kmol/h m^3 bar)

The mass transfer number k_{Ga} can be determined using the Sherwood and Schmidt number.

The use of empirical values is recommended.

For unknown systems the k_{Ga} value can be estimated using diffusion coefficients.

$$k_{Ga(new)} = k_{Ga(known)} * \left[\frac{D_{new}}{D_{known}}\right]^{0.56}$$

$k_{Ga(new)}$ = new mass transfer number

$k_{Ga(known)}$ = known mass transfer number
D_{new} = diffusion coefficient of the new system
D_{known} = diffusion coefficient of the known system

With an increasing pressure gradient Δp_{ln} the k_{Ga} decreases, as it also does with increasing reaction equilibrium.

Systems with high-temperature reactions have high k_{Ga} values, but the heating of the liquid from the heat of the reaction increases the vapour pressure and reduces the driving partial pressure gradient.

Example 8.7.1: 1000 m_N^3/h air with 1 vol.% SO_2 are washed with aqueous NaOH

Outlet concentration : 0.01 vol% $\quad M_{SO2} = 64.1 \quad P = 1$ bar
$y_{in} = 0.01$ molfr. $\quad y_{out} = 0.0001$ molfr. $\quad k_{GA} = 384\,\text{kmol/h}\,\text{m}^2\,\text{bar}$
Absorptive rate $= 10\,m_N^3 = 0.446\,\text{kmol/h}$ $\quad$ Column cross sectional area : $0.196\,\text{m}^2$
$G_M = 0.446/0.196 = 2.27\,\text{kmol/h}\,\text{m}^2$
$P_{in} = 0.01 * 1000 = 10\,\text{mbar} \quad P_{out} = 0.0001 * 1000 = 0.1\,\text{mbar}$
$P^* = 0$ with chemical wash

$$\Delta P_{ln} = \frac{10 - 0.1}{\ln \frac{10}{0.1}} = 2.15\,\text{mbar} = 0.00215\,\text{bar}$$

$$H_{Pack} = \frac{2.27}{384 * 0.00215} = 2.75\,\text{m Packing}$$

Cross-check calculation with NTU_{OG} and H_{OG} = 0.6 m packing:

$$NTU_{OG} = \frac{y_{in} - y_{out}}{\Delta P_{ln}} = \frac{0.01 - 0.001}{0.00215} = 4.6$$
$$H_{Pack} = NTU_{OG} * H_{OG} = 4.6 * 0.6 = 2.76\,\text{m Packing}$$

8.8 Calculation of the Required Theoretical Stages and the Concentrations on the Stages According to Nguyen [11, 12]

This method is simple and fast and allows consideration of tray efficiency.

8.8.1 Determination of the Required Ideal Number of Trays N_{id} *with a Tray Efficiency of* $\eta_B = 1$ *for Absorption*

First of all an operand α_A is determined:

$$\alpha_A = \frac{y_{\text{out}} - A * (m * x_{\text{in}} + B)}{A - 1} \qquad A = \frac{1}{S} = \frac{L}{m * G}$$

$$y = m * x + B$$

G = gas rate (kmol/h)

L = liquid rate (kmol/h)
m = slope of the equilibrium line
B = ordinate section of the equilibrium line
η_B = tray efficiency

Determination of the required ideal number of trays n_{id} with a tray efficiency of η_B = 1:

$$n_{\text{id}} = \frac{\ln\left[\frac{y_{\text{in}} + \alpha_A}{y_{\text{out}} + \alpha_A}\right]}{\ln A}$$

Calculation of the compositions on the individual trays:

$$y_{\text{id}} = \frac{y_{\text{in}} + \alpha_A}{A^n} - \alpha_A \qquad x_{\text{id}} = \frac{y - B}{m}$$

Example 8.8.1.1: Cross-check of absorption Example 8.4.1

$y_{\text{in}} = 0.217$ molfr. $\quad y_{\text{out}} = 0.0105$ molfr. $\quad x_{\text{ein}} = 0 \quad \text{m} = 2 \quad 1/\text{S} = 5.32$

$$\alpha_A = \frac{0.0105 - 5.32 * 0}{5.32 - 1} = 0.002431$$

$$n = \frac{\ln \frac{0.217 + 0.002431}{0.0105 + 0.002431}}{\ln 5.32} = 1.69 \text{ theoretical stages}$$

The results of Examples 8.4.1 and 8.8.1.1 are identical.

Example 8.8.1.2: Calculation of the theoretical trays with $\eta_B = 1$ for absorption

$$
\begin{array}{lll}
y_{\text{in}} = 0.3\,\text{molfr.} & y_{\text{out}} = 0.03\,\text{molfr.} & x_{\text{in}} = 0 \\
A = 1.35 & m = 1 & B = 0.02
\end{array}
$$

$$\alpha_A = \frac{0.03 - 1.35 * (1 * 0 + 0.02)}{1.35 - 1} = 0.00857$$

$$n_{\text{id}} = \frac{\ln \frac{0.3 + 0.00857}{0.03 + 0.00857}}{\ln 1.35} = 6.93$$

Required ideal number of trays is seven.

Calculation of the concentrations (molfr.) on the theoretical trays:

$$
\begin{array}{lll}
\text{Tray}\,1: & y_1 = \dfrac{0.3 + 0.00857}{1.35^1} - 0.00857 = 0.22 & x_1 = \dfrac{0.22 - 0.02}{1} = 0.2 \\
\text{Tray}\,2: & y_2 = \dfrac{0.3 + 0.00857}{1.35^2} - 0.00857 = 0.160 & x_2 = \dfrac{0.1607 - 0.02}{1} = 0.1407 \\
\text{Tray}\,3: & y_3 = \dfrac{0.3 + 0.00857}{1.35^3} - 0.00857 = 0.1168 & x_3 = 0.1168 - 0.02 = 0.0968
\end{array}
$$

$$
\begin{array}{lll}
\text{Tray 4}: & y_4 = 0.0843 & x_4 = 0.0643 \\
\text{Tray 5}: & y_5 = 0.0602 & x_5 = 0.04 \\
\text{Tray 6}: & y_6 = 0.0424 & x_6 = 0.022 \\
\text{Tray 7}: & y_7 = 0.0292 & x_7 = 0.009
\end{array}
$$

8.8.2 Calculation of the Required Real Number of Trays N$_{real}$ with a Tray Efficiency of $\eta_V < 1$ for Absorption

First of all the operand β_A is determined:

$$\beta_A = \frac{1}{1 + \eta_V * \left(\frac{1}{A} - 1\right)} \qquad n_{\text{real}} = \frac{\ln \frac{y_{\text{in}} + \alpha_A}{y_{\text{out}} + \alpha_A}}{\ln \beta_A}$$

Calculation of the concentrations on individual trays:

$$y_{\text{real}} = \frac{y_{\text{in}} + \alpha_A}{\beta_A^n} - \alpha_A \qquad x_{\text{real}} = \frac{y - B}{m}$$

Example 8.8.2.1: Calculation of the theoretical trays with a tray efficiency η_V = 0.5 for absorption Data as in Example 8.8.1.2:

$$\beta_A = \frac{1}{1+0.5*\left(\frac{1}{1.35}-1\right)} = 1.149 \qquad n_{\text{real}} = \frac{\ln\frac{0.3+0.00857}{0.03+0.00857}}{\ln 1.149} = 15$$

With a tray efficiency η_V = 0.5 you arrive at a requirement of 15 actual trays for absorption.

Calculation of the concentrations (molfr.) on the actual trays:

$$\text{Tray 1}: \quad y_1 = \frac{0.3+0.00857}{1.149^1} - 0.00857 = 0.26 \qquad x_1 = 0.26 - 0.02 = 0.24$$

$$\text{Tray 2}: \quad y_2 = \frac{0.3+0.00857}{1.149^2} - 0.00857 = 0.225 \qquad x_2 = 0.225 - 0.02 = 0.205$$

Tray 3 : $y_3 = 0.195$ $x_3 = 0.175$
Tray 4 : $y_4 = 0.168$ $x_4 = 0.148$
Tray 5 : $y_5 = 0.1455$ $x_5 = 0.1255$
Tray 6 : $y_6 = 0.125$ $x_6 = 0.105$
Tray 7 : $y_7 = 0.108$ $x_7 = 0.088$
Tray 10 : $y_{10} = 0.068$ $x_{10} = 0.048$
Tray 12 : $y_{12} = 0.0497$ $x_{12} = 0.0297$
Tray 15 : $y_{15} = 0.0298$ $x_{15} = 0.0098$

8.8.3 Determination of the Required Ideal Number of Trays N_{idL} with $\eta_L = 1$ for Desorption

First of all the operand α_L is determined:

$$\alpha_L = \frac{x_{\text{out}} - \frac{G}{L}*(y_{\text{in}} - B)}{\frac{1}{A}-1} \qquad n_{\text{idL}} = \frac{\ln\frac{x_{\text{out}}+\alpha_L}{x_{\text{in}}+\alpha_L}}{\ln A}$$

Calculation of the concentrations on the trays:

$$x_{\text{idL}} = \frac{x_{\text{out}}+\alpha_L}{A^n} - \alpha_L \qquad y_{\text{idL}} = m * x_{\text{idL}} + B$$

Example 8.8.3.1: Determination of the required theoretical trays for the data from Example 8.4.2 .

$$\alpha_L = \frac{0.529 * 10^{-4} - \frac{24.4}{222.5} * 0}{1/0.701 - 1} = 0.000124$$

$$n = \frac{\ln \frac{0.529 * 10^{-4} + 0.000124}{0.0218 + 0.000124}}{\ln 0.701} = 13.6 \textit{ theoretische Böden}$$

The result is identical to that of Example 8.4.2.

Example 8.8.3.2: Calculation of the theoretical trays for desorption of x = 0.2 to x = 0.02 with a tray efficiency of η_L = 1

$$x_{\text{ein}} = 0.2 \quad x_{\text{aus}} = 0.02 \quad y_{\text{ein}} = 0 \quad m = 1 \quad A = 1.1 \quad B = 0.02$$
$$G = 10\,\text{kmol/h} \qquad L = 11\,\text{kmol/h} \qquad \eta_L = 1$$

$$\alpha_L = \frac{0.02 - \frac{10}{11} * (0 - 0.02)}{\frac{1}{1.1} - 1} = -0.42 \qquad n_{\text{idL}} = \frac{\ln \frac{0.02 + (-0.42)}{0.2 + (-0.42)}}{\ln 1.1} = 6.27$$

Required theoretical trays with η_L = 1 is 6.27.

Calculation of the concentrations (molfr.) on the trays:

Tray 0: $x_0 = \frac{0.02 - 0.42}{1.1^0} + 0.42 = 0.02 \qquad y_0 = 0.02 + 0.02 = 0.04$

Tray 1: $x_1 = \frac{0.02 + (-0.42)}{1.1^1} - (-0.42) = 0.056 \quad y_1 = 1 * 0.056 + 0.02 = 0.076$

Tray 2: $x_2 = \frac{0.02 - 0.42}{1.1^2} + 0.42 = 0.089 \qquad y_2 = 0.089 + 0.02 = 0.109$

Tray 3: $x_3 = \frac{0.02 - 0.42}{1.1^3} + 0.42 = 0.119 \qquad y_3 = 0.119 + 0.02 = 0.139$

Tray 4: $x_4 = \frac{0.02 - 0.42}{1.1^4} + 0.42 = 0.146 \qquad y_4 = 0.146 + 0.02 = 0.166$

Tray 5: $x_5 = \frac{0.02 - 0.42}{1.1^5} + 0.42 = 0.171 \qquad y_5 = 0.171 + 0.02 = 0.191$

Tray 6: $x_6 = \frac{0.02 - 0.42}{1.1^6} + 0.42 = 0.194 \qquad y_6 = 0.214$

Tray 7: $x_7 = \frac{0.02 - 0.42}{1.1^7} + 0.42 = 0.214 \qquad y_7 = 0.234$

8.8.4 Calculation of the Number of the Required Theoretical Trays with a Tray Efficiency of $\eta_L < 1$ for Desorption

First of all some operands have to be determined:

$$\eta_L = \frac{\eta_V}{\eta_V + A*(1-\eta_V)} \qquad \beta_L = 1 + \eta_L*(A-1)$$

Calculation of the number of required trays $n_{\mathrm{rL}} = \dfrac{\ln \frac{x_{\mathrm{out}}+\alpha_L}{x_{\mathrm{in}}+\alpha_L}}{\ln \beta_L}$

Determination of the concentrations on individual trays:

$$x_{\mathrm{real}} = \frac{x_{\mathrm{out}}+\alpha_L}{\beta_L^n} - \alpha_L \qquad y_{\mathrm{real}} = m*x_{\mathrm{real}} + B$$

Example 8.8.3.3: Calculation of the required number of trays for desorption from *x* = 0.2 to *x* = 0.02 considering a tray efficiency of $\eta_V = 0.5$ Data from Example 8.8.3.2:

$$\eta_L = \frac{0.5}{0.5+1.1*(1-0.5)} = 0.476 \qquad \beta_L = 1 + 0.476*(1.1-1) = 1.0476$$

$$n_{\mathrm{iL}} = \frac{\ln \frac{0.02+(-0.42)}{0.2+(-0.42)}}{\ln 1.0476} = 12.85$$

We arrive a requirement of 12.85 trays with a tray efficiency of $\eta_L = 0.476$.
Calculation of the concentrations on the trays:

Tray 0: $x_0 = \dfrac{0.02-0.42}{1.0476^0} + 0.42 = 0.02$ $\quad y_0 = 0.04$ (bottom product)

Tray 1: $x_1 = \dfrac{0.02-0.42}{1.0476^1} - (-0.42) = 0.038$ $\quad y_1 = 1*0.038 + 0.02 = 0.058$

Tray 2: $x_2 = \dfrac{0.02-0.42}{1.0476^2} + 0.42 = 0.0555$ $\quad y_2 = 0.0755$

Tray 4: $x_4 = \dfrac{0.02-0.42}{1.0476^4} + 0.42 = 0.0878$ $\quad y_4 = 0.1079$

Tray 8: $x_8 = \dfrac{0.02-0.42}{1.0476^8} + 0.42 = 0.144$ $\quad y_8 = 0.164$

Tray 12: $x_{12} = \dfrac{0.02-0.42}{1.0476^{12}} + 0.42 = 0.191$ $\quad y_{12} = 0.211$

Tray 13: $x_{13} = \dfrac{0.02-0.42}{1.0476^{13}} + 0.42 = 0.201$ $\quad y_{13} = 0.221$ (feed at the top)

8.9 Graphical Determination of the Number of Stages for Absorption and Desorption

For **linear equilibrium and operating lines** with a constant *L*/*V* ratio the required theoretical number of trays can be very simply determined graphically.

Equilibrium equation: $y = m * x + B$ for the equilibrium compositions.

Equation of the operating line of the absorption for real compositions in gas and liquid:

$$y = \frac{L}{G} * x + y_{\text{out}} - \frac{L}{G} * x_{\text{in}}$$

y_{in} = gas inlet concentration (molfraction)
y_{out} = gas outlet concentration (molfraction)
x_{out} = absorbent inlet loading (molfraction)
G = gas rate (kmol/h)
L = washing liquid rate (kmol/h)

Calculation of the bottoms concentration x_{out} in the washing fluid during absorption:

$$x_{\text{out}} = G/L * (y_{\text{in}} - y_{\text{out}}) + x_{\text{in}}$$

Equation of the operating line of desorption for the compositions in gas and liquid:

$$y = \frac{L}{G} * x + y_{\text{in}} - \frac{L}{G} * x_{\text{out}}$$

x_{in} = liquid inlet concentration (molfraction)
x_{out} = liquid outlet concentration (molfraction)
y_{in} = Stripping gas inlet concentration (molfraction)

Calculation of the top concentration y_{out} of stripping gas whilst desorbing:

$$y_{\text{out}} = \frac{L}{G} * (x_{\text{in}} - x_{\text{out}}) + y_{\text{in}}$$

Mass balance in the column:

$$(y_{\text{in}} - y_{\text{out}}) * G = (x_{\text{out}} - x_{\text{in}}) * L$$

While drawing equilibrium and operating lines some *y* and *x* values are determined.

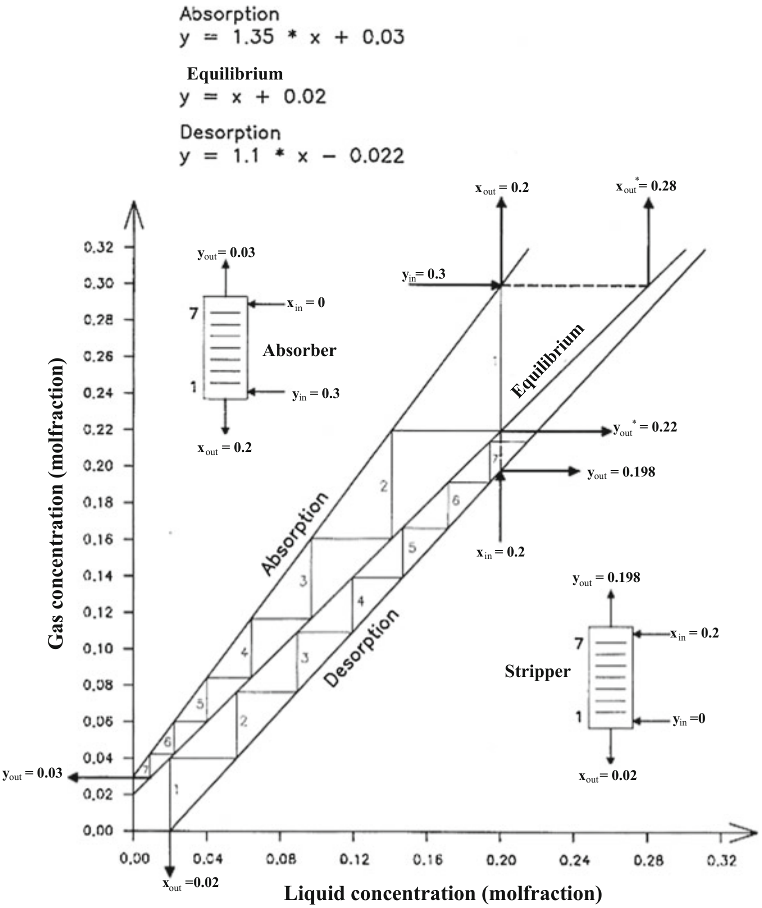


Fig. 8.7 Graphical determination of the number of trays

In the linear region two points are required:
Absorption: top, y_{in} and x_{out}; bottom, y_{out} and x_{in}
Desorption: top, x_{in} and y_{out}; bottom, x_{out} and y_{in}
Slope of the operating or balance line:

$$\frac{L}{G} = \frac{y_{\text{in}} - y_{\text{out}}}{x_{\text{out}} - x_{\text{in}}}$$

Figure 8.7 shows an example of the graphical determination of the number of trays for absorption and desorption.

The equations for the equilibrium and both of the operating lines are given.

The required theoretical stages result from the stages between the equilibrium and balance lines.

For absorption we require 7 theoretical stages.

For desorption we require 7 theoretical stages.

By using a larger washing fluid rate the ratio *L*/*G* becomes larger and the balance line for absorption becomes steeper.

Therefore, the number of required theoretical trays for absorption decreases.

By using a larger stripping gas rate the ratio *L*/*G* becomes smaller and the balance line for desorption becomes shallower, so that fewer theoretical stages are required for stripping out.

Example 8.9.1: Cross-checking the graphically determined number of trays in Fig. 8.7 with the calculation method in Sect. 8.8.0 Absorption calculation according to Sect. 8.8.1:

$$y_{\text{in}} = 0.3 \quad y_{\text{out}} = 0.03 \quad x_{\text{in}} = 0 \quad A = 1.35 \quad m = 1 \quad B = 0.02$$

$$\alpha_A = \frac{0.03 - 1.35 * (1 * 0 + 0.02)}{1.35 - 1} = 0.00857$$

$$n_{\text{id}} = \frac{\ln \frac{0.3 + 0.00857}{0.03 + 0.00857}}{\ln 1.35} = 6.93$$

Required ideal number of trays is seven.

Desorption calculation according to Sect. 8.8.3:

$$x_{\text{in}} = 0.2 \quad x_{\text{out}} = 0.02 \quad y_{\text{in}} = 0 \quad m = 1 \quad A = 1.1 \quad B = 0.02$$

$$G = 10\,\text{kmol/h} \quad L = 11\,\text{kmol/h} \quad \eta_L = 1$$

$$\alpha_L = \frac{0.02 - \frac{10}{11} * (0 - 0.02)}{\frac{1}{1.1} - 1} = -0.42 \qquad n_{\text{idL}} = \frac{\ln \frac{0.02 + (-0.42)}{0.2 + (-0.42)}}{\ln 1.1} = 6.27$$

Required ideal number of trays with $\eta_B = 1$ is 6.27.

The calculated results according to Sect. 8.8 are consistent with the graphically determined required numbers of trays for the absorption and desorption in Fig. 8.7.

Example 8.9.2: Graphical determination of the number of trays for absorption with two different absorbent rates Gas inlet concentration y_{in} = 0.25 = 25 vol.%

Gas outlet concentration y_{out} = 0.03 = 3 vol.%

Washing liquid inlet concentration x_{in} = 0

Equilibrium: $y = m * x = 0.9 * x$

Example 8.9.2.1: Washing fluid rate *L* = 100 kmol/h

***G* = 100 kmol/h**

***L*/*G* = 1 = slope of the operating line**

Equation of operating line a:

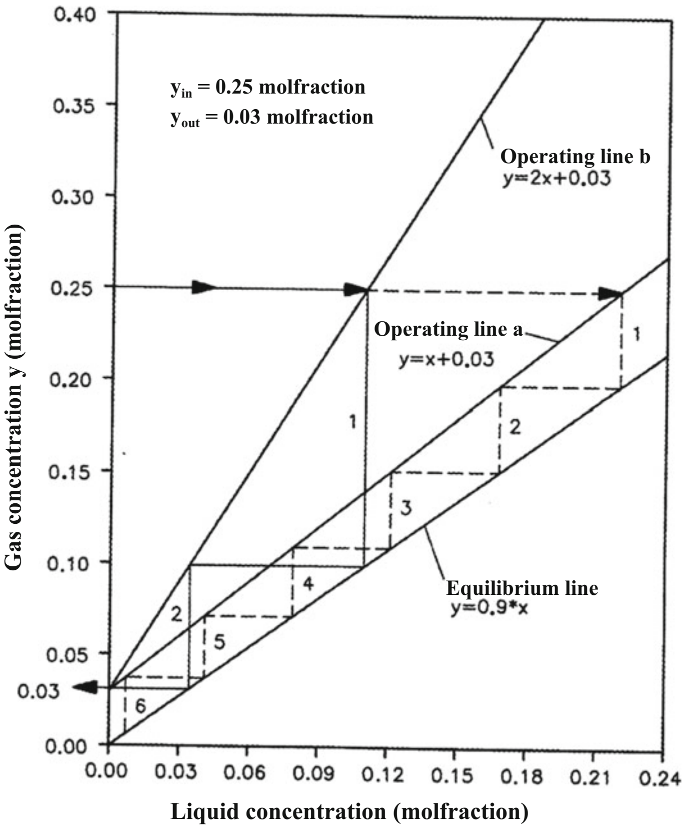


Fig. 8.8 Graphical determination of the number of trays for absorption with two different absorbent rates

$$y = \frac{L}{G} * x + y_{\mathrm{out}} - \frac{L}{G} * x_{\mathrm{in}} = x + 0.03 - 1 * 0 = x + 0.03$$

From the graphical representation of equilibrium and balance lines in Fig. 8.8 a requirement of about **5.2 separation stages for absorption** results.

Calculation cross-check according to Sect. 8.4:

$$y_{\mathrm{in}} = 0.25 \qquad y_{\mathrm{out}} = 0.03 \qquad x_{\mathrm{in}} = 0$$

$$S = m * \frac{L}{G} = 0.9 * 1 = 0.9 \qquad M = \frac{0.25}{0.003} = 8.33$$

$$\mathrm{NT} = \frac{\lg\left[(1-S) * M + S\right]}{\lg \frac{1}{S}}$$

$$\mathrm{NT} = \frac{\lg\left[(1-0.9) * 8.33 + 0.9\right]}{\lg \frac{1}{0.9}} = 5.22$$

From the calculation there is a requirement for 5.22 theoretical trays.

Example 8.9.2.2: Washing fluid rate L = 200 kmol/h

G = 100 kmol/h

L/G = 2 = slope of the operating line

Operating line b: $y = 2 * x + 0.03$

Figure 8.8 shows that the required number of trays reduces to **two theoretical trays** with a doubling of the washing liquid rate.

Calculation cross-check according to Sect. 8.4:

$$S = m * \frac{G}{L} = 0.9 * \frac{100}{200} = 0.45 \qquad M = \frac{0.25}{0.03} = 8.33$$

$$\mathrm{NT} = \frac{\lg[(1-0.45) * 8.33 + 0.45]}{\lg 1/0.45} = 2$$

According to the calculation **two theoretical trays** are required.

Example 8.9.3: Graphical determination of the number of trays for desorption with different stripping gas rates Liquid inlet loading $x_{\text{in}} = 0.1 = 10$ mol%

Liquid outlet loading $x_{\text{out}} = 0.01 = 1$ mol%

Stripping gas inlet concentration $y_{\text{in}} = 0$

Example 8.9.3.1: Graphical determination of the number of trays Equilibrium equation: $y = m * x = 2 * x$

(a) Stripping gas rate $G = 100\,\mathrm{kmol/h}$ $L = 100\,\mathrm{kmol/h}$

$L/G = 1 =$ slope of the operating line

Equation of **operating line a**:

$$y = \frac{L}{G} * x + y_{\text{in}} - \frac{L}{G} * x_{\text{out}} = x + 0 - 0.01 = x - 0.01$$

From the graphical representation in Fig. 8.9 a requirement of approximately **2.5 separation stages** results.

This is consistent with the calculated required number of trays in Example 8.9.3.2.

(b) Striping gas rate $G = 200\,\mathrm{kmol/h}$ $L = 100\,\mathrm{kmol/h}$

$L/G = 0.5 =$ slope of the operating line

$$\text{Equation of operating line } b: y = 0.5 * x - 0.005$$

By doubling the stripping gas rate the **separation stages required for stripping are reduced from 2.5 to 1.5 trays**.

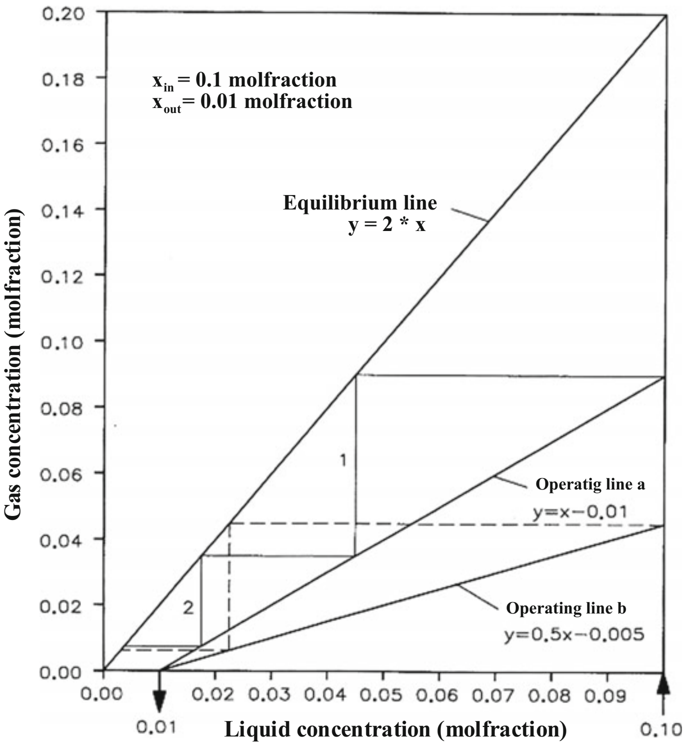


Fig. 8.9 Graphical determination of the number of trays for desorption with different stripping gas rates

The calculation of the number of trays in Example 8.9.3.2 gives the same result.

Example 8.9.3.2: Determination of the number of trays by calculation for a desorption with two stripping gas rates

$$x_{\text{in}} = 0.1\,\text{molfr.} \qquad x_{\text{out}} = 0.01\,\text{molfr.} \qquad y_{\text{in}} = 0\,\text{molfr.}$$

$$\text{Equilibrium:}\, y = 2 * x$$

$$\text{Stripping gas rate}\, G = 100\,\text{kmol/h} \qquad L/G = 1$$

$$S = m * \frac{G}{L} = 2 * 1 = 2 \qquad \frac{1}{S} = 0.5 \qquad M = \frac{0.1}{0.01} = 10$$

$$\text{NT} = \frac{\lg[(1 - 1/S) * M + 1/S]}{\lg S}$$

$$\text{NT} = \frac{\lg[(1 - 0.5) * 10 + 0.5]}{\lg 2} = 2.45$$

The result is consistent with the graphical determination of the number of trays in Fig. 8.9.

Stripping gas rate *G* = 200 kmol/h *L*/*G* = 0.5

$$S = m * \frac{G}{L} = 2 * 2 = 4 \qquad \frac{1}{S} = 0.25 \qquad M = 10$$

$$\mathrm{NT} = \frac{\lg[(1 - 0.25) * 10 + 0.25]}{\lg 4} = 1.47$$

The result is identical to the graphical determination of the number of trays in Fig. 8.9.

8.10 Procedure for Absorber and Stripper Design for Linear Equilibrium and Operating Lines

8.10.1 Design of an Absorption Column

The requirements are as follows (Fig. 8.10):

1. Data collection: gas rates, inlet loading, and outlet loading.
2. Determination of the equation of equilibrium.

$$y = K * x = \frac{p_i}{P_{tot}} = \frac{x * p_{0i}}{P_{tot}} = \frac{H}{P_{tot}} * x = \frac{\gamma * p_{0i} * x}{P_{tot}} (\text{molfraction})$$

3. Determination of the maximum washing fluid loading in the equilibrium with the concentration in the entering gas stream.

$$x^*_{\text{out}} = \frac{y_{\text{in}}}{K}\ (\text{molfr.}) \qquad X^*_{\text{out}} = \frac{x^*}{1 - x^*_{\text{out}}}\ (\text{kmol/kmol})$$

4. Calculation of the required **minimum absorbent rate**.

$$L_{\min} = G * \frac{Y_{\text{in}} - Y_{\text{out}}}{X^*_{\text{out}} - X_{\text{in}}}\ (\text{kmol/h})$$

Actual washing liquid rate $L_{\text{real}} \approx 1.5 * L_{\min}$

5. Checking of the **temperature increase** Δt via the condensation or reaction heat Q.

$$\Delta t = \frac{Q}{L_{\text{real}} * c_L} \quad (^\circ\text{C})$$

Q = released heat (kJ/h) = m (kg/h) * r (kJ/kg)
c_L = specific heat capacity (kJ/kg K)
m = condensed quantity (kg/h)
L_{real} = washing liquid rate (kg/h)

6. Calculation of the **minimum absorbent rate for maximum temperature increase** Δt.

$$L = \frac{Q}{\Delta t * c_L} \quad (\text{kg/h})$$

In high gas inlet concentrations, and low absorbent rates, severe heating can occur!

This can deteriorate the absorption effect.

7. Calculation of the required transfer units NTU_{OG}, or theoretical trays NT, for the given problem.

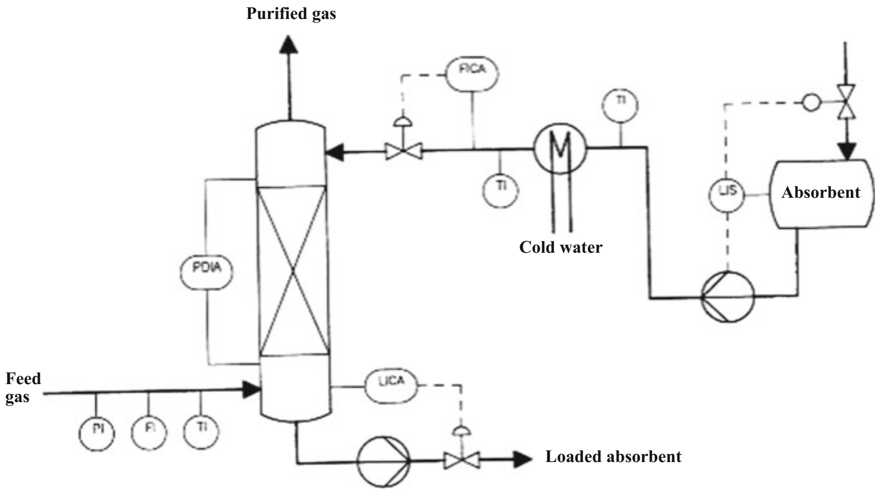


Fig. 8.10 Flow diagram of an absorption unit

$$\mathrm{NTU_{OG}} = \frac{\ln\left[(1-S)*M+S\right]}{1-S} \qquad M = \frac{y_{\mathrm{in}} - m*x_{\mathrm{in}}}{y_{\mathrm{out}} - m*x_{\mathrm{in}}}$$

$$\mathrm{NT} = \frac{\lg\left[(1-S)*M+S\right]}{\lg\frac{1}{S}} \qquad S = m*\frac{G}{L}$$

The required number of separation stages reduces with increasing washing liquid rate.

A larger absorbent rate, with a low concentration of the absorptive, increases the effort required during the cleaning of the wash medium.

Remark In the absorption of **water soluble solvents** in water the equilibrium line is **not linear**. The K value rises both with increasing vapour pressure at higher temperatures and increasing activity coefficients at lower concentrations of the solvent in the liquid.

Example 8.10.1.1: Water wash for exhaust air containing methanol

1. Inlet conditions:

   5000 m^3/h air with a loading of 100 g/m_N^3 methanol.
   Inlet methanol concentration y_{in} = 0.07 molfraction.
   Molar inlet loading = 0.075269 kmol methanol/kmol air.
   Required outlet loading S = 150 mg/m_N^3.
   Outlet concentration y_{out} = 0.000105.
   Molar outlet loading Y_{out} = 0.000105 kmol/kmol.
   Mass balance inlet:

$$4055\,\mathrm{m_N^3/h\ inert\ gas} = 5249\,\mathrm{kg/h\ with}\ 305\,\mathrm{m_N^3/h\ methanol\ vapour} = 436\,\mathrm{kg/h\ methanol}$$
$$\mathrm{Methanol\ rate\ in\ the\ outlet} = 0.6\,\mathrm{kg/h} \qquad \mathrm{Washed\ out\ methanol} = 435.4\,\mathrm{kg/h}$$

2. Equilibrium for a water wash at 30 °C:

$$\mathrm{Vapour\ pressure}\, p_{0i} = 218\,\mathrm{mbar} \quad \mathrm{Activity\ coefficient}\,\gamma = 1.89$$

$$K = \frac{1.89*218}{1013} = 0.4 \qquad y = 0.4*x$$

3. Maximum washing liquid loading X_{out} (kmol/kmol) in the equilibrium to the gas inlet concentration:

y_{in} = 0.07 molefraction methanol

$$x^*_{out} = \frac{y_{in}}{K} = \frac{0.07}{0.4} = 0.175 \text{ Molfr. methanol}$$
$$X^*_{out} = \frac{0.175}{1 - 0.175} = 0.212 \text{ kmol/kmol}$$

4. Minimum absorbent rate for absorption with a wash water with $\boldsymbol{x_{in}}$ **= 0.00013**.

$$L_{min} = \frac{0.075269 - 0.000105}{0.212 - 0.00013} * \frac{4055}{22.4} = 64.2 \text{ kmol/h Water}$$

$$= 1155.2 \text{ kg water/h}$$

Chosen:
L_{real} = 3011 kg/h wash water at 30 °C

5. Check the temperature increase of the condensed methanol (435.4 kg/h)

$$\text{Released heat } Q = m_{\text{Methanol}} * r \qquad r = \text{condensation heat} = 1104 \text{ kJ/kg}$$

$$Q = 435.4 * 1104 = 480{,}680 \text{ kJ/h}$$

$$\Delta t = \frac{Q}{L * c_L} = \frac{480680}{3011 * 4.2} = 38\,^\circ\text{C}$$

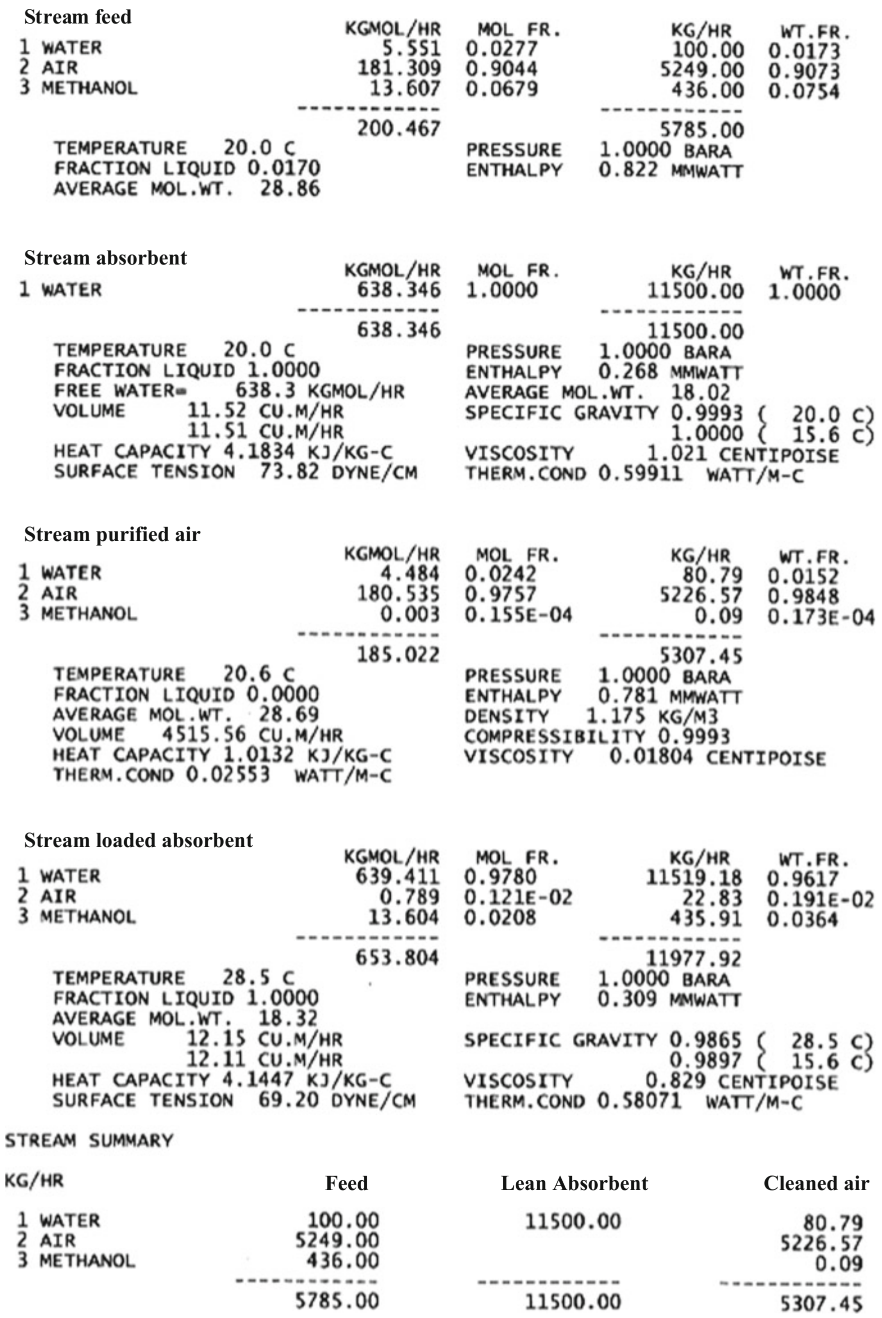
The washing water heats up from around 38 °C to a flow temperature of 68 °C and deteriorates the absorption, because m becomes greater. A temperature rise around 10 °C is the maximum allowable.

6. Calculation of the minimum water rate for an allowable temperature rise Δt = 10 °C.

$$L = \frac{Q}{\Delta t * c_L} = \frac{480680}{10 * 4.2} = 11445 \text{ kg/h Water}$$

7. Calculation of the required transfer units and the required theoretical trays.

At 30 °C with L = 11,500 kg/h for a constant equilibrium line with $y = 0.4 * x$ at 30 °C.



Stream feed

```
                                 KGMOL/HR   MOL FR.        KG/HR   WT.FR.
1 WATER                             5.551   0.0277        100.00   0.0173
2 AIR                             181.309   0.9044       5249.00   0.9073
3 METHANOL                         13.607   0.0679        436.00   0.0754
                             ------------            ------------
                                  200.467                5785.00
   TEMPERATURE    20.0 C                  PRESSURE   1.0000 BARA
   FRACTION LIQUID 0.0170                 ENTHALPY   0.822 MMWATT
   AVERAGE MOL.WT.   28.86
```

Stream absorbent

```
                                 KGMOL/HR   MOL FR.        KG/HR   WT.FR.
1 WATER                           638.346   1.0000      11500.00   1.0000
                             ------------            ------------
                                  638.346               11500.00
   TEMPERATURE    20.0 C                  PRESSURE   1.0000 BARA
   FRACTION LIQUID 1.0000                 ENTHALPY   0.268 MMWATT
   FREE WATER=     638.3 KGMOL/HR         AVERAGE MOL.WT.  18.02
   VOLUME       11.52 CU.M/HR             SPECIFIC GRAVITY 0.9993 (  20.0 C)
                11.51 CU.M/HR                              1.0000 (  15.6 C)
   HEAT CAPACITY 4.1834 KJ/KG-C           VISCOSITY      1.021 CENTIPOISE
   SURFACE TENSION  73.82 DYNE/CM         THERM.COND 0.59911  WATT/M-C
```

Stream purified air

```
                                 KGMOL/HR   MOL FR.        KG/HR   WT.FR.
1 WATER                             4.484   0.0242         80.79   0.0152
2 AIR                             180.535   0.9757       5226.57   0.9848
3 METHANOL                          0.003   0.155E-04       0.09   0.173E-04
                             ------------            ------------
                                  185.022                5307.45
   TEMPERATURE    20.6 C                  PRESSURE   1.0000 BARA
   FRACTION LIQUID 0.0000                 ENTHALPY   0.781 MMWATT
   AVERAGE MOL.WT.   28.69                DENSITY    1.175 KG/M3
   VOLUME     4515.56 CU.M/HR             COMPRESSIBILITY 0.9993
   HEAT CAPACITY 1.0132 KJ/KG-C           VISCOSITY    0.01804 CENTIPOISE
   THERM.COND 0.02553   WATT/M-C
```

Stream loaded absorbent

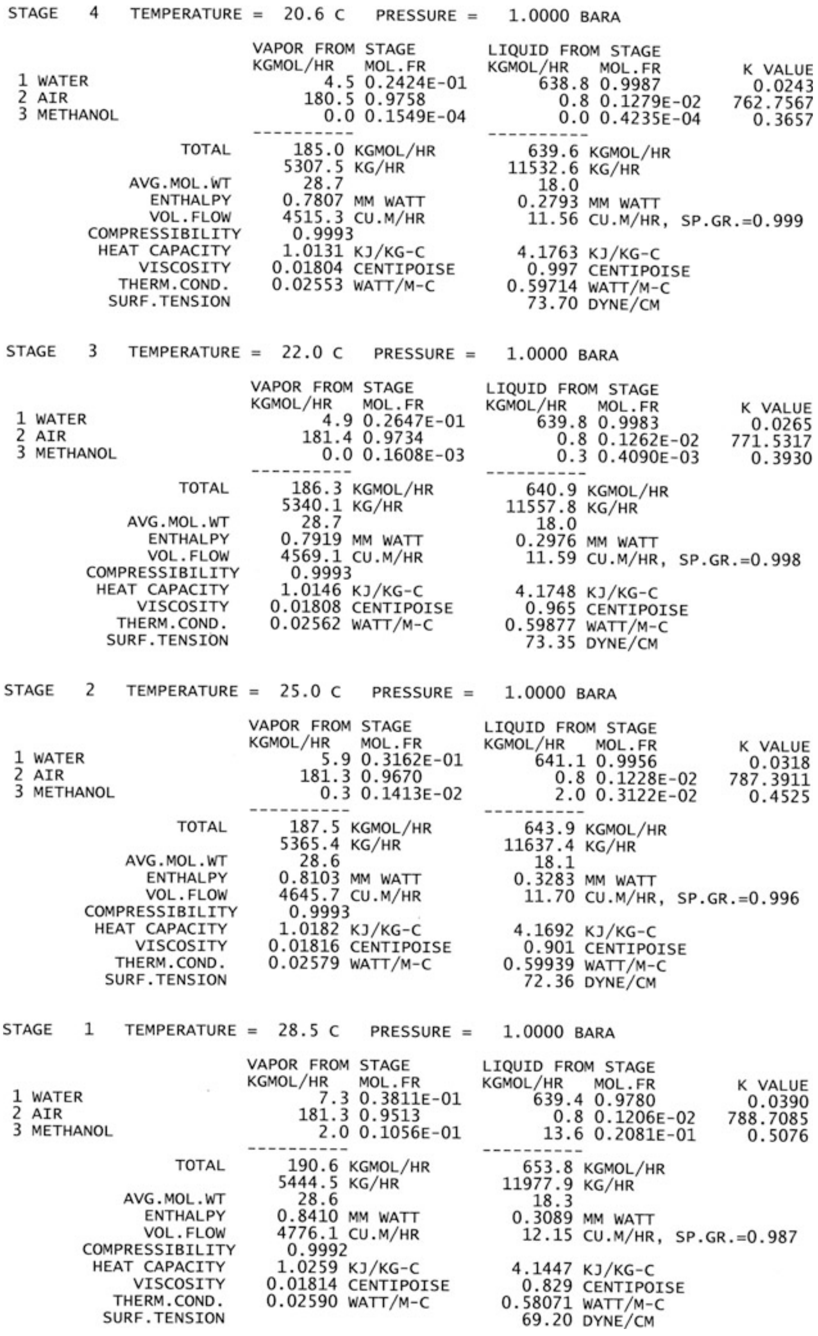
```
                                 KGMOL/HR   MOL FR.        KG/HR   WT.FR.
1 WATER                           639.411   0.9780      11519.18   0.9617
2 AIR                               0.789   0.121E-02      22.83   0.191E-02
3 METHANOL                         13.604   0.0208        435.91   0.0364
                             ------------            ------------
                                  653.804               11977.92
   TEMPERATURE    28.5 C                  PRESSURE   1.0000 BARA
   FRACTION LIQUID 1.0000                 ENTHALPY   0.309 MMWATT
   AVERAGE MOL.WT.   18.32
   VOLUME       12.15 CU.M/HR             SPECIFIC GRAVITY 0.9865 (  28.5 C)
                12.11 CU.M/HR                              0.9897 (  15.6 C)
   HEAT CAPACITY 4.1447 KJ/KG-C           VISCOSITY      0.829 CENTIPOISE
   SURFACE TENSION  69.20 DYNE/CM         THERM.COND 0.58071  WATT/M-C
```

```
STREAM SUMMARY

KG/HR                        Feed        Lean Absorbent        Cleaned air

 1 WATER                   100.00           11500.00                 80.79
 2 AIR                    5249.00                                  5226.57
 3 METHANOL                436.00                                     0.09
                     ------------       ------------          ------------
                          5785.00           11500.00               5307.45
```

Fig. 8.11 Mass balance for the methanol wash with water in Example 8.10.1.1



```
STAGE    4    TEMPERATURE =  20.6 C    PRESSURE =   1.0000 BARA

                              VAPOR FROM STAGE       LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR     KGMOL/HR    MOL.FR        K VALUE
 1 WATER                           4.5 0.2424E-01       638.8 0.9987           0.0243
 2 AIR                           180.5 0.9758             0.8 0.1279E-02     762.7567
 3 METHANOL                        0.0 0.1549E-04         0.0 0.4235E-04       0.3657
                              ----------             ----------
                 TOTAL           185.0 KGMOL/HR         639.6 KGMOL/HR
                                5307.5 KG/HR          11532.6 KG/HR
           AVG.MOL.WT             28.7                   18.0
             ENTHALPY           0.7807 MM WATT         0.2793 MM WATT
             VOL.FLOW           4515.3 CU.M/HR          11.56 CU.M/HR, SP.GR.=0.999
      COMPRESSIBILITY           0.9993
        HEAT CAPACITY           1.0131 KJ/KG-C         4.1763 KJ/KG-C
            VISCOSITY          0.01804 CENTIPOISE       0.997 CENTIPOISE
          THERM.COND.          0.02553 WATT/M-C       0.59714 WATT/M-C
         SURF.TENSION                                   73.70 DYNE/CM

STAGE    3    TEMPERATURE =  22.0 C    PRESSURE =   1.0000 BARA

                              VAPOR FROM STAGE       LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR     KGMOL/HR    MOL.FR        K VALUE
 1 WATER                           4.9 0.2647E-01       639.8 0.9983           0.0265
 2 AIR                           181.4 0.9734             0.8 0.1262E-02     771.5317
 3 METHANOL                        0.0 0.1608E-03         0.3 0.4090E-03       0.3930
                              ----------             ----------
                 TOTAL           186.3 KGMOL/HR         640.9 KGMOL/HR
                                5340.1 KG/HR          11557.8 KG/HR
           AVG.MOL.WT             28.7                   18.0
             ENTHALPY           0.7919 MM WATT         0.2976 MM WATT
             VOL.FLOW           4569.1 CU.M/HR          11.59 CU.M/HR, SP.GR.=0.998
      COMPRESSIBILITY           0.9993
        HEAT CAPACITY           1.0146 KJ/KG-C         4.1748 KJ/KG-C
            VISCOSITY          0.01808 CENTIPOISE       0.965 CENTIPOISE
          THERM.COND.          0.02562 WATT/M-C       0.59877 WATT/M-C
         SURF.TENSION                                   73.35 DYNE/CM

STAGE    2    TEMPERATURE =  25.0 C    PRESSURE =   1.0000 BARA

                              VAPOR FROM STAGE       LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR     KGMOL/HR    MOL.FR        K VALUE
 1 WATER                           5.9 0.3162E-01       641.1 0.9956           0.0318
 2 AIR                           181.3 0.9670             0.8 0.1228E-02     787.3911
 3 METHANOL                        0.3 0.1413E-02         2.0 0.3122E-02       0.4525
                              ----------             ----------
                 TOTAL           187.5 KGMOL/HR         643.9 KGMOL/HR
                                5365.4 KG/HR          11637.4 KG/HR
           AVG.MOL.WT             28.6                   18.1
             ENTHALPY           0.8103 MM WATT         0.3283 MM WATT
             VOL.FLOW           4645.7 CU.M/HR          11.70 CU.M/HR, SP.GR.=0.996
      COMPRESSIBILITY           0.9993
        HEAT CAPACITY           1.0182 KJ/KG-C         4.1692 KJ/KG-C
            VISCOSITY          0.01816 CENTIPOISE       0.901 CENTIPOISE
          THERM.COND.          0.02579 WATT/M-C       0.59939 WATT/M-C
         SURF.TENSION                                   72.36 DYNE/CM

STAGE    1    TEMPERATURE =  28.5 C    PRESSURE =   1.0000 BARA

                              VAPOR FROM STAGE       LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR     KGMOL/HR    MOL.FR        K VALUE
 1 WATER                           7.3 0.3811E-01       639.4 0.9780           0.0390
 2 AIR                           181.3 0.9513             0.8 0.1206E-02     788.7085
 3 METHANOL                        2.0 0.1056E-01        13.6 0.2081E-01       0.5076
                              ----------             ----------
                 TOTAL           190.6 KGMOL/HR         653.8 KGMOL/HR
                                5444.5 KG/HR          11977.9 KG/HR
           AVG.MOL.WT             28.6                   18.3
             ENTHALPY           0.8410 MM WATT         0.3089 MM WATT
             VOL.FLOW           4776.1 CU.M/HR          12.15 CU.M/HR, SP.GR.=0.987
      COMPRESSIBILITY           0.9992
        HEAT CAPACITY           1.0259 KJ/KG-C         4.1447 KJ/KG-C
            VISCOSITY          0.01814 CENTIPOISE       0.829 CENTIPOISE
          THERM.COND.          0.02590 WATT/M-C       0.58071 WATT/M-C
         SURF.TENSION                                   69.20 DYNE/CM
```

Fig. 8.12 Compositions and equilibrium constant *K* on the four trays for the absorption of methanol with water in Example 8.10.1.1

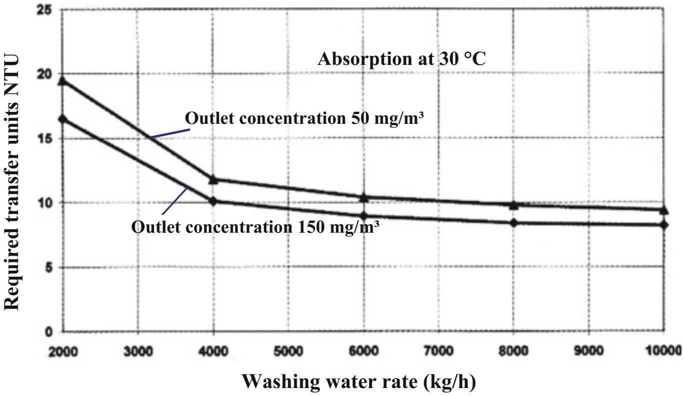


Fig. 8.13 Required transfer units $\mathrm{NTU_{OG}}$ for the purification of exhaust air containing methanol as a function of the wash water rate at a water temperature of 30 °C

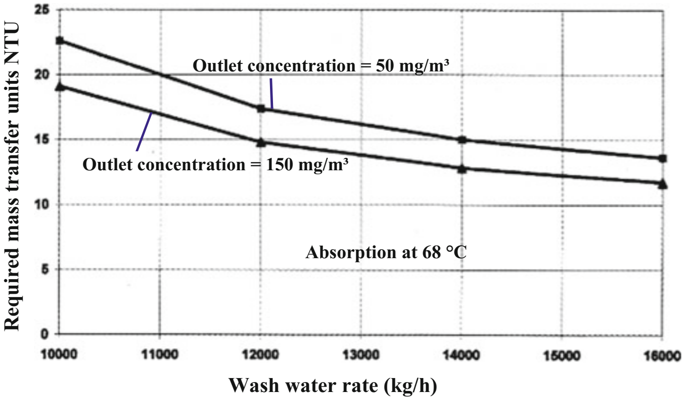


Fig. 8.14 Required transfer units $\mathrm{NTU_{OG}}$ for the purification of exhaust air containing methanol as a function of the wash water rate at a water temperature of 68 °C

$$S = \frac{m * G}{L} = \frac{0.4 * 4055/22.4}{11500/18} = 0.113$$

$$\text{Transfer units } \mathrm{NT_{OG}} = \frac{\ln[(1-S) * M + S]}{1-S} = \frac{\ln[(1-0.113) * 1320 + 0.113]}{1-0.113} = 8$$

$$M = \frac{y_{ein} - m * x_{ein}}{y_{aus} - m * x_{ein}} = \frac{0.07 - 0.4 * 0.00013}{0.000105 - 0.4 * 0.00013} = 1320$$

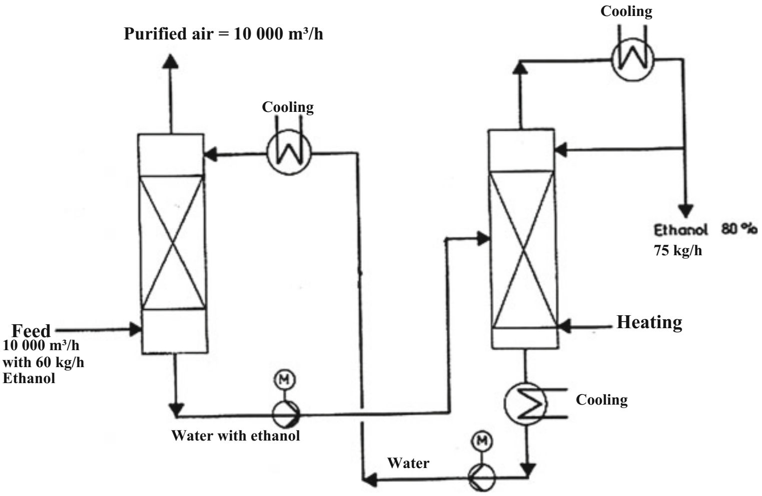


Fig. 8.15 Flow diagram of a water wash for exhaust air containing ethanol

$$\text{Theoretical trays NT} = \frac{\lg[(1-0.113)*1320+0.113]}{\lg\frac{1}{0.113}} = 3.2$$

In Figs. 8.11 and 8.12 the results of the computer simulation with a variable *K* value on the different trays are shown.

Tray 4: $K = 0.3657$ bei 20.6 °C

Tray 3: $K = 0.393$ bei 22 °C

Tray 2: $K = 0.4525$ bei 25 °C

Tray 1: $K = 0.5076$ bei 28.5 °C

The result scarcely differs from calculations by hand calculation $K = 0.4$.

Four theoretical stages are required.

In Figs. 8.13 and 8.14 the required transfer units for the cleaning of exhaust air containing methanol on outlet loadings of 150 and 50 mg/m_N^3, at wash water temperatures of 30 °C and at 68 °C, are shown.

Recommendation:

It is preferably to use low washing liquid temperatures with the absorption.

Example 8.10.1.2: Water wash for exhaust air containing ethanol with fractionation for the separation of the ethanol and for purification of the wash water (Fig. 8.15)

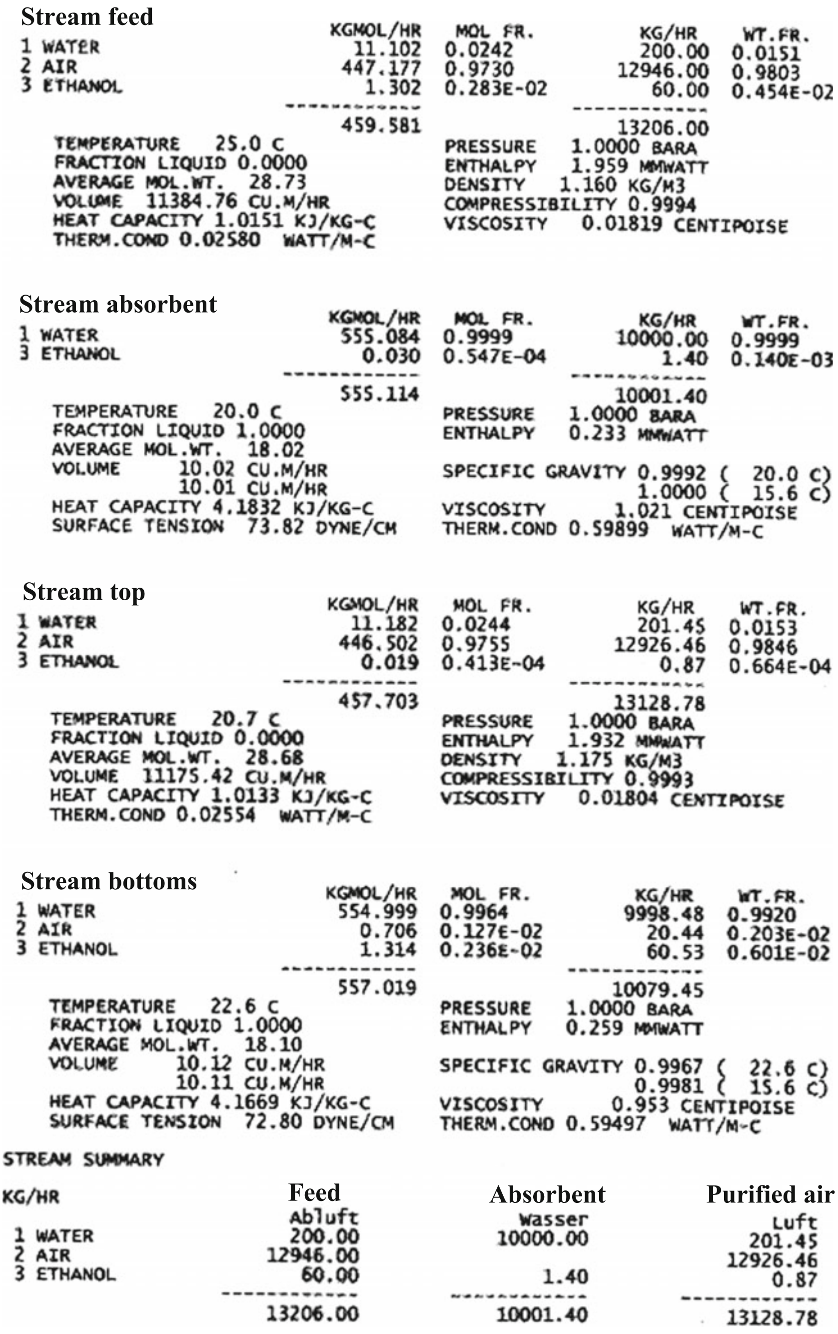
Problem definition: see mass balance in Fig. 8.16

Equilibrium at 20 °C: $m = 0.51$

Inlet ethanol concentration $y_\text{in} = 0.283 * 10^{-2}$ molfraction ethanol

Desired outlet concentration $y_\text{out} = 0.413*10^{-4}$ molfraction ethanol

Washing liquid loading: $0.547 * 10^{-4}$ molfraction ethanol in wash water



Stream feed

```
                          KGMOL/HR  MOL FR.          KG/HR    WT.FR.
1 WATER                     11.102  0.0242          200.00   0.0151
2 AIR                      447.177  0.9730        12946.00   0.9803
3 ETHANOL                    1.302  0.283E-02        60.00   0.454E-02
                      ------------            ------------
                           459.581                13206.00
    TEMPERATURE    25.0 C           PRESSURE    1.0000 BARA
    FRACTION LIQUID 0.0000          ENTHALPY    1.959 MMWATT
    AVERAGE MOL.WT.   28.73         DENSITY    1.160 KG/M3
    VOLUME  11384.76 CU.M/HR        COMPRESSIBILITY 0.9994
    HEAT CAPACITY 1.0151 KJ/KG-C    VISCOSITY    0.01819 CENTIPOISE
    THERM.COND 0.02580   WATT/M-C
```

Stream absorbent

```
                          KGMOL/HR  MOL FR.          KG/HR    WT.FR.
1 WATER                    555.084  0.9999        10000.00   0.9999
3 ETHANOL                    0.030  0.547E-04         1.40   0.140E-03
                      ------------            ------------
                           555.114                10001.40
    TEMPERATURE    20.0 C           PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000          ENTHALPY    0.233 MMWATT
    AVERAGE MOL.WT.   18.02
    VOLUME          10.02 CU.M/HR   SPECIFIC GRAVITY 0.9992 (  20.0 C)
                    10.01 CU.M/HR                    1.0000 (  15.6 C)
    HEAT CAPACITY 4.1832 KJ/KG-C    VISCOSITY       1.021 CENTIPOISE
    SURFACE TENSION  73.82 DYNE/CM  THERM.COND 0.59899  WATT/M-C
```

Stream top

```
                          KGMOL/HR  MOL FR.          KG/HR    WT.FR.
1 WATER                     11.182  0.0244          201.45   0.0153
2 AIR                      446.502  0.9755        12926.46   0.9846
3 ETHANOL                    0.019  0.413E-04         0.87   0.664E-04
                      ------------            ------------
                           457.703                13128.78
    TEMPERATURE    20.7 C           PRESSURE    1.0000 BARA
    FRACTION LIQUID 0.0000          ENTHALPY    1.932 MMWATT
    AVERAGE MOL.WT.   28.68         DENSITY    1.175 KG/M3
    VOLUME  11175.42 CU.M/HR        COMPRESSIBILITY 0.9993
    HEAT CAPACITY 1.0133 KJ/KG-C    VISCOSITY    0.01804 CENTIPOISE
    THERM.COND 0.02554   WATT/M-C
```

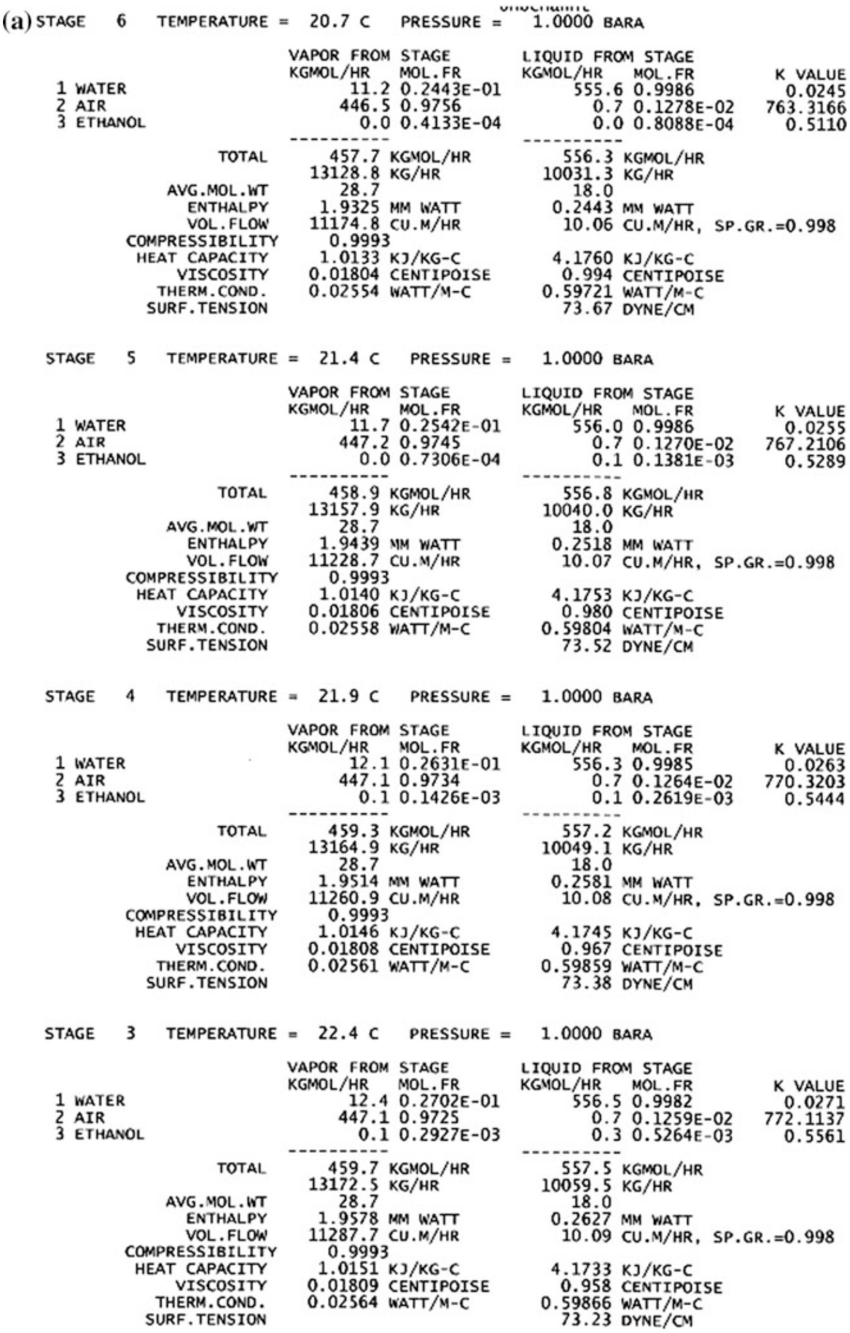
Stream bottoms

```
                          KGMOL/HR  MOL FR.          KG/HR    WT.FR.
1 WATER                    554.999  0.9964         9998.48   0.9920
2 AIR                        0.706  0.127E-02        20.44   0.203E-02
3 ETHANOL                    1.314  0.236E-02        60.53   0.601E-02
                      ------------            ------------
                           557.019                10079.45
    TEMPERATURE    22.6 C           PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000          ENTHALPY    0.259 MMWATT
    AVERAGE MOL.WT.   18.10
    VOLUME          10.12 CU.M/HR   SPECIFIC GRAVITY 0.9967 (  22.6 C)
                    10.11 CU.M/HR                    0.9981 (  15.6 C)
    HEAT CAPACITY 4.1669 KJ/KG-C    VISCOSITY       0.953 CENTIPOISE
    SURFACE TENSION  72.80 DYNE/CM  THERM.COND 0.59497  WATT/M-C
```

```
STREAM SUMMARY

KG/HR                      Feed          Absorbent       Purified air
                          Abluft           Wasser               Luft
 1 WATER                  200.00         10000.00             201.45
 2 AIR                  12946.00                            12926.46
 3 ETHANOL                 60.00             1.40               0.87
                    ------------     ------------       ------------
                        13206.00         10001.40           13128.78
```

Fig. 8.16 Mass balance for an ethanol wash (Example 8.10.1.2)



```
STAGE    6    TEMPERATURE =   20.7 C     PRESSURE =    1.0000 BARA

                          VAPOR FROM STAGE        LIQUID FROM STAGE
                          KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR          K VALUE
 1 WATER                        11.2 0.2443E-01        555.6 0.9986             0.0245
 2 AIR                         446.5 0.9756              0.7 0.1278E-02       763.3166
 3 ETHANOL                       0.0 0.4133E-04          0.0 0.8088E-04         0.5110
                          ----------              ----------
                 TOTAL         457.7 KGMOL/HR          556.3 KGMOL/HR
                             13128.8 KG/HR           10031.3 KG/HR
           AVG.MOL.WT           28.7                    18.0
             ENTHALPY         1.9325 MM WATT          0.2443 MM WATT
             VOL.FLOW        11174.8 CU.M/HR           10.06 CU.M/HR, SP.GR.=0.998
      COMPRESSIBILITY         0.9993
        HEAT CAPACITY         1.0133 KJ/KG-C          4.1760 KJ/KG-C
            VISCOSITY        0.01804 CENTIPOISE        0.994 CENTIPOISE
          THERM.COND.        0.02554 WATT/M-C        0.59721 WATT/M-C
         SURF.TENSION                                  73.67 DYNE/CM

STAGE    5    TEMPERATURE =   21.4 C     PRESSURE =    1.0000 BARA

                          VAPOR FROM STAGE        LIQUID FROM STAGE
                          KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR          K VALUE
 1 WATER                        11.7 0.2542E-01        556.0 0.9986             0.0255
 2 AIR                         447.2 0.9745              0.7 0.1270E-02       767.2106
 3 ETHANOL                       0.0 0.7306E-04          0.1 0.1381E-03         0.5289
                          ----------              ----------
                 TOTAL         458.9 KGMOL/HR          556.8 KGMOL/HR
                             13157.9 KG/HR           10040.0 KG/HR
           AVG.MOL.WT           28.7                    18.0
             ENTHALPY         1.9439 MM WATT          0.2518 MM WATT
             VOL.FLOW        11228.7 CU.M/HR           10.07 CU.M/HR, SP.GR.=0.998
      COMPRESSIBILITY         0.9993
        HEAT CAPACITY         1.0140 KJ/KG-C          4.1753 KJ/KG-C
            VISCOSITY        0.01806 CENTIPOISE        0.980 CENTIPOISE
          THERM.COND.        0.02558 WATT/M-C        0.59804 WATT/M-C
         SURF.TENSION                                  73.52 DYNE/CM

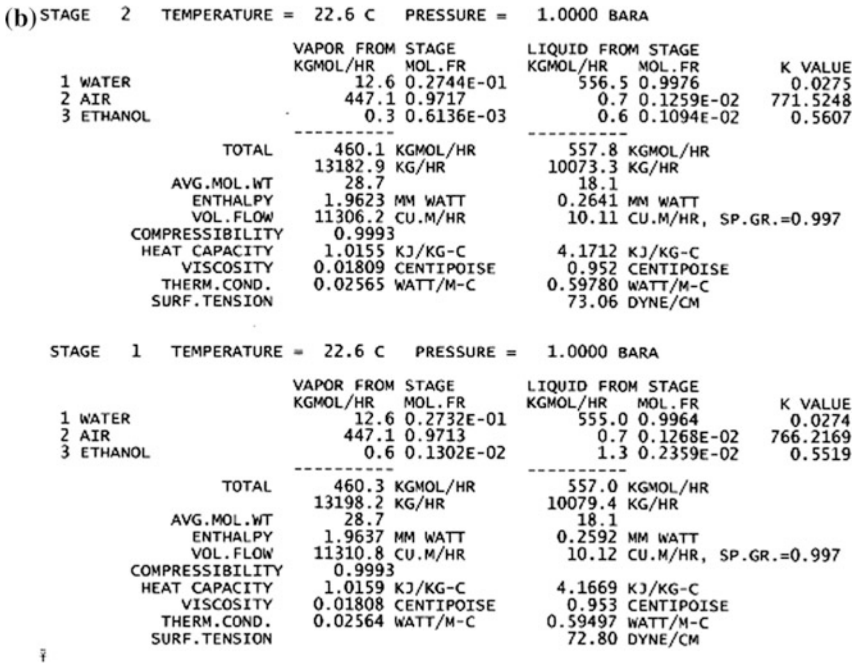
STAGE    4    TEMPERATURE =   21.9 C     PRESSURE =    1.0000 BARA

                          VAPOR FROM STAGE        LIQUID FROM STAGE
                          KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR          K VALUE
 1 WATER                        12.1 0.2631E-01        556.3 0.9985             0.0263
 2 AIR                         447.1 0.9734              0.7 0.1264E-02       770.3203
 3 ETHANOL                       0.1 0.1426E-03          0.1 0.2619E-03         0.5444
                          ----------              ----------
                 TOTAL         459.3 KGMOL/HR          557.2 KGMOL/HR
                             13164.9 KG/HR           10049.1 KG/HR
           AVG.MOL.WT           28.7                    18.0
             ENTHALPY         1.9514 MM WATT          0.2581 MM WATT
             VOL.FLOW        11260.9 CU.M/HR           10.08 CU.M/HR, SP.GR.=0.998
      COMPRESSIBILITY         0.9993
        HEAT CAPACITY         1.0146 KJ/KG-C          4.1745 KJ/KG-C
            VISCOSITY        0.01808 CENTIPOISE        0.967 CENTIPOISE
          THERM.COND.        0.02561 WATT/M-C        0.59859 WATT/M-C
         SURF.TENSION                                  73.38 DYNE/CM

STAGE    3    TEMPERATURE =   22.4 C     PRESSURE =    1.0000 BARA

                          VAPOR FROM STAGE        LIQUID FROM STAGE
                          KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR          K VALUE
 1 WATER                        12.4 0.2702E-01        556.5 0.9982             0.0271
 2 AIR                         447.1 0.9725              0.7 0.1259E-02       772.1137
 3 ETHANOL                       0.1 0.2927E-03          0.3 0.5264E-03         0.5561
                          ----------              ----------
                 TOTAL         459.7 KGMOL/HR          557.5 KGMOL/HR
                             13172.5 KG/HR           10059.5 KG/HR
           AVG.MOL.WT           28.7                    18.0
             ENTHALPY         1.9578 MM WATT          0.2627 MM WATT
             VOL.FLOW        11287.7 CU.M/HR           10.09 CU.M/HR, SP.GR.=0.998
      COMPRESSIBILITY         0.9993
        HEAT CAPACITY         1.0151 KJ/KG-C          4.1733 KJ/KG-C
            VISCOSITY        0.01809 CENTIPOISE        0.958 CENTIPOISE
          THERM.COND.        0.02564 WATT/M-C        0.59866 WATT/M-C
         SURF.TENSION                                  73.23 DYNE/CM
```

Fig. 8.17 **a** Compositions and equilibrium constants on Tray 6 (at the *top*) through to Tray 3, for Example 8.10.1.2. **b** Compositions and equilibrium constants on Trays 2 and 1 (*bottoms*) for Example 8.10.1.2



```
(b)STAGE   2   TEMPERATURE =  22.6 C    PRESSURE =    1.0000 BARA

                              VAPOR FROM STAGE        LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR       K VALUE
   1 WATER                        12.6 0.2744E-01        556.5 0.9976          0.0275
   2 AIR                         447.1 0.9717              0.7 0.1259E-02    771.5248
   3 ETHANOL                       0.3 0.6136E-03          0.6 0.1094E-02      0.5607
                              ----------              ----------
                    TOTAL        460.1 KGMOL/HR          557.8 KGMOL/HR
                               13182.9 KG/HR           10073.3 KG/HR
              AVG.MOL.WT          28.7                    18.1
                ENTHALPY        1.9623 MM WATT          0.2641 MM WATT
                VOL.FLOW       11306.2 CU.M/HR           10.11 CU.M/HR, SP.GR.=0.997
          COMPRESSIBILITY       0.9993
           HEAT CAPACITY        1.0155 KJ/KG-C          4.1712 KJ/KG-C
               VISCOSITY       0.01809 CENTIPOISE        0.952 CENTIPOISE
              THERM.COND.      0.02565 WATT/M-C        0.59780 WATT/M-C
             SURF.TENSION                                73.06 DYNE/CM

   STAGE   1   TEMPERATURE =  22.6 C    PRESSURE =    1.0000 BARA

                              VAPOR FROM STAGE        LIQUID FROM STAGE
                              KGMOL/HR    MOL.FR      KGMOL/HR    MOL.FR       K VALUE
   1 WATER                        12.6 0.2732E-01        555.0 0.9964          0.0274
   2 AIR                         447.1 0.9713              0.7 0.1268E-02    766.2169
   3 ETHANOL                       0.6 0.1302E-02          1.3 0.2359E-02      0.5519
                              ----------              ----------
                    TOTAL        460.3 KGMOL/HR          557.0 KGMOL/HR
                               13198.2 KG/HR           10079.4 KG/HR
              AVG.MOL.WT          28.7                    18.1
                ENTHALPY        1.9637 MM WATT          0.2592 MM WATT
                VOL.FLOW       11310.8 CU.M/HR           10.12 CU.M/HR, SP.GR.=0.997
          COMPRESSIBILITY       0.9993
           HEAT CAPACITY        1.0159 KJ/KG-C          4.1669 KJ/KG-C
               VISCOSITY       0.01808 CENTIPOISE        0.953 CENTIPOISE
              THERM.COND.      0.02564 WATT/M-C        0.59497 WATT/M-C
             SURF.TENSION                                72.80 DYNE/CM
```

◄**Fig. 8.17** (continued)

Calculations for a linear equilibrium line:

$$S = m * \frac{G}{L} = 0.51 * \frac{459.58}{555.1} = 0.422$$

$$M = \frac{y_{\text{ein}} - m * x_{\text{ein}}}{y_{\text{aus}} - m * x_{\text{ein}}} = \frac{0.283 * 10^{-2} - 0.51 * 0.547 * 10^{-4}}{0.413 * 10^{-4} - 0.51 * 0.547 * 10^{-4}} = 209$$

$$\text{NT} = \frac{\lg[(1-S) * M + S]}{\lg \frac{1}{S}} = \frac{\lg((1-0.422) * 209 + 0.422)}{\lg \frac{1}{0.422}} = 5.57$$

$$\text{NTU} = \frac{\ln[(1-S) * M + S]}{1-S} = \frac{\ln[(1-0.422) * 209 + 0.422]}{1-0.422} = 8.3$$

In Figs. 8.16 and 8.17 the results of the computer simulation, with variable *K* values on the different trays, are given. The results are largely consistent with hand calculations.

In both cases six theoretical trays are required.

Conclusion:

In the calculation with the constant equilibrium line, and in the computer simulation with variable *K* values, six theoretical stages for the absorption of the ethanol are required.

From the Fig. 8.17a, b it can be seen that the equilibrium constant on the different trays changes because the temperature and the concentrations of the ethanol in the liquid phase vary.

The vapour pressure increases with rising temperature. This causes the K value to rise.

With decreasing ethanol concentration in the liquid phase the activity coefficient rises.

8.10.2 Design of a Desorption/Stripper Column

1. Collection of data for the problem: liquid rates, inlet loadings and outlet loadings, and stripping medium (Fig. 8.18).
2. Determination of the equilibrium equation.

$$y = K * x = \frac{p_i}{P_{\text{tot}}} = \frac{x * p_{0\text{i}}}{P_{\text{tot}}} = \frac{H}{P_{\text{tot}}} * x = \frac{\gamma * p_{0\text{i}} * x}{P_{\text{tot}}}$$

3. Determination of the maximum gas composition y^* from the stripping gas in the equilibrium to the stripping gas entering the loaded washing liquid.

$$y^*_{\text{aus}} = m * x_{\text{in}} \ (\text{Molfr.}) \qquad Y^*_{\text{out}} = \frac{y^*_{\text{out}}}{1 - y^*_{\text{out}}} \ (\text{kmol/kmol})$$

4. Determination of the minimum stripping gas rate $G_{\min}$.

$$G_{\min} = L * \frac{X_{\text{in}} - X_{\text{out}}}{Y^*_{\text{out}} - Y_{\text{in}}} \ (\text{kmol/h})$$

5. Checking the cooling by evaporation.

$$\Delta t = \frac{Q\,(\text{kJ/h})}{L\,(\text{kg/h}) * c_L\,(\text{kJ/kg K})} \ (^{\circ}\text{C})$$

6. Calculation of the required transfer units NTU_{OL}, or theoretical trays NT, for a linear equilibrium line with a constant K value.

$$\mathrm{NTU}_{\mathrm{OL}} = \frac{\ln[(1 - 1/S) * M + 1/S]}{1 - 1/S} \qquad M = \frac{x_{\mathrm{in}} - y_{\mathrm{in}}/m}{x_{\mathrm{out}} - y_{\mathrm{in}}/m}$$

$$NT = \frac{\lg[(1 - 1/S) * M + 1/S]}{\lg S} \qquad S = m * \frac{G}{L}$$

Calculation of NTU_{OL} with a logarithmic concentration gradient:

$$NTU_{\mathrm{OL}} = \frac{x_{\mathrm{out}} - x_{\mathrm{in}}}{\Delta x_{\ln}}$$

$$\Delta x_{\ln} = \frac{\left(x_{\mathrm{in}} - x^*_{\mathrm{in}}\right) - \left(x_{\mathrm{out}} - x^*_{\mathrm{out}}\right)}{\ln \frac{\left(x_{\mathrm{in}} - x^*_{\mathrm{in}}\right)}{\left(x_{\mathrm{out}} - x^*_{\mathrm{out}}\right)}}$$

Note:

When stripping water soluble solvents out of water with steam the equilibrium constant K changes with the concentration and the temperature because the vapour pressure and activity coefficient change.

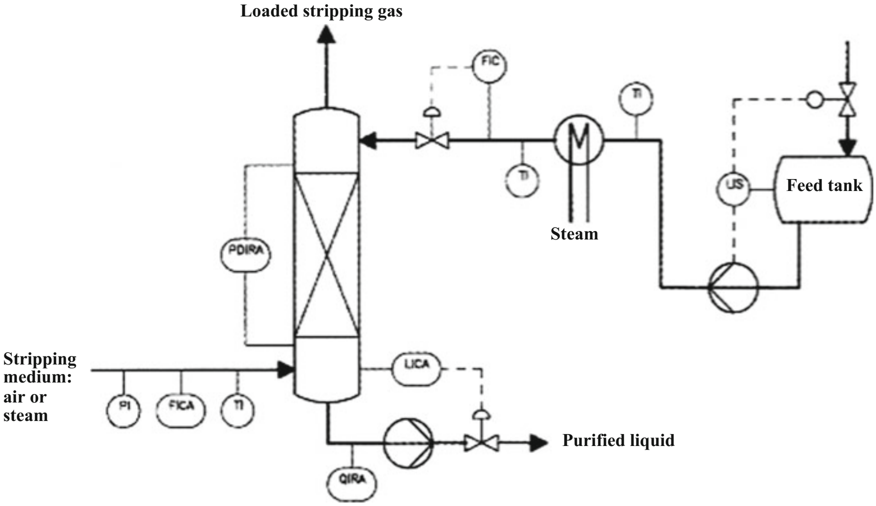


Fig. 8.18 Flow diagram of a stripping column

Example 8.10.2.1: Desorption of hexane from wash oil with steam

1. Data for the design

$$\text{Inlet conditions}: 6728\,\text{kg oil}\,(M = 360)\,\text{with}\,223\,\text{kg hexane}\,(M = 86)$$
$$B_{\text{in}} = 0.033\,\text{kg hexane/kg oil} \qquad X_{\text{in}} = 0.1388\,\text{kmol hexane/kmol oil}$$
$$x_{\text{in}} = 0.1218\,\text{molfraction hexane in the oil}$$
$$\text{Outlet conditions}: \text{Desorption to}\,0.1\,\text{weight}\,\%\,\text{hexane in the oil}\,(7\,\text{kg hexane})$$
$$x_{\text{out}} = 0.004\,\text{molfraction hexane in the oil}$$
$$X_{\text{out}} = 0.00402\,\text{kmol hexane/kmol oil} \qquad B_{\text{out}} = 0.00096\,\text{kg hexane/kg oil}$$

2. $\text{Equilibrium at}\,120\,^\circ\text{C and}\,P_{\text{ges}} = 1013\,\text{mbar} \qquad p_{0\text{Hexan}} = 3971\,\text{mbar}$

$$K = \frac{p_{0\text{i}}}{P_{\text{ges}}} = \frac{3971}{1013} = 3.93$$

3. Maximum stripping gas loading in the equilibrium to the entering loaded oil

$$x_{\text{in}} = 0.1218 \quad \text{molfr.} \qquad y*_{\text{out}} = 3.93 * 0.1218 = 0.479\,\text{molfr.}$$

$$Y^*_{\text{out}} = \frac{0.479}{1 - 0.479} = 0.918\,\text{kmol/kmol}$$

4. Determine minimum stripping steam rate G_{min} ($y_{\text{in}} = 0$)

$$G_{\text{min}} = \frac{6728}{360} * \frac{0.1388 - 0.00402}{0.918 - 0} = 2.74\,\text{kmol steam/h} = 49.4\,\text{kg/h}$$

Chosen:
360 kg/h steam

$$B = \frac{223 - 7}{360} = 0.6\,\text{kg Hexan/kg Dampf}$$
$$Y_{\text{out}} = 0.1255\,\text{kmol Hexan/kmol Dampf}$$

5. Cooling by evaporation of 216 kg hexane: $Q = 216 * 333 = 72{,}000$ kJ/h

$$\Delta t = \frac{72{,}000}{6728 * 2.1} = 5.1\,^\circ\text{C} \qquad c_L = 2.1\,\text{kJ/kg K for washing media}$$

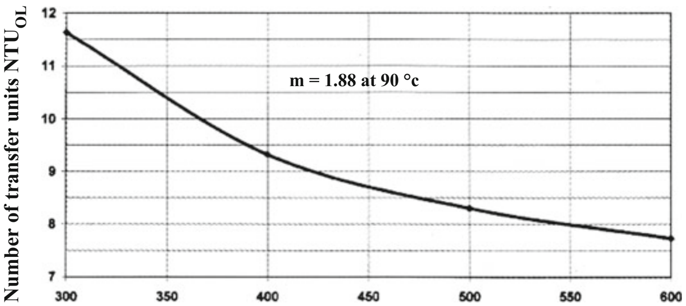


Fig. 8.19 Required transfer units NTU_{OL} for the desorption of hexane from wash oil to a rest loading of 100 mg/kg oil as function of the stripping steam rate

6. Calculation of the transfer units NTU_{OL}

$$\frac{1}{S} = \frac{6728/360}{3.93 * 360/18} = 0.2377 \qquad M = \frac{0.1218 - 0}{0.004 - 0} = 30.45$$

$$NTU_{OL} = \frac{\ln[(1 - 0.2377) * 30.45 + 0.2377]}{1 - 0.2377} = 4.14$$

With the logarithmic concentration difference:

$$x_{in} = 0.1218 \qquad x_{out} = 0.004 \qquad y_{in} = 0 * x^*_{out} = 0 \quad Y_{out} = 0.1255$$

$$y_{out} = \frac{0.1255}{0.1255 + 1} = 0.1115 \qquad x^*_{in} = \frac{0.1115}{3.93} = 0.02839$$

$$\Delta x_{ln} = \frac{(0.1218 - 0.02839) - (0.004 - 0)}{\ln\frac{(0.1218-0.02839)}{(0.004-0)}} = 0.02838$$

$$NTU_{OL} = \frac{0.1218 - 0.004}{0.02838} = 4.15$$

Figure 8.19 shows how the number of required transfer units reduces with increasing stripping steam rate.

8.11 Water Purification Air Stripper [13–16]

Air strippers are used for the purification of water contaminated with solvents.

The function of an air stripper for water purification can be seen in Fig. 8.20.

The water polluted with solvents is introduced at the top of the stripping column and streams through the mass transfer units—trays or packings—from top to bottom.

The air streaming from bottom to top in the countercurrent direction enters the column in the bottom and functions as a carrier gas capturing the solvents from the water.

The recycle air from the adsorber can be used in order to reduce the fresh air requirement.

The stripping air is cooled down to the wet-bulb temperature as it streams through the column because the air only carries water up to the saturation limit. Cooling deteriorates the effectiveness of the stripper since the equilibrium factor (m) reduces with decreasing temperature.

The stripping air, loaded with solvent that is streaming out on the top of the column, is subsequently purified in an active carbon adsorber. In an adsorber plant in which steam is used for the regeneration the condensate which is contaminated with a solvent is fed back from the regeneration after the decanter for the solvent separation in the stripping column.

Alternatively, the stripping air, loaded with the solvent, can be purified by oxidation.

Due to the low solvent compositions in the water the design becomes simple:

$$\text{Minimum stripping air rate } G_{\min} \approx \frac{L}{m} \qquad G_{\text{real}} = 10 * G_{\min}$$

$$\text{NTU}_{\text{OL}} = \frac{1}{1 - 1/S} * \ln\left[(1 - 1/S) * \frac{x_{\text{in}}}{x_{\text{out}}} + \frac{1}{S}\right]$$

Minimum transfer units for very large excess air rate

$$\text{NTU}_{\text{OL}} \approx \ln \frac{x_1}{x_2}$$

What is important for the required separation effort—number of trays and stripping air rate—are the equilibrium and the required purification grade R.

$$R = \frac{x_{\text{out}}}{x_{\text{in}}}$$

In Fig. 8.21 the number of required theoretical trays for $R = 0.0001$ is plotted as a function of the stripping air rate for four solvents with different equilibrium constants $K = \text{m}$.

From Fig. 8.21 the following relationships can be derived:

The higher the equilibrium constant K, the lower the required separation effort.

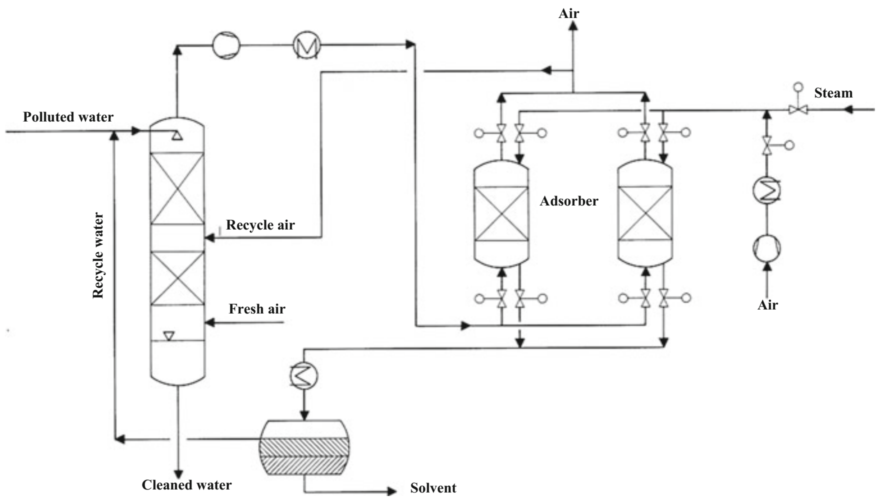


Fig. 8.20 Air stripper for water containing solvents

For instance, for trichloroethene with $K = 650$ only 4 theoretical stages and 2000 m^3/h of stripping air are needed. For 1,2 dichloromethane with $K = 61.2$, on the other hand, you need 10 trays and 5000 m^3/h of stripping air.

The design follows for the component with the lowest equilibrium constant K.

If water soluble material is contained in the water, for instance acetone, the equilibrium seriously deteriorates due to their mutual interaction.

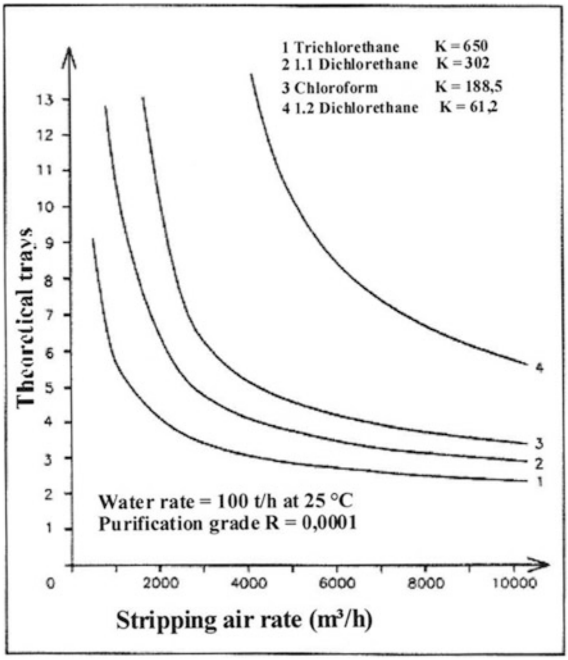
Basically, the required number of theoretical trays reduces with increasing stripping air rate. After falling below a critical stripping air rate the required number of trays increases rapidly with the required purification level.

A low stripping air rate, with high solvent concentration, should be preferred in order to reduce the effort for air purification in the adsorber.

Example 8.11.1: 1000 kg/h water (55.55 kmol/h) with 100 ppm solvent (100 g) is to be purified to 5 ppm (5 g)

$$\begin{array}{ll}
\text{Trichlorethene with } m = 650 & \text{Dichlormethane with } m = 137.6 \\
G_{\text{min}} = \frac{55.55}{650} = 0.085\ \text{kmol/h} & G_{\text{min}} = \frac{55.55}{137.6} = 0.403\ \text{kmol/h} \\
G_{\text{min}} = 1.9\ \text{m}_N^3/h & G_{\text{min}} = 9\ \text{m}_N^3/h \\
G_{\text{real}} = 10 * 1.9 = 19\ \text{m}_N^3/\text{h} & G_{\text{real}} = 10 * 9 = 90\ \text{m}_N^3/\text{h} \\
\text{Air loading } C = \frac{95}{19} = 5\ \text{g/m}_N^3 & \text{Air loading } C = \frac{95}{90} = 1.05\ \text{g/m}_N^3 \\
\text{NTU}_{\text{OL}} = \ln\frac{100}{5} = 3 & \text{NTU}_{\text{OL}} = \ln\frac{100}{5} = 3
\end{array}$$

Fig. 8.21 Required number of theoretical trays for the stripping of different solvents from water as a function of the stripping air rate



Calculations for other stripping air rates:

Trichloroethene			Dichloromethane		
Stripping air	NTU	C	Stripping air	NTU	C
(m_N^3/h)	–	(g/m_N^3)	(m_N^3/h)	–	(g/m_N^3)
2.1	11.1	45.5	8.9	22.4	10.6
2.4	7.7	39.7	9.3	15.3	10.2
3.0	5.6	31.5	10	10.6	9.4
4.2	4.4	22.4	11.6	7.5	8.2
5.8	3.9	16.4	13.5	6	7
7.7	3.6	12.3	15.4	5.3	6.2
38.6	3.1	2.5	38.6	3.6	2.5
77.2	3.05	1.2	77.2	3.2	1.2

Conclusion:

With a larger stripping air rate the required number of separation stages and the solvent concentration C in the escaping stripping air are reduced.

The number of the required theoretical trays NT for a specific purification level R is determined as follows:

$$\mathrm{NT} = \frac{\lg\left[\frac{1}{R} + \left(1 - \frac{1}{R}/S\right)\right]}{\lg[\eta * (S-1) + 1]} \quad \text{for } S \neq 1 \qquad \eta = \text{Tray efficiency}$$

$$\mathrm{NT} = \frac{1/R - 1}{\eta} \quad \text{for } S = 1$$

In Fig. 8.22 the required number of theoretical trays for purification level R, along with the tray efficiency, are plotted as a function of the stripping factor S.

Example 8.11.2: Required number of theoretical trays for stripping out trichloroethene from water at 25 °C Equilibrium constant $K = 650$

$$\begin{array}{ll} x_{\mathrm{in}} = 100\,\mathrm{ppm} = 0.0001\,\mathrm{molfr.} & x_{\mathrm{out}} = 0.01\,\mathrm{ppm} = 1 * 10^{-8}\mathrm{molfr.} \\ L = 17.514\,\mathrm{kmol/h} & G = 47.14\,\mathrm{kmol/h} \quad \eta = 0.6 \end{array}$$

$$R = \frac{0.01}{100} = 0.0001 \qquad S = \frac{m * G}{L} = 650 * \frac{47.14}{17514} = 1.75$$

$$\mathrm{NT} = \frac{\lg\left[1/0.0001 + (1 - 1/0.0001)/1.75\right]}{\lg[0.6 * (1.75 - 1) + 1]} = 22.5$$

The **composition on the individual trays** is calculated as follows:

$$x_n = \frac{S-1}{S * [\eta * (S-1) + 1]^{\mathrm{NT}} - 1} * x_{\mathrm{in}} \quad \mathrm{x_n} = \text{Concentration on the tray } n$$

Example 8.11.3: Calculation of the concentration on tray 15

$$\eta = 1 \quad S = 1.75 \quad x_{\mathrm{in}} = 100\,\mathrm{ppm}\,(\mathrm{molar})$$

$$x_{15} = \frac{1.75 - 1}{1.75 * [1 * (1.75 - 1) + 1]^{15}} * 100 = 0.0097\ \mathrm{ppm}\,(\mathrm{molar}) = 1 * 10^{-8}\,\mathrm{Molfr.}$$

Conversion to weight-ppm:

$$x_{\mathrm{Gew}} = \frac{x_m}{1 - x_m} * \frac{M_{\mathrm{LM}}}{18} = \frac{1 * 10^{-8}}{1 - 1 * 10^{-8}} * \frac{131.4}{18} = 7.3 * 10^{-8} = 0.073\,\mathrm{weight\ ppm}$$

The calculation of the concentration on the last bottom tray is very helpful if different solvents must be stripped out from the water.

The column is initially designed for the component with the lowest equilibrium constant *K*.

For this problem, a certain number NT of theoretical trays for the specific purification level *R*, and the stripping factor *S*, of the component with the lowest equilibrium value *K* follow.

Subsequently, the composition of the other components in the bottoms draw with the given number of theoretical trays NT is determined.

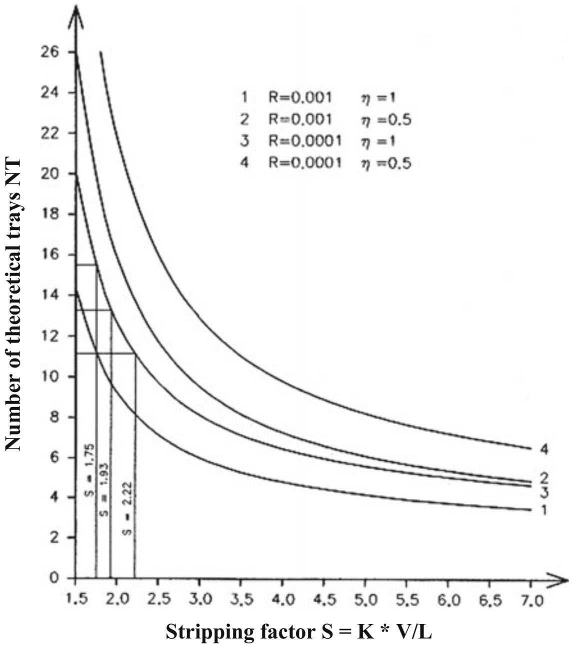


Fig. 8.22 Required theoretical stages as a function of the stripping factor for different purification grades R and efficiencies η

8.12 Steam Stripper [17–21]

8.12.1 Process Description

Steam strippers have the advantage that the vapour–solvent mixture exiting at the top of the column can be condensed.

With the air stripper the exhaust air, containing the solvent, must be purified by adsorption or burning.

Since a steam stripper operates under atmospheric conditions at 100 °C the vapour pressure, and thus also the equilibrium constant K, is much higher than with air stripping at 30 °C.

Due to the mostly high activity coefficients of solvents in water, even relatively high boiling components such as toluene, xylene, fluorine, and anthracene can be stripped out.

In Fig. 8.23 a simple steam stripper for a water soluble solvent is shown.

The polluted water is preheated to about 90 °C by heat exchange with the hot purified water drawn at the bottom and is then fed to the column top.

The steam introduced to the column bottom heats the water, streaming downward from the column top, to 100 °C. The steam which is not used in the column for heating streams together with the stripped out solvents into the condenser, in which the mixture is liquified.

The distillate of solvent and water should form two phases.

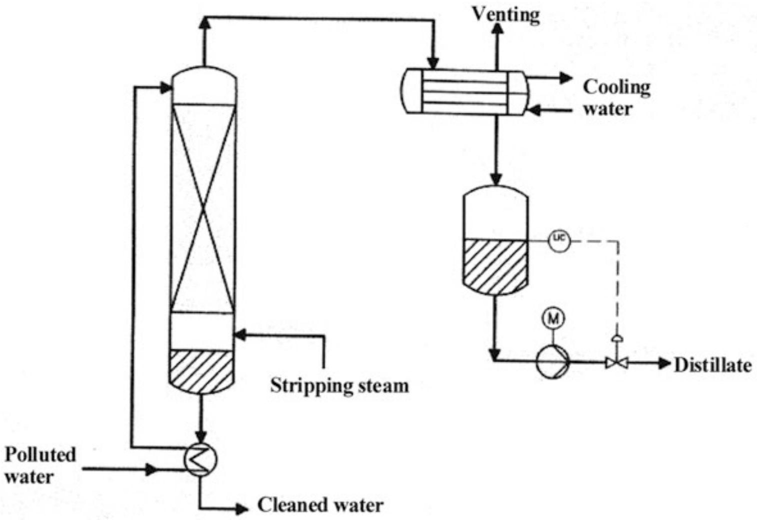


Fig. 8.23 Flow diagram of a steam stripper

The separation can then occur by decantation.

The large amount of purified water is drawn out from the bottom.

Water soluble solvents should be considered as non-ideal systems.

The vapour–liquid equilibrium is greatly determined by the activity coefficient which strongly increases with a decreasing concentration of the solvent in water.

The separation behaviour strongly changes on different trays of a column.

In such cases the column design should be carried out with a computer program.

A typical example is an ethyl acetate stripper.

A small amount of ethyl acetate with an almost azeotropic composition is stripped off from a large amount of water.

Example 8.12.1.1: Steam stripper design for stripping ethyl acetate from water The mass balance is given in Fig. 8.26.

Chosen: Five theoretical trays for the stripping out of ethyl acetate

Feed: 4000 kg water/h with 0.04 weight% ethyl acetate

Desired purification of water <0.1 kg/h ethyl acetate

Result of the computer simulation:

Tray	1	2	3	4	5
Temperature (°C)	99.6	99.2	94	80.2	74.9
$x_{\text{ethyl acetate}}$ (molfr.)	$0.41*10^{-5}$	$0.68*10^{-4}$	$0.92*10^{-3}$	$0.57*10^{-2}$	$0.12*10^{-1}$
$y_{\text{ethyl acetate}}$ (molfr.)	$0.1*10^{-2}$	$0.17*10^{-1}$	0.186	0.524	0.618
K-value	252	248	202	92	51

From Fig. 8.24 it follows that the equilibrium is non-linear.

Figure 8.25 shows the strong change in the equilibrium constant on the different trays with different liquid compositions.

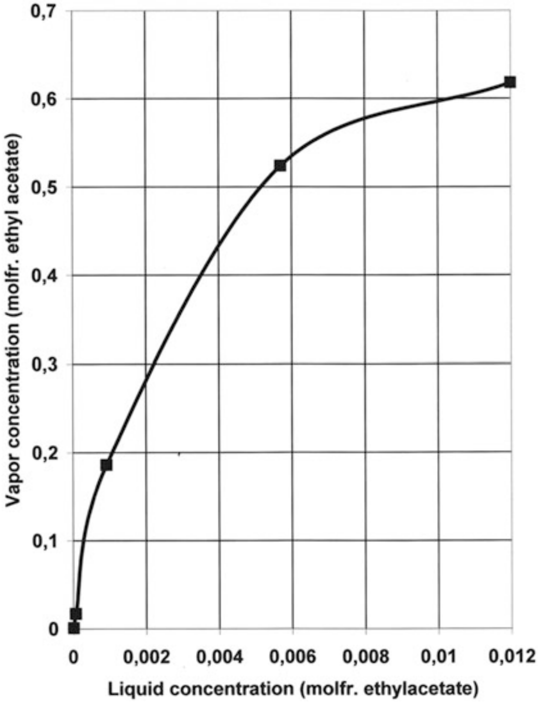


Fig. 8.24 Vapour–liquid equilibrium for an ethyl acetate–water stripper

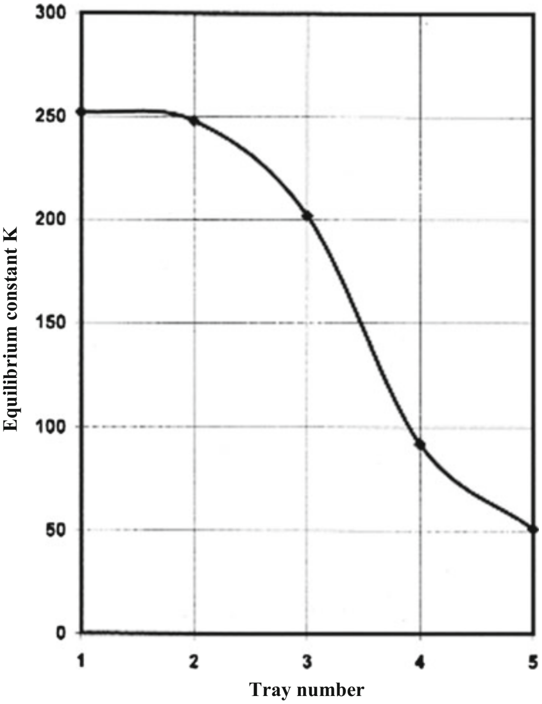
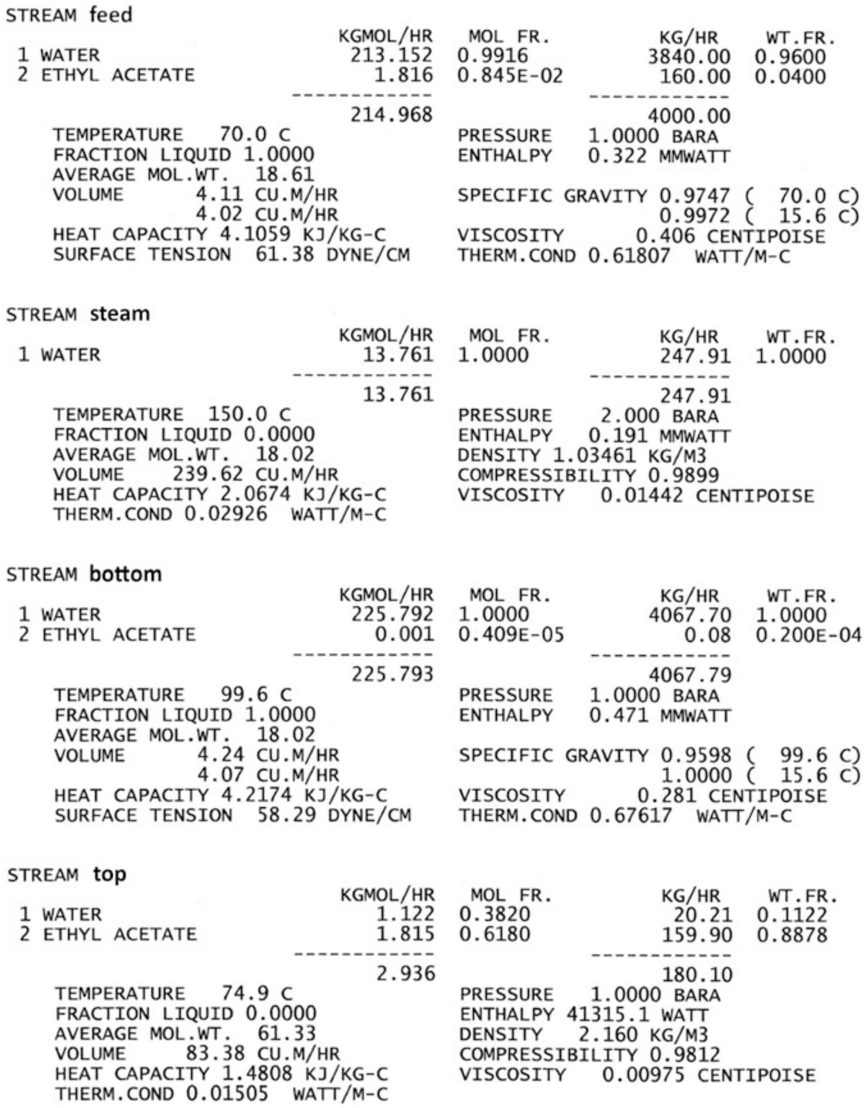


Fig. 8.25 Equilibrium constants for the ethyl acetate–water stripper on different trays



```
STREAM feed
                               KGMOL/HR   MOL FR.        KG/HR    WT.FR.
 1 WATER                        213.152  0.9916         3840.00  0.9600
 2 ETHYL ACETATE                  1.816  0.845E-02       160.00  0.0400
                           ------------            ------------
                                214.968                 4000.00
    TEMPERATURE    70.0 C                PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000               ENTHALPY    0.322 MMWATT
    AVERAGE MOL.WT.   18.61
    VOLUME        4.11 CU.M/HR           SPECIFIC GRAVITY 0.9747 (  70.0 C)
                  4.02 CU.M/HR                            0.9972 (  15.6 C)
    HEAT CAPACITY 4.1059 KJ/KG-C         VISCOSITY      0.406 CENTIPOISE
    SURFACE TENSION  61.38 DYNE/CM       THERM.COND 0.61807  WATT/M-C

STREAM steam
                               KGMOL/HR   MOL FR.        KG/HR    WT.FR.
 1 WATER                         13.761  1.0000          247.91  1.0000
                           ------------            ------------
                                 13.761                  247.91
    TEMPERATURE  150.0 C                 PRESSURE     2.000 BARA
    FRACTION LIQUID 0.0000               ENTHALPY    0.191 MMWATT
    AVERAGE MOL.WT.   18.02              DENSITY 1.03461 KG/M3
    VOLUME     239.62 CU.M/HR            COMPRESSIBILITY 0.9899
    HEAT CAPACITY 2.0674 KJ/KG-C         VISCOSITY    0.01442 CENTIPOISE
    THERM.COND 0.02926  WATT/M-C

STREAM bottom
                               KGMOL/HR   MOL FR.        KG/HR    WT.FR.
 1 WATER                        225.792  1.0000         4067.70  1.0000
 2 ETHYL ACETATE                  0.001  0.409E-05         0.08  0.200E-04
                           ------------            ------------
                                225.793                 4067.79
    TEMPERATURE    99.6 C                PRESSURE    1.0000 BARA
    FRACTION LIQUID 1.0000               ENTHALPY    0.471 MMWATT
    AVERAGE MOL.WT.   18.02
    VOLUME        4.24 CU.M/HR           SPECIFIC GRAVITY 0.9598 (  99.6 C)
                  4.07 CU.M/HR                            1.0000 (  15.6 C)
    HEAT CAPACITY 4.2174 KJ/KG-C         VISCOSITY      0.281 CENTIPOISE
    SURFACE TENSION  58.29 DYNE/CM       THERM.COND 0.67617  WATT/M-C

STREAM top
                               KGMOL/HR   MOL FR.        KG/HR    WT.FR.
 1 WATER                          1.122  0.3820           20.21  0.1122
 2 ETHYL ACETATE                  1.815  0.6180          159.90  0.8878
                           ------------            ------------
                                  2.936                  180.10
    TEMPERATURE    74.9 C                PRESSURE    1.0000 BARA
    FRACTION LIQUID 0.0000               ENTHALPY 41315.1 WATT
    AVERAGE MOL.WT.   61.33              DENSITY     2.160 KG/M3
    VOLUME       83.38 CU.M/HR           COMPRESSIBILITY 0.9812
    HEAT CAPACITY 1.4808 KJ/KG-C         VISCOSITY    0.00975 CENTIPOISE
    THERM.COND 0.01505  WATT/M-C
```

Fig. 8.26 Mass balance for an ethyl acetate–water stripper

8.12.2 Steam Stripper for the Stripping Out of Non-Water-Soluble Components from Water

Figure 8.27 shows the application of a steam stripper with reboiler for stripping out non-water-soluble chlorinated hydrocarbons from water.

A steam stripper with reboiler has the advantage that the steam condensate does not make contact with the waste water [23].

In the following text a simplified calculation of the required theoretical trays NT, and the mass transfer units NTU, for a steam stripper are shown.

For low solubilities of non-water-soluble materials linear equilibrium, and operating lines, result.

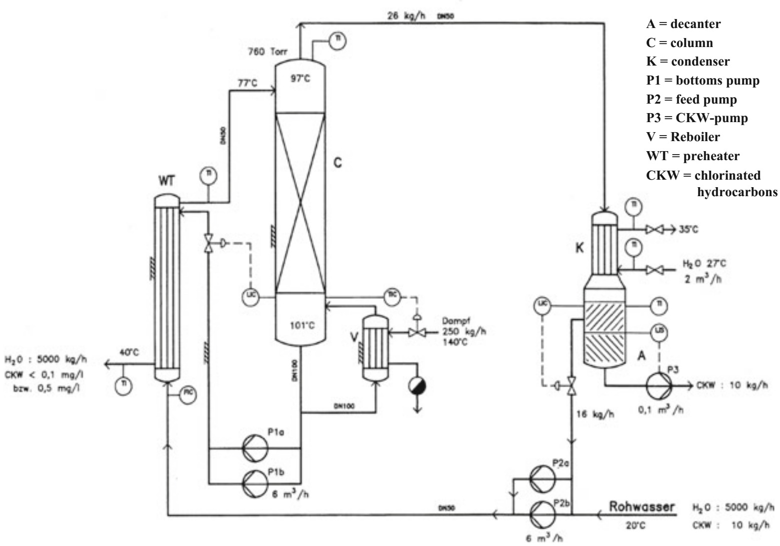


Fig. 8.27 Steam stripper for the stripping out of chlorinated hydrocarbons from water

$$\text{Required theoretical stages NT} = \frac{\ln\left[\frac{x_{\text{in}}}{x_{\text{out}}} * (S-1) + 1\right]}{\ln S} - 1 \qquad (S \neq 1)$$

$$\text{Stripping efficiency } f = \frac{x_{\text{in}} - x_{\text{out}}}{x_{\text{in}}} = 1 - \frac{x_{\text{out}}}{x_{\text{in}}}$$

$$\text{Required transfer units NTU} = \frac{S}{S-1} * \ln\left[\frac{\left[\frac{x_{\text{in}}}{x_{\text{out}}} * (S-1) + 1\right]}{S}\right]$$

Example 8.12.2.1: Determination of NT and NTU for desorption

$S = 1.75 \quad x_{\text{in}} = x_F = 100\,\text{mol ppm (feed)} \quad x_{\text{out}} = x_S = 1\,\text{mol ppm(bottom)}$

$$\text{NT} = \frac{\ln[100/1 * (1.75-1) + 1]}{\ln 1.75} - 1 = 6.74$$

$$f = \frac{x_{\text{in}} - x_{\text{out}}}{x_{\text{in}}} = 1 - \frac{x_{\text{out}}}{x_{\text{in}}} = \frac{100-1}{100} = 1 - \frac{1}{100} = 0.99$$

$$\text{NTU} = \frac{1.75}{0.75} * \ln\left[\frac{100 * 0.75 + 1}{1.75}\right] = 8.8$$

Cross-check of the stripping efficiency:

$$f = \frac{S^{N+1} - S}{S^{N+1} - 1} = \frac{1.75^{7.74} - 1.75}{1.75^{7.74} - 1} = 0.99$$

$$\frac{x_S}{x_F} = \frac{S-1}{S^{N+1} - 1} = \frac{1.75 - 1}{1.75^{7.74} - 1} = 0.00999$$

$$\frac{x_F}{x_S} = \frac{1}{0.00999} = 100$$

Calculation of the tray concentrations from top to bottom:

Tray 1:

$$x_1 = \frac{S-1}{S^{N+1} - 1} * x_F = \frac{1.75 - 1}{1.75^{1+1} - 1} * 100 = 36.4\text{ ppm}$$

Tray 2:

$$x_2 = \frac{1.75 - 1}{1.75^{2+1} - 1} * 100 = 17.2\text{ ppm}$$

Tray 3:

$$x_3 = \frac{1.75 - 1}{1.75^{3+1} - 1} * 100 = 8.95\text{ ppm}$$

Tray 6.74::

$$x_{6.74} = \frac{1.75 - 1}{1.75^{6.74+1} - 1} * 100 = 1\text{ ppm}$$

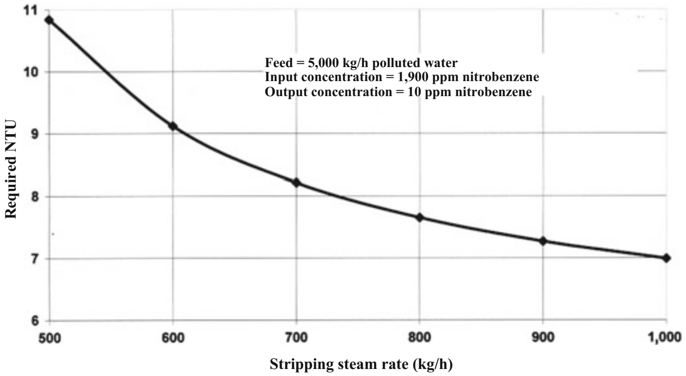


Fig. 8.28 With increasing stripping steam rate the number of required mass transfer units NTU for steam stripping falls

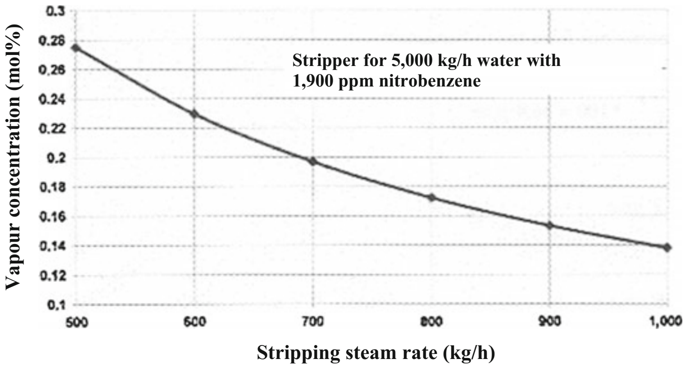


Fig. 8.29 The concentration of the organic component in the exiting vapour at the top of the column decreases with increasing stripping steam rate

In Figs. 8.28 and 8.29 the results of a stripping design for the stripping out of nitrobenzene from water are given.

Conclusion from Figs. 8.28 **and** 8.29:

The more stripping steam the fewer separation stages are needed, however, a larger stripping steam rate reduces the nitrobenzene composition in the distillate which must lie over the solubility concentration for decanting.

8.12.3 Steam Stripping of Non-Water-Soluble Materials with Water Phase Reflux

With the steam stripper shown in Fig. 8.30 the decanted water is returned as reflux into the column.

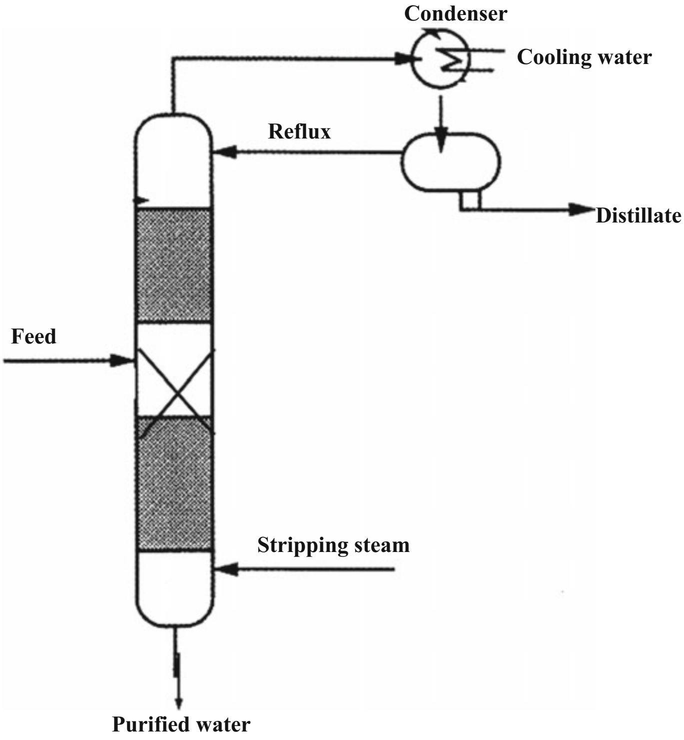


Fig. 8.30 Steam stripper for chlorinated hydrocarbons with a water reflux from the decanter

As a consequence of this an improvement in the stripping efficiency is achieved (see Table 8.2).

Calculation of a steam stripper with reflux and tray efficiency η = 1:

$$k = \frac{1 + R_r * \gamma_{\text{org}}/\gamma_{\text{ow}}}{R_r + 1} \qquad R_r = R * \frac{1 + c_p * (t_K - t_R)}{r}$$

$$\text{NTU} = \frac{S}{S-1} * \ln\left[\frac{x_{\text{in}}}{x_{\text{out}}} * k * \frac{S-1}{S} + 1 + k * \frac{S-1}{S}\right]$$

$$\text{NT} = \frac{\ln\left[S + \frac{f*k*(S-1)}{1-f}\right]}{\ln S} - 1$$

$$f = \frac{x_{\text{in}} - x_{\text{out}}}{x_{\text{in}}} = 1 - \frac{x_{\text{out}}}{x_{\text{in}}}$$

Control :

$$f = \frac{S^{N+1} - S}{S^{N+1} - S - k * (1 - S)}$$

c_p = specific heat capacity (Wh/kg K)
R = reflux ratio = reflux flow rate/distillate flow
R_r = actual reflux flow rate considering the subcooled reflux
f = stripping efficiency
r = evaporation heat (Wh/kg)
S = Stripping factor = m*G/L
t_K = top temperature (°C)
t_R = reflux temperature (°C)
x_{in} = composition of the organic component in the water inlet (ppm)
x_{out} = composition of the organic component in the water outlet (ppm)
γ_{org} = activity coefficient of the organic phase in the organic phase (γ = 1)
γ_{ow} = activity coefficient of the organic phase in water (γ high)

Example 8.12.2: Steam stripper with and without reflux

$$\begin{array}{llll} S = 1.6585 & R_r = 10 & x_{\text{in}} = 200\,\text{ppm} & x_{\text{out}} = 1\,\text{ppm} \\ \gamma_{\text{org}} = 1 & \gamma_{\text{ow}} = 300 & m = 16.6\,\text{at}\,100\,°\text{C} & \end{array}$$

$$\text{With reflux}\ \ R = 10 \qquad k = \frac{1 + 10 * 1/300}{11} = 0.0939$$

$$f = \frac{200 - 1}{200} = 0.995$$

$$\text{NTU} = \frac{1.6585}{0.6585} * \ln\left[\frac{200}{1} * 0.0939 * \frac{0.6585}{1.6585} + 1 + 0.0939 * \frac{0.6585}{1.6585}\right] = 5.39$$

$$\text{NT} = \frac{\ln\left[1.6585 + \frac{0.995 * 0.0939 * (1.6585 - 1)}{1 - 0.995}\right]}{\ln 1.6585} - 1 = 4.21$$

$$\text{Without reflux}\ \ R = 0 \qquad k = 1$$

$$\text{NTU} = \frac{1.6585}{0.6585} * \ln\left[\frac{200 * 1 * 0.6585}{1 * 1.6585} + 1 + 1 * \frac{0.6585}{1.6585}\right] = 11.06$$

$$\text{NT} = \frac{\ln[(200/1) * (1.6585 - 1) + 1]}{\ln 1.6585} - 1 = 8.66$$

Table 8.2 Stripping efficiency of different components with and without reflux

Component	Equilibrium constant K	Stripping efficiency (%)			
		R = 0		R = 10	
		S = 0.05	S = 0.1	S = 0.05	S = 0.1
Toluene	1133	99.99	100	100	100
Xylene	1202	99.99	100	100	100
Fluorene	49.3	96.02	99.35	100	100
Nitrobenzene	16.6	67.64	39.99	95.76	100
Anthracene	15	63.40	87.69	95	100
Phenol	2.03	10.14	20.16	49.67	68.83

S Specific stripping steam rate (kg Steam/kg water)

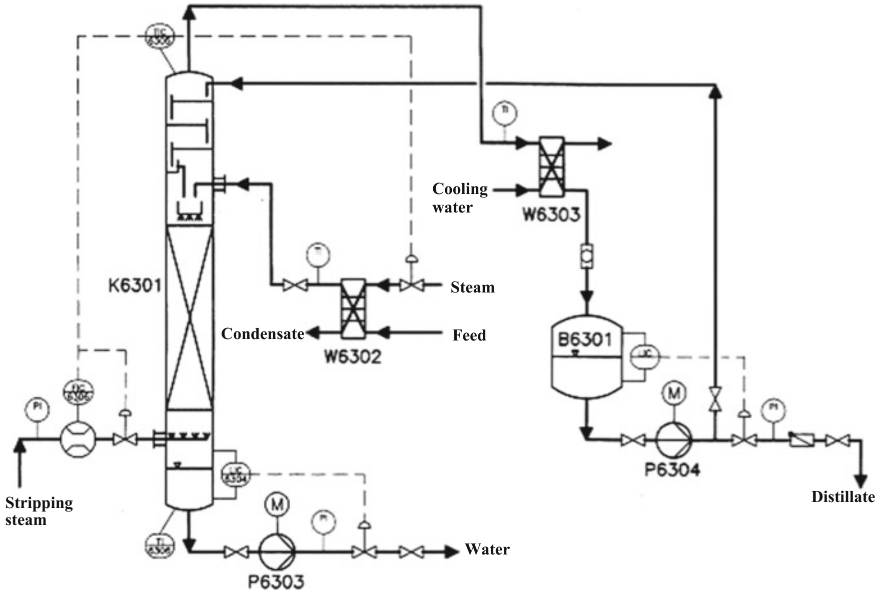


Fig. 8.31 Steam stripper with rectification section and reflux

In Table 8.2 the calculation results for the different components with reflux (R = 10) and without reflux (R = 0) are listed for different specific stripping steam rates S in kg steam/kg waste water.

Conclusion:

The more volatile toluene and xylene can be easily stripped out.

With higher boiling nitrobenzene and anthracene more steam and reflux is required.

A larger specific stripping steam rate S improves the stripping efficiency, however, this is at the expense of a higher steam requirement.

A more effective separation of the organic components can be achieved using a fractionator on top of the stripping section of the column as shown in Fig. 8.31.

In the fractionation section the organic components are gathered and the polluted distillate is reduced. The considerably lower liquid rate in the fractionation section of the column has to be considered in the fluid dynamic design.

The separation of the organic components works best if in the stripped out distillate the solubility limit of the organic phase is exceeded and two phases form in the decanter (Fig. 8.32).

The decanted organic phase is drawn out as distillate.

The overdistilled water with the solvable solvent goes back to the stripper and is drawn out from the bottom of the column after cleaning.

The operation is shown in Fig. 8.32.

The decanter design is covered in Chap. 7.

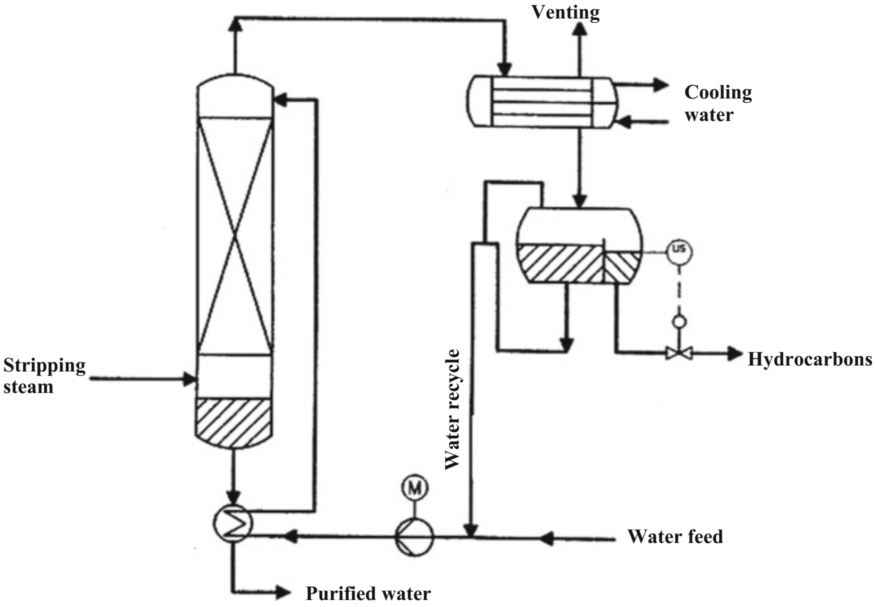


Fig. 8.32 Steam stripper with solvent recovery by phase separation

Example 8.12.3: Steam stripper with a decanter for the separation of nitrobenzene from water

$$\text{Data for nitrobenzene} : M = 123 \quad \text{Solubility in water} = 1.900\,\text{ppm}$$
$$\text{Activity coefficient at infinite dilution}\,\gamma_\infty = 621$$
$$\text{Vapour pressure at } 100\,^\circ\text{C} : \quad P_0 = 27\,\text{mbar} \qquad \text{Boiling point}\,Kp = 210.9\,^\circ\text{C}$$
$$\text{Equilibrium constant}\,K = 16.6 = \text{y/x at } 100\,^\circ\text{C}$$
$$\text{Inlet concentration}\,x_{\text{in}} = 1.460\,\text{ppm} \qquad \text{Required outlet concentration}\,x_{\text{out}} = 1\,\text{ppm}$$
$$\text{Liquid flow}\,L = 6.000\,\text{kg/h} = 277.8\,\text{kmol/h}$$
$$\text{Stripping steam flow}\,G = 400\ \text{kg/h} = 38.9\,\text{kmol/h}$$
$$\text{Absorptive inlet} = 6.000 * 1.460 * 10^{-6} = 8.76\,\text{kg/h} \approx \text{distillate flow}$$

$$f = 1 - \frac{1}{1460} = 0.9993 \qquad R \approx \frac{400}{8.76} \approx 45.6$$
$$R_r = 45.6 * \left[1 + \frac{0.6 * (100 - 50)}{90}\right] = 45.6 * 1.33 = 60.8$$
$$\text{Reflux rate } R_M = R_r * D = 60.8 * 8.76 = 532.6\ \text{kg/h}$$

$$\text{Vapor rate } G = (R_r + 1) * D = 61.8 * 8.76 = 541.4\ \text{kg/h}$$

$$L = 6000 + 532.6 = 6532.6\ \text{kg/h}$$

$$S = 16.6 * \frac{541.4}{6532.6} = 1.376$$

$$k = \frac{1 + 60.8 * \frac{1}{621}}{60.8 + 1} = 0.0177$$

$$\text{NT} = \frac{\ln\left[1.376 + \frac{0.9993*0.0177*(1.376-1)}{1-0.9993}\right]}{\ln 1.376} - 1 = 7.48 - 1 = 6.48$$

Cross-check calculation of f:

$$f = \frac{S^{N+1} - S}{S^{N+1} - S - k * (1 - S)} = \frac{1.376^{7.48} - 1.376}{1.376^{7.48} - 1.376 - 0.0177 * (1 - 1.376)} = 0.9993$$

Top concentration of nitrobenzene y_K

$$y_K = \frac{x_{\text{ein}} * F - B * x_{\text{aus}}}{G} = \frac{1460 * 6000 - 6532.6 * 1}{541.4} = \frac{8753467}{541.4} = 16168\ \text{ppm}$$

$$y_K = x_K = \frac{f * F * x_{\text{ein}}}{G} = \frac{0.9993 * 6000 * 1460}{541.4} = 16168\ \text{pp}$$

The nitrobenzene concentration in the overdistilled mixture of water and nitrobenzene lies clearly over the solubility limit of 1900 ppm.

Two phases form in the decanter.

If the solubility limit is not exceeded in the stripped off distillate, and phase separation in the decanter is not possible, then the process given in Fig. 8.33 can be applied.

The steam stripper is equipped with a fractionator at the top and is operated with reflux in order to enrich the solvent composition in the distillate, up to the point that the solubility limit in the water phase is exceeded and two phases are formed in the decanter.

The solvent can be drawn off.

Example 8.12.4: Water with 100 ppm nitrobenzene must be stripped down to a residual content of 1 ppm. At a specific stripping steam use of 0.1 kg steam/kg water the nitrobenzene concentration in the distillate is 1000 ppm The solubility limit lies at 1900 ppm and a phase separation is therefore not possible.

With two rectification trays the composition can be increased to over 6000 ppm, so that the solubility limit is exceeded and two phases form in the decanter.

For the recovery or the draw out of the solvent it is advantageous to operate the phase separation in the decanter at low temperature because the solubility of the organic solvents mostly increases with rising temperature.

The used stripping steam rate for the stripping out of the solvent should be minimized.

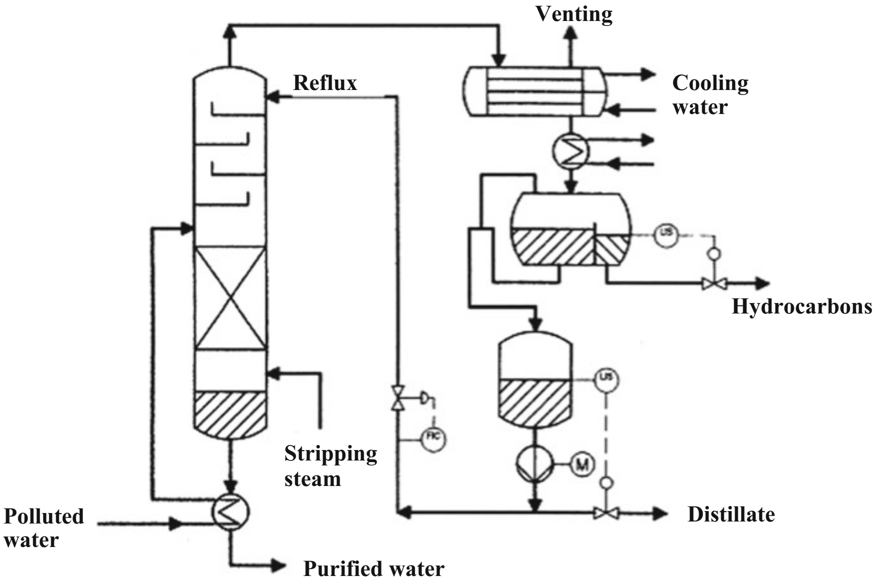


Fig. 8.33 Steam stripper with fractionator at the top and a decanter

A large amount of stripping steam dilutes the distillate drawn off from the top and thus lowers the effectivity of the pollutant removal by decantation because the dissolved part in the water goes back into the stripper.

Regarding the column design a lower liquid loading in the fractionation section is to be considered.

The diameter in the fractionation section must be reduced (Fig. 8.34) or packing cross-flow trays need to be used in the rectification section.

The control scheme for a waste water column is shown in Fig. 8.35.

8.13 Comparison of Air and Steam Strippers

Advantages of an air stripper:

For the stripping out only electricity is necessary for the functioning of the air blower.

No lime precipitation by heating.

Cheap and corrosion resistant material.

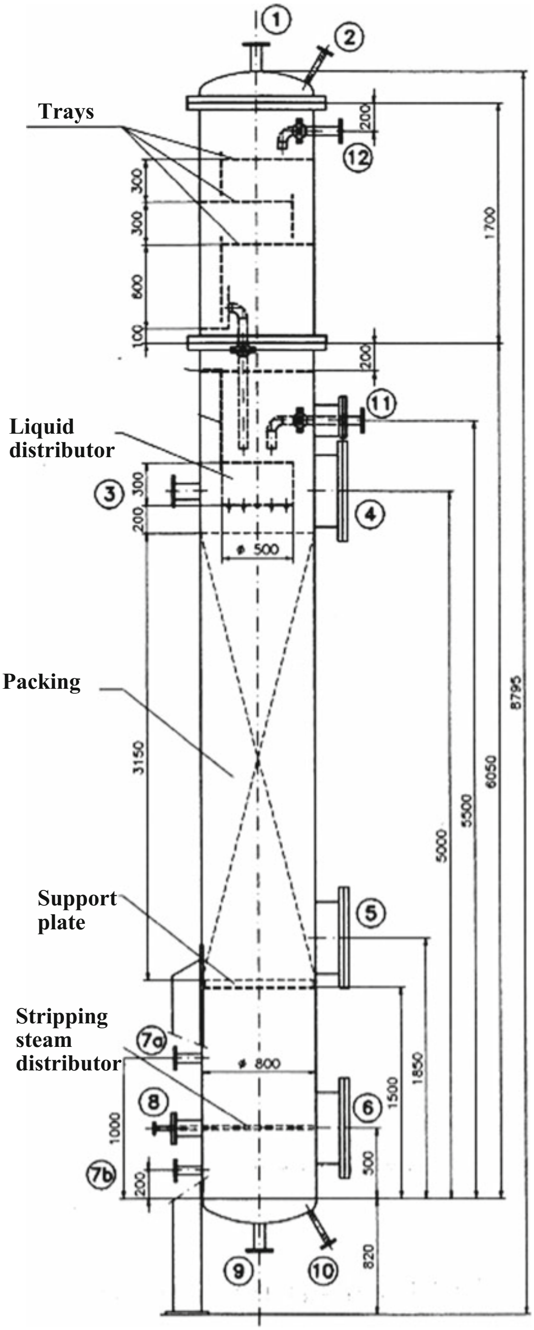
Disadvantages of an air stripper:

The exiting solvent–air mixture is not condensable.

Due to the low equilibrium factor K the degree of purification is worse.

With high boiling components large amounts of air are required (see Fig. 8.36).

Post-cleaning of the exiting air by adsorption or burning.



Nozzles
1 Vapour outlet
2 Temperature
3 Reserve
4 Manway packing
5 Manway packing
6 Manway
7 Level
8 stripping steam
9 bottoms product
10 temperature
11 water feed
12 reflux

Fig. 8.34 Packing–steam stripper with a tray column as a fractionating extension

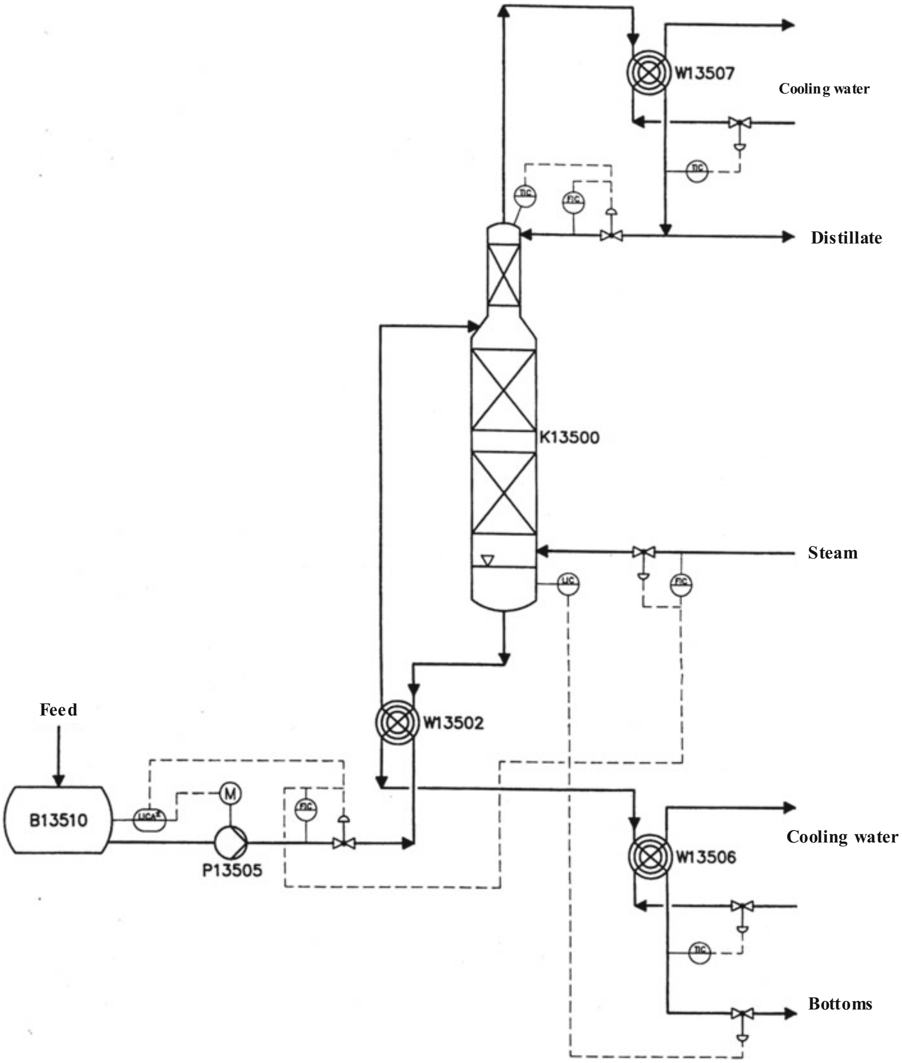


Fig. 8.35 Control scheme of a waste water stripper with a fractionator extension

Due to steam desorption of the adsorber new pollutant mixtures are generated.

The high moisture content and the low solvent composition in the stripping air disturb the adsorption and make the burning more expensive.

Advantages of a steam stripper:

Higher equilibrium factor m at 100 °C in the column ➔ less stripping gas (Fig. 8.36).

Adequate for high boiling components due to the high activity coefficient.

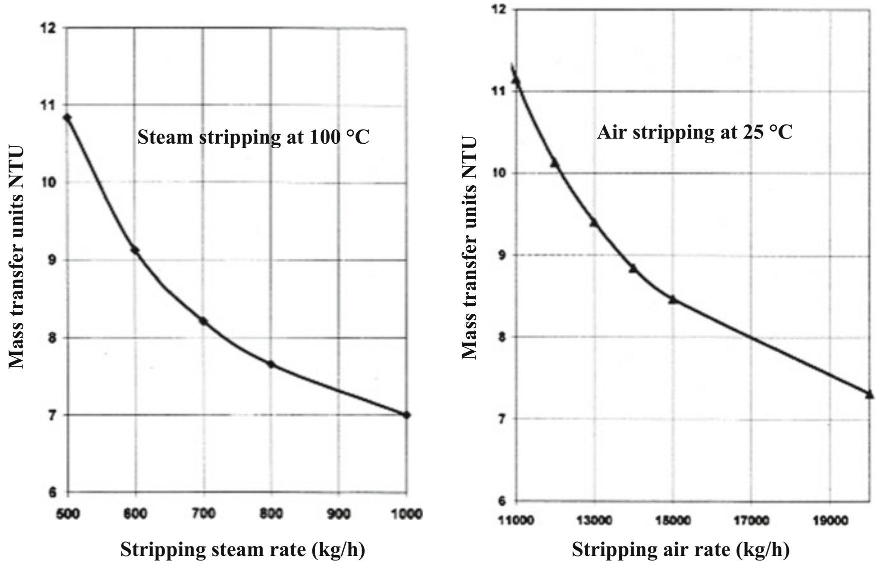


Fig. 8.36 Required transfer Units NTU as a function of the stripping gas rate for the lowering of the nitrobenzene concentration in water from 1900 to 10 ppm

The solvent–vapour mixture is condensable so that no extensive post-cleaning by adsorption or burning is necessary.

With a decanter, solvent discharge is very easy.

Using fractionation extension and reflux the degree of purification can be optimized.

Disadvantages of a steam stripper:

No linear equilibrium in water soluble solvents.

Steam and cooling water required.

Calcifications and salt precipitations possible.

8.14 Ammonia Stripper

An ammonia stripper is a column in which the water, fed to the column at the top, flows downwards with the free ammonia being stripped out with steam in a countercurrent fashion.

The purified water is drawn from the bottom of the column, having come from the top–an ammonia–water concentrate.

Since only the strippable ammonia, i.e., free molecular ammonia but not the ionogene chemically bound ammonia, can be drawn out of the water by steam stripping the water must be brought to a pH value of 10.4–11 before entering the steam stripper.

Due to the temperature increase the dissociation equilibrium is additionally shifted to the free NH_3. The increase in pH value occurs with the use of caustic soda or lime milk.

The caustic soda changes the pH value very quickly so that an inline mixer can be used. In using lime milk a longer residence time is necessary due to the low reaction velocity. The alcalizing solid materials, which should be removed before entering the column, can be precipitated.

The flow diagram of an ammonia stripper with a rectification section is given in Fig. 8.37.

The plant operates at atmospheric pressure. The water, containing ammonia from the vessel B1, is preheated with the run-off hot water in the heat exchanger WT1; alkalized by the addition of caustic soda; and then fed into the column K between the stripping and rectification sections.

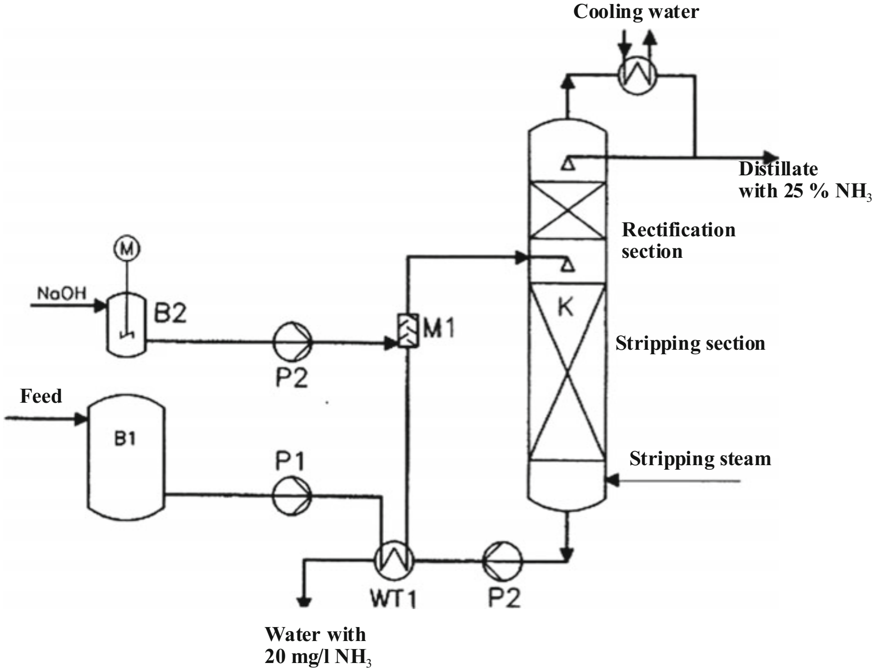


Fig. 8.37 Flow diagram of an ammonia stripper

In the stripping section the NH_3 concentration is lowered according to the required purity specification, for instance from 1.5 g/l in the inlet to 20 mg/l in the water outlet.

The stripping section therefore is used for water purification.

In the upper rectification section a rising of the ammonia concentration occurs, for instance from 1.5 g/l to of 25% ammonia water which can be used for the denitrification of flue gases.

The stripping steam supply can be directly fed as steam into the column or occur indirectly by stripping steam generation in a reboiler. Since the evaporator becomes blocked over time, by calcification and fouling, a direct steam supply is more reliable. The condenser for the water vapour containing 25% ammonia and 75% water must be configured as an integral condenser.

In a differential condenser the ammonia is strongly enriched and is therefore no longer condensable with cooling water.

Ammonia stripper design

The required theoretical number of trays for water purification can be graphically determined.

This is shown in Fig. 8.38a, b for two different stripping steam rates.

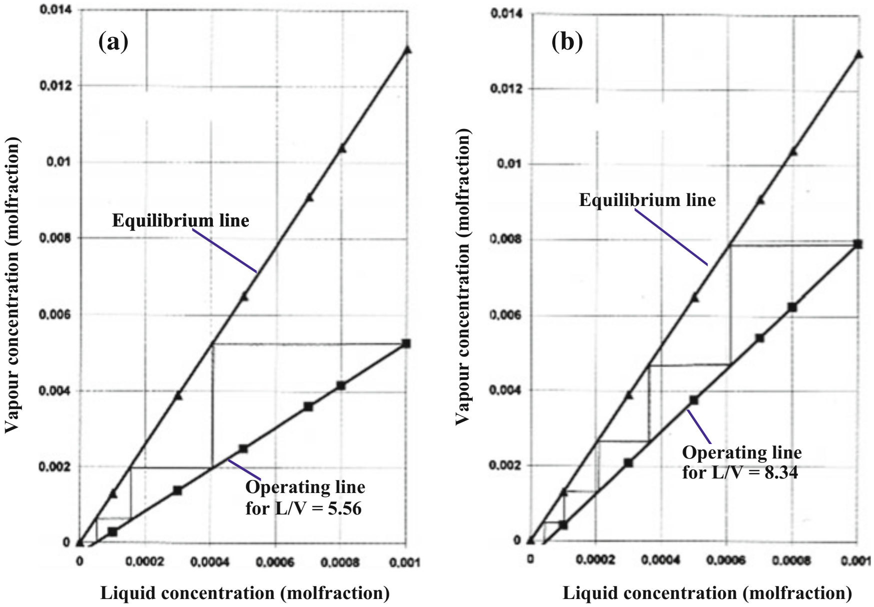


Fig. 8.38 Mcabe–Thiele diagram for the determination of the theoretical number of trays for an ammonia stripper with different stripping steam rates

Example 8.14.1: Determination of the number of trays needed for an ammonia stripper using graphical and calculation methods Water inlet flow L = 10,000 kg/h = 555.55 kmol/h

Inlet concentration: 0.001 molfr. NH_3

Outlet concentration: 0.00005 molfr. NH_3

(a) **Stripping steam flow: 1800 kg/h = 100 kmol/h**

Graphical determination of number of theoretical trays with Fig. 8.38a:

$$\frac{L}{V} = \frac{555.55}{100} = 5.56 \qquad \text{Required theoretical stages} \quad n_{\text{th}} = 2.9$$

Determination of the number of theoretical trays by calculation:

$$S = 13 * \frac{100}{555.55} = 2.34$$

$$\text{NT} = \frac{\ln\left[\frac{0.001}{0.00005} * (2.34 - 1) + 1\right]}{\ln 2.34} - 1 = 2.9$$

With a stripping steam rate of **1800 kg/h = 100 kmol/h you need 2.9 theoretical trays**.

(b) **Stripping steam flow: 1200 kg/h steam = 66.66 kmol/h**

Graphical determination of the number of theoretical trays with Fig. 8.38b:

$$\frac{L}{V} = \frac{555.55}{66.66} = 8.34 \qquad \text{Required theoretical stages} \quad n_{\text{th}} = 4.6$$

Determination of the number of theoretical trays by calculation:

$$S = m * \frac{V}{L} = 13 * \frac{66.66}{555.55} = 1.56$$

$$\text{NT} = \frac{\ln\left[\frac{x_{\text{ein}}}{x_{\text{aus}}} * (S - 1) + 1\right]}{\ln S} - 1 = \frac{\ln\left[\frac{0.001}{0.00005} * (1.56 - 1) + 1\right]}{\ln 1.56} - 1 = 4.6$$

For a stripping steam flow of **1200 kg/h = 66.66 kmol/h you need 4.6 theoretical trays.**

The calculated results are largely consistent with the graphical determination of the number of trays in Fig. 8.38a, b.

Figure 8.39 shows the **optimization possibilities** for ammonia strippers.

At low inlet compositions of 1–1.5 g/l NH_3 it is energetically unfavorable to purify the water in a column to 20–50 mg/l and to produce 25% ammonia water at the same time (Fig. 8.39a with 450 kg/h steam).

In such cases it is more sensible to install two columns in series.

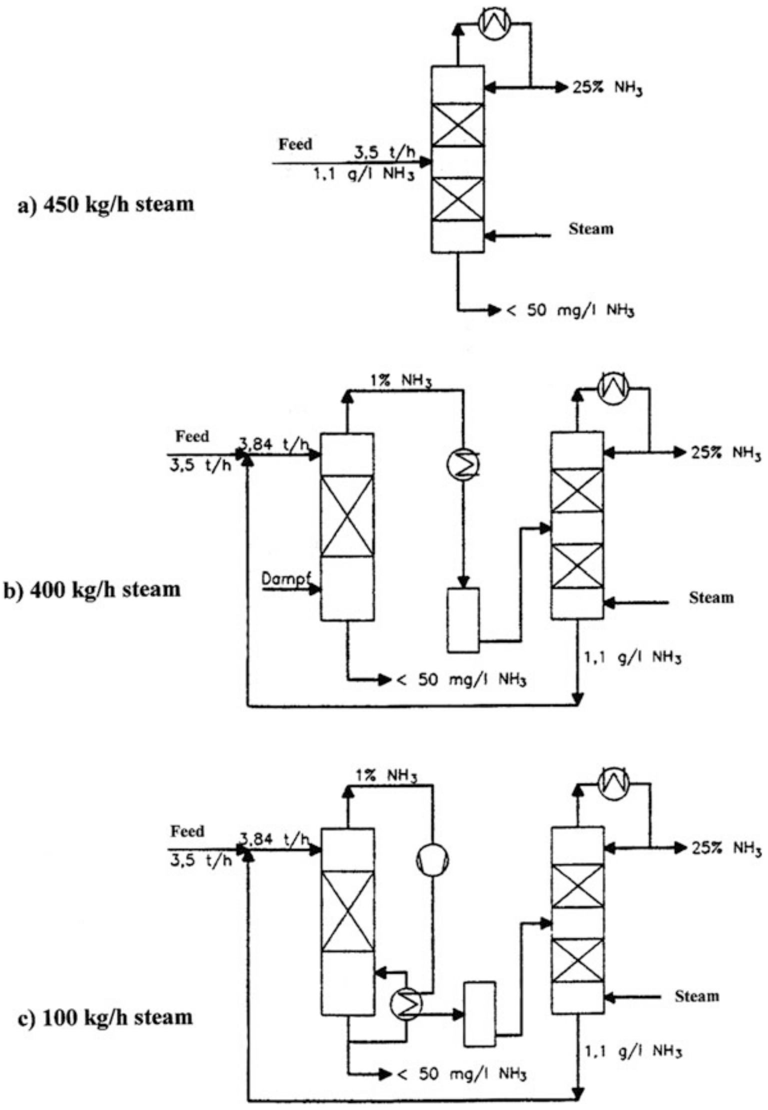


Fig. 8.39 Optimization possibilities for ammonia strippers

The first column is used as a stripper and produces 1% NH_3 water as distillate which is enriched in the second column to 25% NH_3 (Fig. 8.39b with 400 kg/h steam).

In Fig. 8.39c heating steam is saved by a vapour recompression process.

Because the vapour exiting at the top of the column contains only a little ammonia, this water vapour can be used as heating steam in the reboiler of the column after mechanical compression in order to produce stripping steam. The required energy for this process is 100 kg/h steam and 16 kWh electricity.

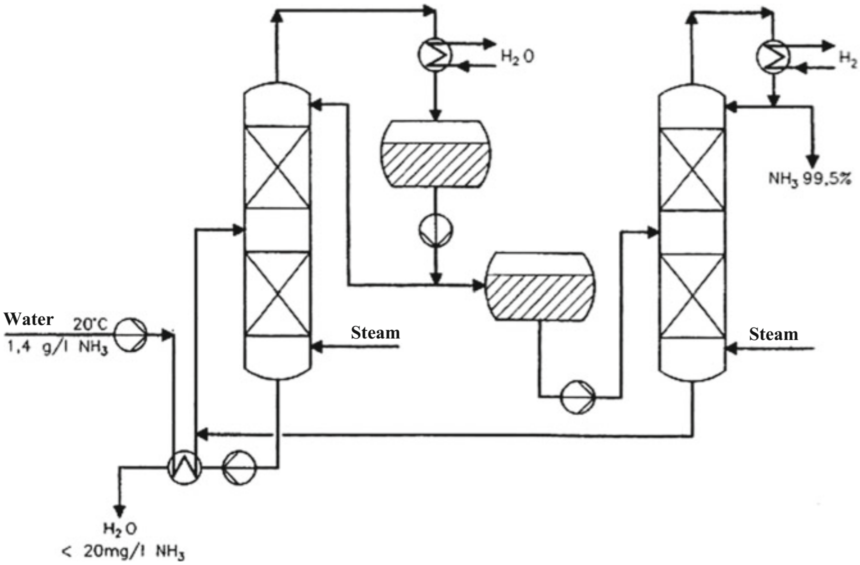


Fig. 8.40 Ammonia stripper for 99.5% NH_3

Figure 8.40 shows a flow diagram of a plant used for the production of 99.5% NH_3.

In the first column the ammonia is driven out of the water at atmospheric pressure, for instance from 1.4 g/l to 20 mg/l, producing a distillate of ammonia–water.

The second column, used for enrichment to a highly concentrated ammonia, must be operated under a pressure of 15–16 bar in order to condense the gaseous ammonia with cooling water.

8.15 Sour Gas Stripper [22]

Sour gas strippers are used in refineries and petrochemical plants for the removal of hydrogen sulfide and ammonia from wash waters of plants in which products are treated with hydrogen, for instance for cracking or desulfurising (Fig. 8.41).

In addition, in coking plants the wash water from the gas wash in sour gas strippers must be freed from H_2S and NH_3

The stripped out gases are burned in a furnace

For the design of such a stripper the so-called “sour gas equilibrium model” is used.

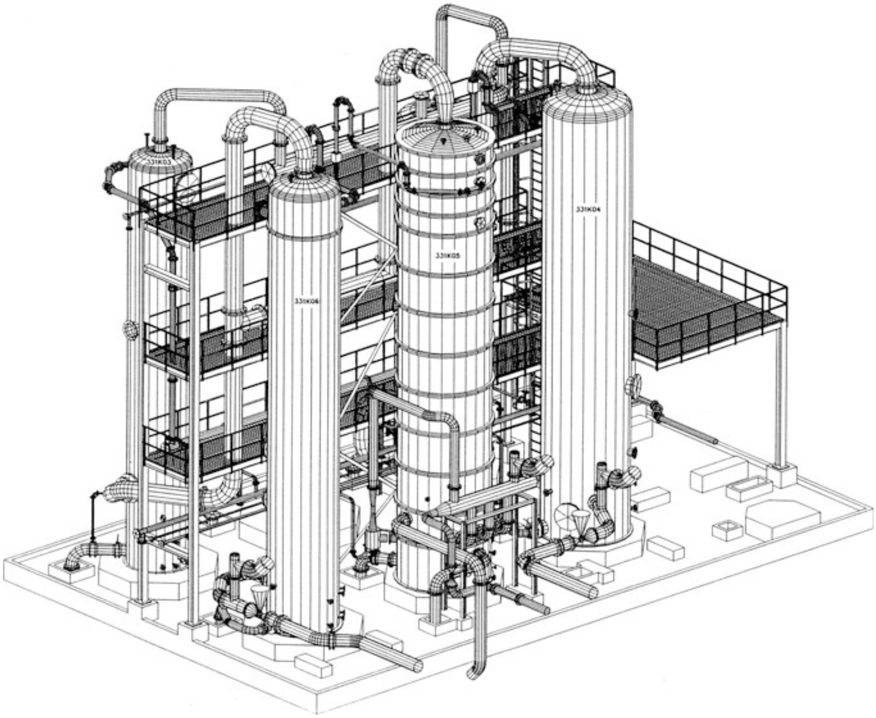


Fig. 8.41 Sour gas washer and stripper in a coking plant

Figure 8.42 shows the flow diagram of a simple conventional sour gas stripper utilising direct-steam feed-in.

The sour water is fed in at the top of the column. The water is warmed up using stripping steam entering the bottom of the column and strips out the pollution components H_2S and NH_3.

The vapours exiting the column top—consisting of water vapour, hydrogen sulfide, and ammonia—proceed to thermal afterburning.

The simple process shown in Fig. 8.42 has the following disadvantages:

1. A high heating steam requirement for the heating the sour water.
2. Using direct-steam feed-in the waste water rate increases.
3. Because the stripping steam is not condensed out a large gas flow with much water vapour streams into the TNV. This places strain on the thermal afterburning and expends fuel.

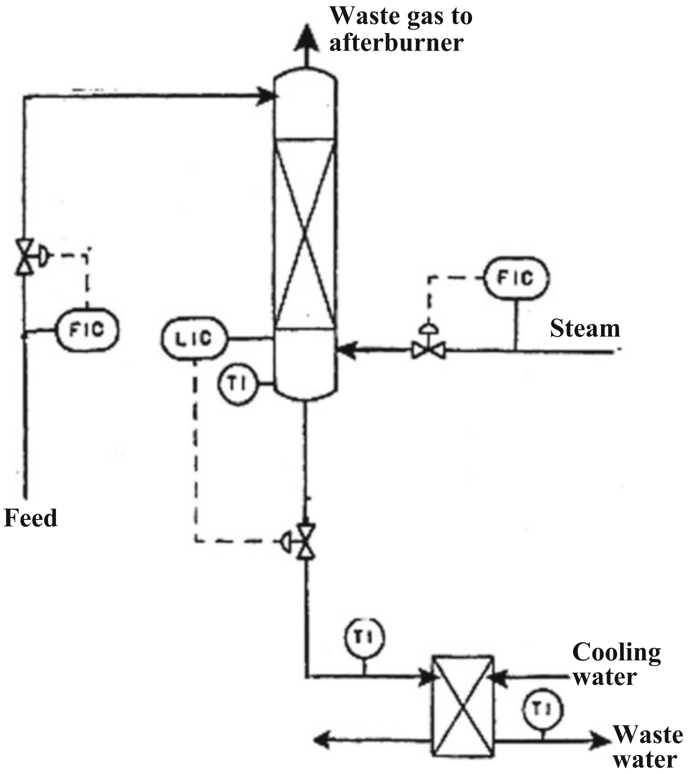


Fig. 8.42 Simple sour gas stripper

An optimized process for sour gas stripping is shown in Fig. 8.43 [22].

Advantages:

The feed is preheated with purified hot water drawn from the bottoms of the column in order to save heating steam.

The stripping steam is generated indirectly in a reboiler with steam heating so that the waste water flow rate is not increased by the condensed stripping steam.

The stripping steam exiting at the top of the column is largely condensed in an air-cooled partial condenser so that the amount of gas that goes to the TNV is reduced by a factor of 10.

A lot of fuel is saved for heating the waste steam from 100 to 800 °C.

The water condensed out of the partial condenser is separated from the gas in a phase separator and goes back to the feed drum.

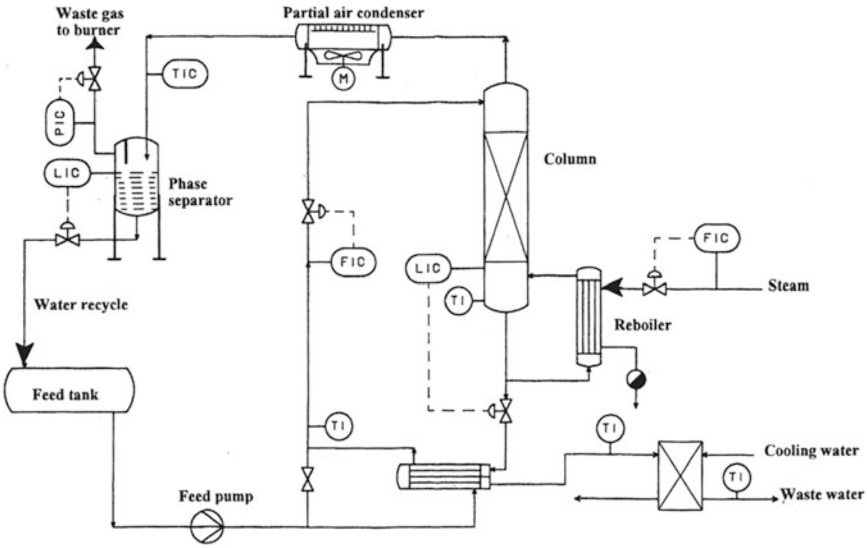


Fig. 8.43 Optimized sour gas stripper

The following results table for a design illuminates the advantage of such an optimized process:

Feed: **2000 kg/h sour water with 5 kg/h H_2S and 6 kg/h NH_3**

Simple direct steam stripper with feed preheating:

Stripping steam flow: 400 kg/h

Waste water: 2121 kg/h water with 5.6 ppm H_2S and 78.2 ppm NH_3

Flue gas to the TNV: 413 m^3/h: 277.7 kg/h H_2O + 4.99 kg/h H_2S + 5.93 kg/h NH_3

Optimized process with a reboiler and a partial condenser:

Heating steam flow: 400 kg/h

Waste water: 1977 kg/h water with 4 ppm H_2S and 69 ppm NH_3

Flue gas to the TNV: 45 m^3/h: 22.9 kg/h H_2O + 4.98 kg/h H_2S + 5.77 kg/h NH_3

Due to the somewhat complicated equilibrium of H_2O– H_2S– NH_3 the design is mostly carried out via computer.

Figure 8.44 shows the result of a computer calculation with the curves of the concentration in the column.

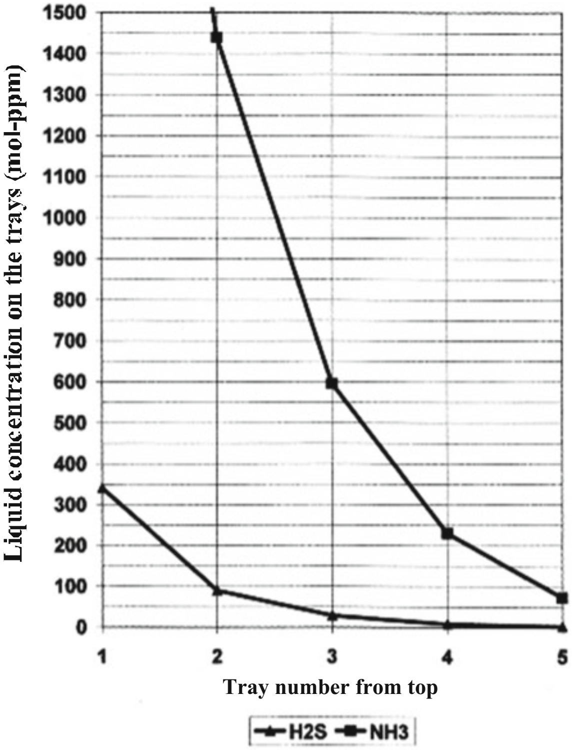


Fig. 8.44 Curve of the concentration of hydrogen sulfide and ammonia on the column trays from top to bottom

In the highly diluted region the calculation can be carried out approximately using the equilibrium constants for H_2S and NH_3 in water.

Example 8.15.1: Calculation of the required theoretical trays for a sour gas stripper

$L = 127.4\,\mathrm{kmol/h} \qquad V = 22.2\,\mathrm{kmol/h}$

$x_{\mathrm{in}} = 1.318\,\mathrm{ppm\,H_2S} \quad x_{\mathrm{out}} = 2\,\mathrm{ppm\,H_2S} \quad x_{\mathrm{in}} = 3.600\,\mathrm{ppm\,NH_3} \quad x_{\mathrm{out}} = 40\,\mathrm{ppm\,NH_3}$

$$H_2S: \quad S = m * \frac{V}{L} = 16 * \frac{22.2}{127.4} = 2.79$$

$$\mathrm{NT} = \frac{\ln\left[\frac{x_{\mathrm{ein}}}{x_{\mathrm{aus}}} * (S-1) + 1\right]}{\ln S} - 1 = \frac{\ln\left[\frac{1318}{2} * (2.79-1) + 1\right]}{\ln 2.79} = 5.89$$

$$\mathrm{NH_3}: \quad S = 12 * \frac{22.2}{127.4} = 2.09$$

$$\mathrm{NT} = \frac{\ln\left[\frac{3600}{40} * (2.09-1) + 1\right]}{\ln 2.09} = 5.23$$

Figure 8.45 shows an arrangement sketch for a sour gas stripper with a reboiler, air-cooled partial condenser, phase separator, and feed preheater.

Figure 8.46 shows the bidding request sketch for the column with a reboiler.

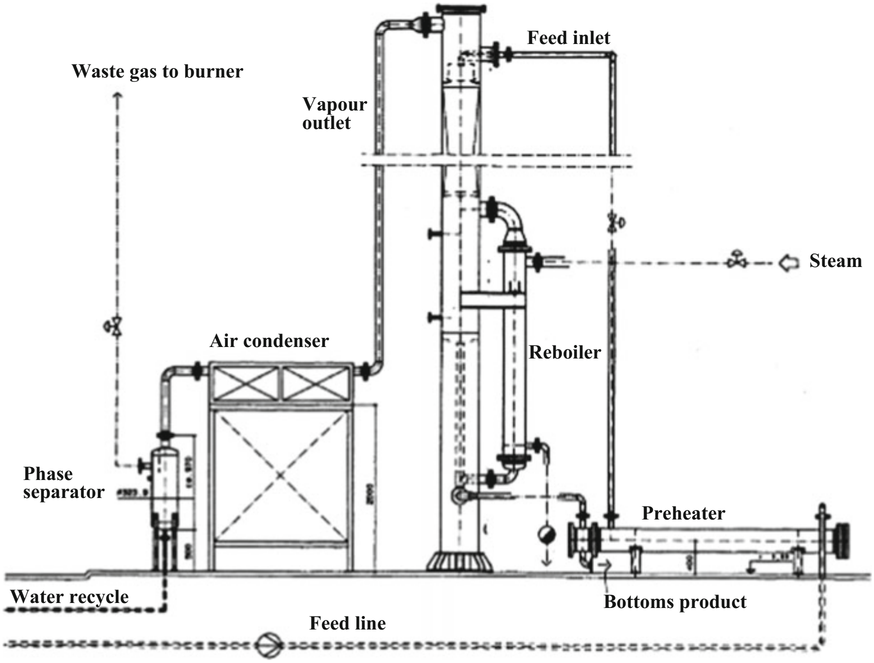
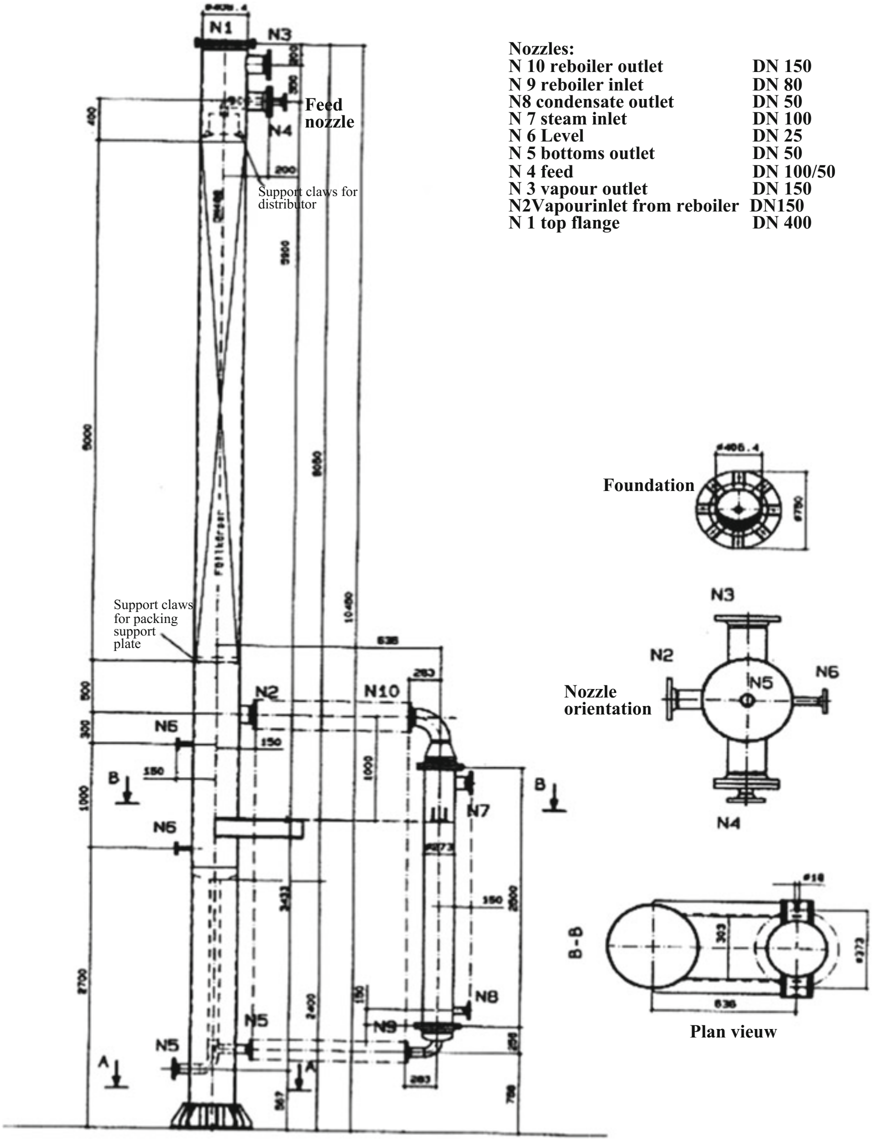


Fig. 8.45 Arrangement sketch for a sour gas stripper



Nozzles:

N 10 reboiler outlet	**DN 150**
N 9 reboiler inlet	**DN 80**
N8 condensate outlet	**DN 50**
N 7 steam inlet	**DN 100**
N 6 Level	**DN 25**
N 5 bottoms outlet	**DN 50**
N 4 feed	**DN 100/50**
N 3 vapour outlet	**DN 150**
N2Vapourinlet from reboiler	**DN150**
N 1 top flange	**DN 400**

Fig. 8.46 Bidding request sketch for a column with a reboiler for a sour gas stripper

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Chapter 9
Fluid Dynamic Dimensioning of Trays and Tray Efficiency

9.1 Fluid Dynamic Design Criteria

In the cross-stream trays the liquid flows horizontally over the tray and the vapour flows vertically from the bottom to the top through the horizontally streaming liquid.

In order to improve the contact between vapour and liquid, and to increase the flexibility of the columns, sieve, valve, tunnel, or bubble cap trays are used.

The different types of trays are shown in the Figs. (9.1, 9.2, 9.3 and 9.4) [7].

In the fluid dynamic design the maximum allowable vapour loading and liquid loading of the column is determined.

The vapour velocity should be chosen such that only a few droplets are entrained to the next higher tray. A high droplet entrainment deteriorates the separation effect and increases the flooding risk.

A high vapour flow velocity increases the pressure loss so that the boiling temperatures in the bottoms are elevated.

A leaking at too low vapour flow velocity must be avoided because this reduces the tray efficiency.

The down-flow velocity of the liquid in the downcomer to the tray below should be low enough that sufficient residence time is available for the outgassing of the liquid. and a flooding by the liquid buildup in the downcomer is avoided.

To check the design the **pressure drops in the rectification section and the stripping section** are calculated because the vapour and liquid loadings are often very different in the rectification and the stripping sections of the column, especially in vacuum columns.

High vapour velocities in the risers of the bubble cap trays, in the holes of the sieve trays, or in the valves of a valve tray, cause large dry pressure losses.

High liquid heights on the trays due to large submergences, weir heights, and weir overflow heights cause large wet pressure losses.

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_9

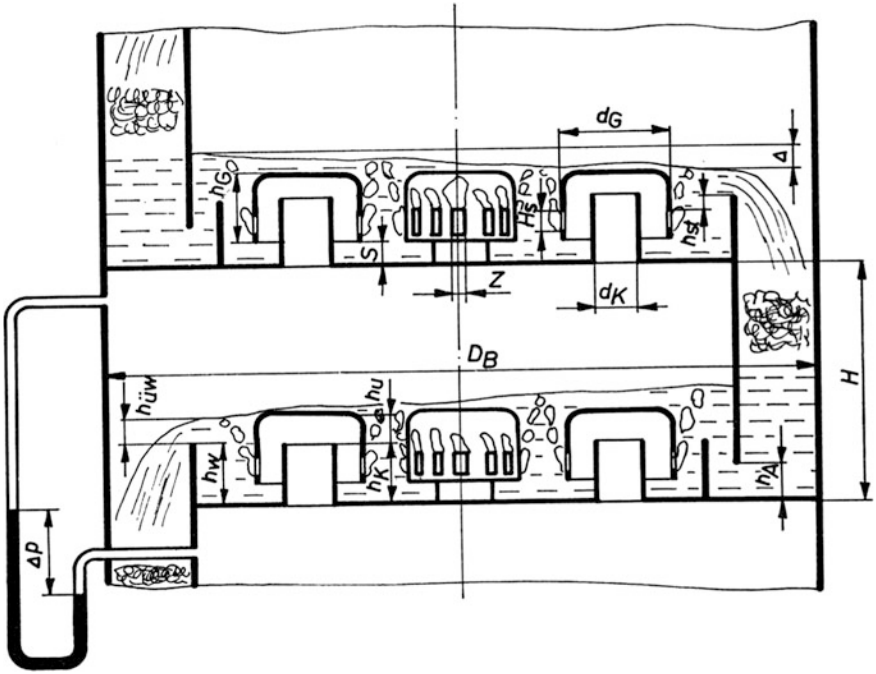


Fig. 9.1 Bubble cap tray column from Hoppe and Mittelstrass [7]

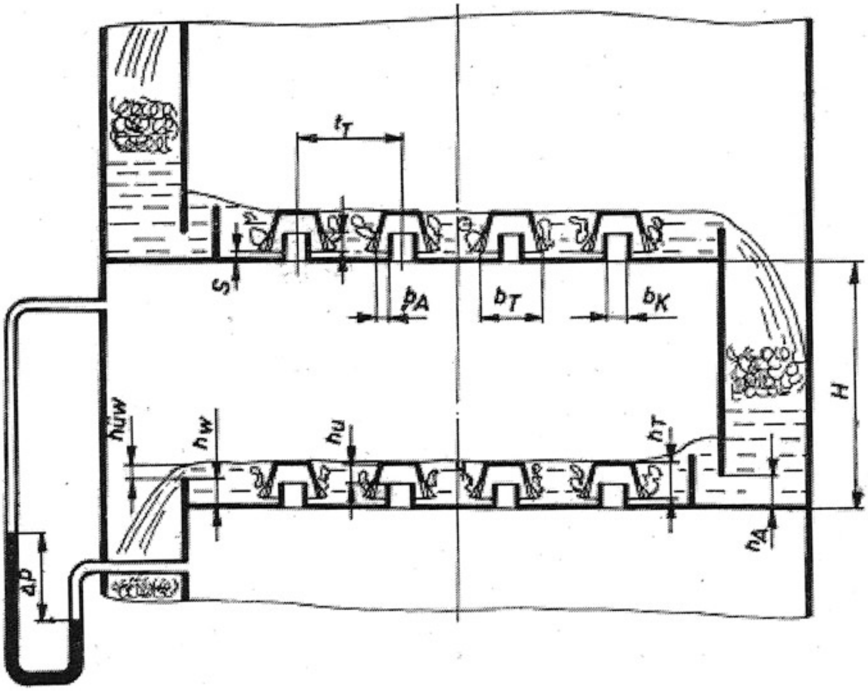


Fig. 9.2 Tunnel cap tray column from Hoppe and Mittelstrass [7]

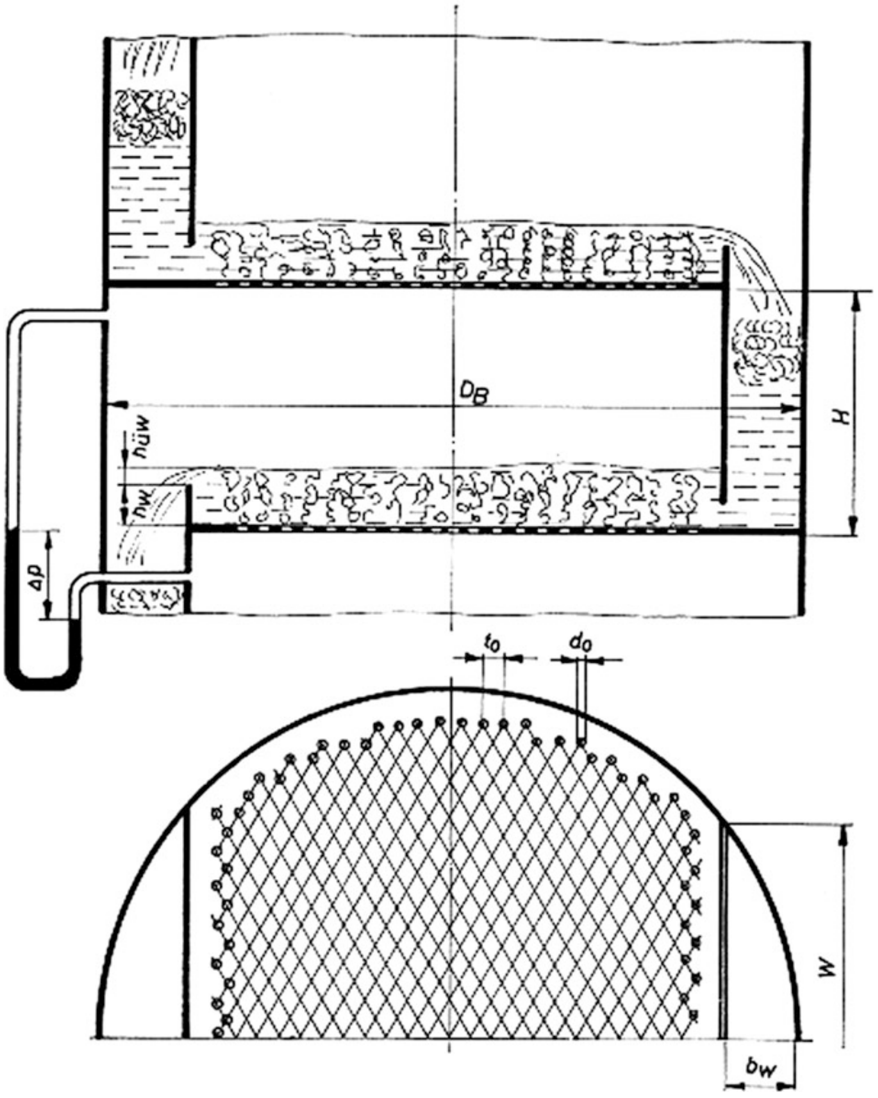


Fig. 9.3 Sieve tray column from Hoppe and Mittelstrass [7]

Initial design remarks

As a first approach the allowable vapour velocity w_D in the column can be determined using the loading factor F. The F value is dependent on the tray spacing, the type of tray, and the pressure in the column.

$$F = w_D * \sqrt{\rho_V} \approx 1.0 - 1.7 \text{ for tray columns}$$

$$w_D = \frac{F}{\sqrt{\rho_V}} \quad \rho_V = \text{vapor density } (\mathrm{kg/m^3})$$

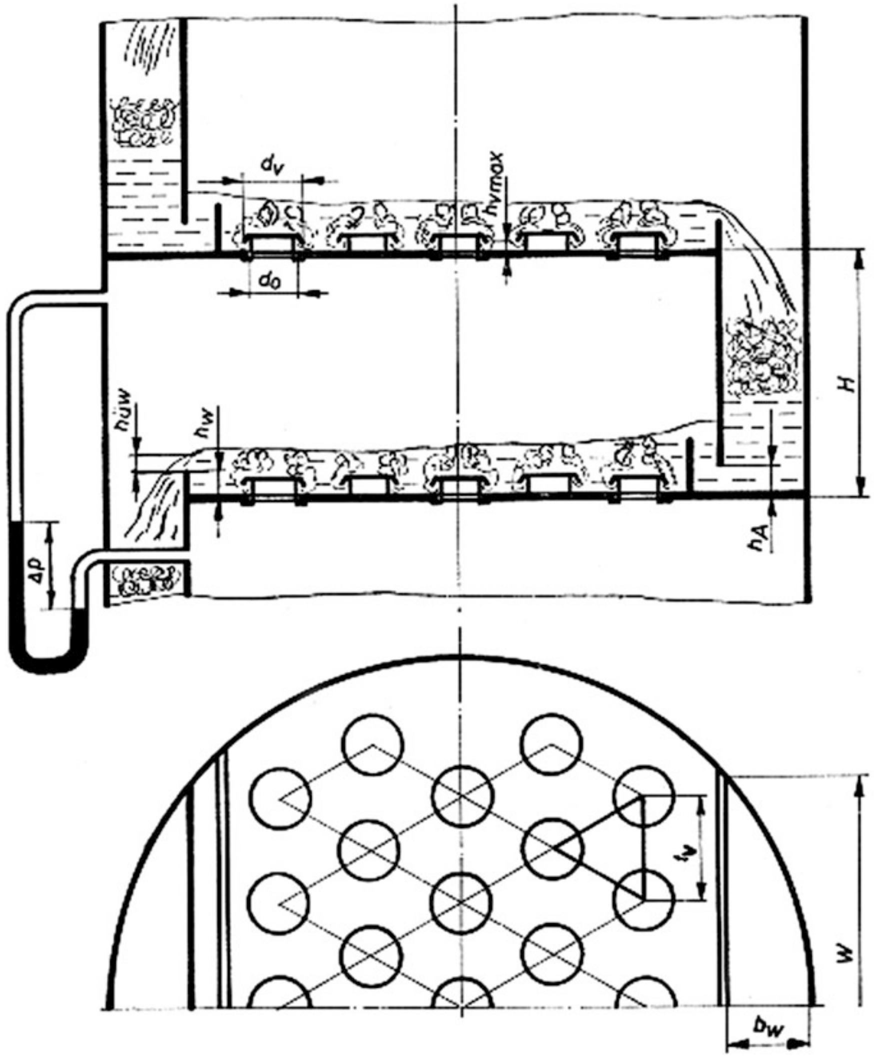


Fig. 9.4 Valve tray column from Hoppe and Mittelstrass [7]

Recommended gas velocity: 80% of the maximum allowable flow velocity
Active area for the vapour flow: 80% of the column cross sectional area
Liquid down-flow cross section: 20% of the column cross sectional area
Free hole area ≈ 8–16% of the active cross sectional area for the vapour
Weir height ≈ 30–80 mm
Weir overflow height ≈ 5–40 mm
Tray spacing ≈ 400–600 mm.

9.1.1 Required Flow Cross Section for the Vapour Loading [1–7]

The required flow cross section results from the vapour rate and the allowable flow velocity w_D in the column. The flow velocity is dependent on the tray spacing. The larger the tray spacing the fewer droplets will be entrained to the next tray above.

An increase in the tray spacing also increases the allowable flow velocity of the vapour.

The maximum allowable flow velocity w_{max} is determined by the gas loading factor C_{SB}, which is a function of the flow parameter F_{LV}.

In Figs. 9.5 and 9.6; Tables 9.1 and 9.2 the gas loading factor C_{SB}, according to different models, is shown as a function of the flow parameter F_{LV} for different tray spacings.

$$F_{LV} = \frac{L}{G} * \sqrt{\frac{\rho_V}{\rho_L}} \quad C_{SB} = f(F_{LV})$$

Using the gas loading factor C_{SB}, the maximum allowable flow velocity w_{max} of the vapour in the column is determined:

$$w_{max} = C_{SB} * \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} * \left(\frac{0.02}{\sigma}\right)^{-0.2} (\mathrm{m/s})$$

σ = surface tension (N/m)
G = vapour rate (kg/h)
L = liquid rate (kg/h)
ρ_V = vapour density (kg/m^3)
ρ_L = liquid density (kg/m^3)

In practice 80–85% of the maximum flow velocity w_{max} is used for the design of the column as the allowable flow velocity w_D for the vapour.

$$w_D = 0.8 * w_{max} = 0.8 * C_{SB} * \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} * \left(\frac{0.02}{\sigma}\right)^{-0.2} (\mathrm{m/s})$$

$$\text{Flow Parameter } F_{LV} = \frac{L}{G} * \sqrt{\frac{\rho_V}{\rho_L}}$$

G = gas flow (kg/h)
L = liquid flow (kg/h)
ρ_G = gas density (kg/m^3)
ρ_L = liquid density (kg/m^3).

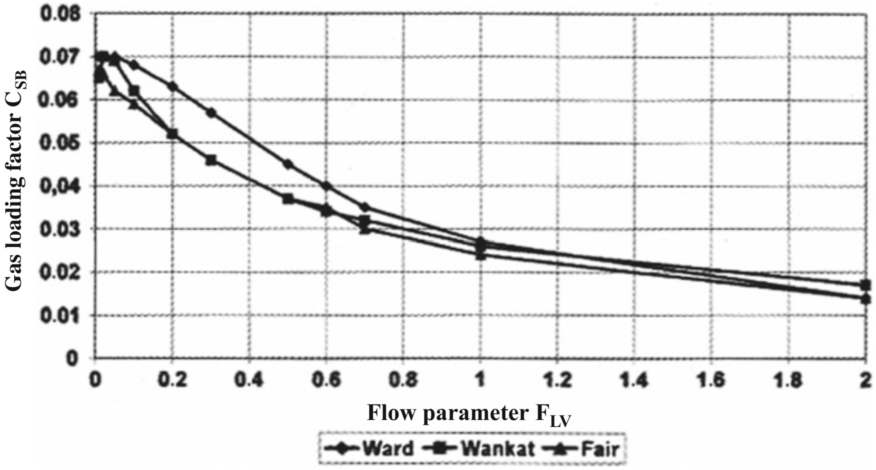


Fig. 9.5 Gas loading factor C_{SB} according to Ward, Wankat, and Fair as a function of the flow parameter F_{LV} for a tray spacing of 300 mm

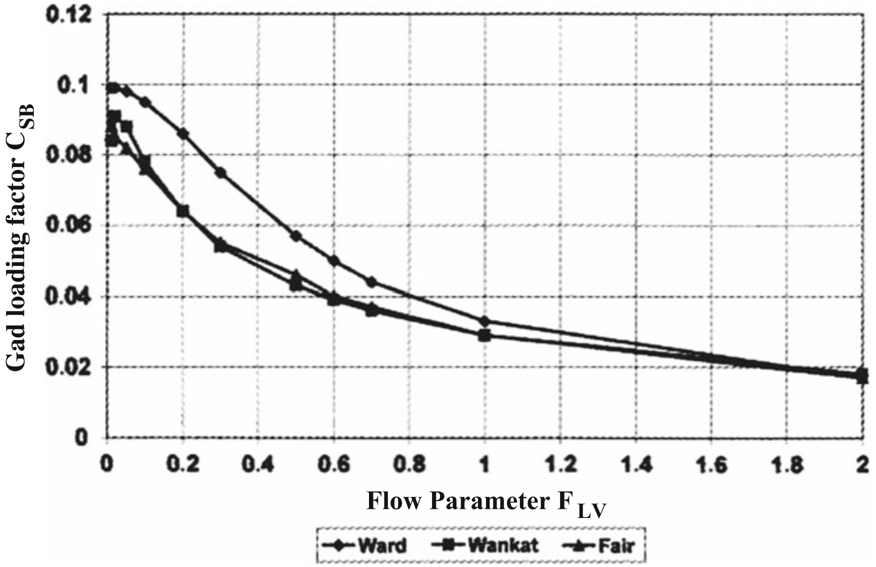


Fig. 9.6 Gas loading factor C_{SB} according to Ward, Wankat, and Fair as a function of the flow parameter F_{LV} for a tray spacing of 450 mm

Table 9.1 Gas loading factors C_{SB} according to Kessler and Wankat for different tray spacings as a function of the flow parameter F_{LV}

Tray spacing H (mm)					
	230	305	457	610	914
F_{LV} = 0.05	0.055	0.069	0.088	0.117	0.153
F_{LV} = 0.10	0.05	0.062	0.078	0.104	0.134
F_{LV} = 0.2	0.042	0.052	0.064	0.083	0.106
F_{LV} = 0.3	0.037	0.046	0.054	0.07	0.088
F_{LV} = 0.4	0.033	0.041	0.048	0.061	0.076
F_{LV} = 0.5	0.03	0.037	0.043	0.054	0.067
F_{LV} = 0.6	0.027	0.034	0.039	0.048	0.060
F_{LV} = 0.7	0.025	0.032	0.036	0.044	0.054
F_{LV} = 0.8	0.024	0.029	0.033	0.04	0.049
F_{LV} = 0.9	0.022	0.028	0.031	0.037	0.045

Table 9.2 Gas loading factors C_{SB} according to Ward, Kessler and Wankat, and fair for different tray spacings and flow parameters

	H = 457 mm			H = 610 mm		
	Ward	Kessler	Fair	Ward	Kessler	Fair
F_{LV} = 0.05	0.098	0.088	0.082	0.122	0.117	0.111
F_{LV} = 0.10	0.095	0.078	0.076	0.117	0.104	0.101
F_{LV} = 0.2	0.086	0.064	0.064	0.104	0.083	0.085
F_{LV} = 0.3	0.075	0.054	0.055	0.089	0.07	0.073
F_{LV} = 0.5	0.057	0.043	0.046	0.066	0.054	0.055
F_{LV} = 0.6	0.050	0.039	0.040	0.057	0.048	0.049
F_{LV} = 0.7	0.044	0.036	0.037	0.051	0.044	0.046
F_{LV} = 1.0	0.033	0.029	0.029	0.037	0.035	0.037

Example 9.1.1: Determination of the allowable vapour flow velocity w_D

Reflux ratio $R = 4$ $L/G = 4/5 = 0.8$ $\rho_V = 3.125\ \mathrm{kg/m^3}$
$\rho_L = 800\ \mathrm{kg/m^3}$ Flow parameter $F_{LV} = 0.05$ $\sigma = 0.05\ \mathrm{N/m}$

From Fig. 9.6, for a tray spacing H = 450 mm, the gas loading factors C_{SB} are taken for the flow parameter F_{LV} = 0.05.

According to Fair: C_{SB} = 0.082

$$w_D = 0.8 * C_{SB} * \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} * \left(\frac{0.02}{\sigma}\right)^{-0.2}$$

$$= 0.8 * 0.082 * \sqrt{\frac{800 - 3.125}{3.125}} * \left(\frac{0.02}{0.05}\right)^{-2} = 1.26\ \mathrm{m/s}$$

According to Wankat and Kessler: C_{SB} = 0.088

$$w_D = 0.8 * 0.088 * \sqrt{\frac{800 - 3.125}{3.125}} * \left(\frac{0.02}{0.05}\right)^{-0.2} = 1.35\ \mathrm{m/s}$$

The required column cross section A_{D} for the vapour flow is calculated for the vapour flow rate V with an allowable flow velocity w_{D}.

$$A_{\mathrm{D}} = \frac{V(\mathrm{m}^3/\mathrm{h})}{3600 * w_{\mathrm{D}}} \ (\mathrm{m}^2)$$

The column diameter D_{K} results from the required flow cross section A_{D} for the vapour flow rate and the required flow cross section A_{F} for the liquid (see Sect. 9.1.3).

Example 9.1.2: Determination of the required column cross section A_{D} for the vapour flow

$$w_{\mathrm{D}} = 1.45\ \mathrm{m/s} \quad \text{Vapour flow } G = 15.000\ \mathrm{kg/h} \quad \rho_{\mathrm{V}} = \ 3\ \mathrm{kg/m}^3$$

$$A_{\mathrm{D}} = \frac{G/\rho_{\mathrm{V}}}{3600 * w_{\mathrm{D}}} = \frac{15.000/3}{3600} * \frac{1}{1.45} = 0.96\ \mathrm{m}^2$$

For a check of the allowable flow velocity of the vapour in the column the comparable **air velocity w_{L}** can be used.

Most of the tray columns are operated with comparable air velocities of 1.4–2.5 m/s based on the vapour cross section.

$$w_{\mathrm{L}} = w_{\mathrm{D}} * \sqrt{\frac{\rho_{\mathrm{V}}}{\rho_{\mathrm{air}}}} = w_{\mathrm{D}} * \sqrt{\frac{\rho_{\mathrm{V}}}{1.21}} = w_{\mathrm{D}} * 0.909 * \sqrt{\rho_{\mathrm{V}}}$$
$$w_{\mathrm{D}} = 1.1 * \frac{w_{\mathrm{L}}}{\sqrt{\rho_{\mathrm{V}}}}$$

w_{L} = comparable air velocity (m/s)
ρ_{V} = vapour density (kg/m^3)
ρ_{air} = air density = 1.21 kg/m^3.

Example 9.1.3: Calculation of the comparable air velocity for w_{D} = 1.45 m/s

$$\text{Vapor density } \rho_{\mathrm{V}} = 3.125\ \mathrm{kg/m}^3$$
$$w_{\mathrm{L}} = w_{\mathrm{D}} * 0.909 * \sqrt{\rho_{\mathrm{V}}} = 1.45 * 0.909 * \sqrt{3.125} = 2.33\ \mathrm{m/s}$$

Cross-check:

$$w_{\mathrm{D}} = 1.1 * \frac{w_{\mathrm{L}}}{\sqrt{\rho_{\mathrm{V}}}} = 1.1 * \frac{2.33}{\sqrt{3.125}} = 1.45\ \mathrm{m/s}.$$

Example 9.1.4: Determination of the allowable vapour loading *G* (kg/h) at different comparable air velocities w_L

$$\rho_D = 0.08\ \mathrm{kg/m^3} \quad A_D = 1.77\ \mathrm{m^2} = \text{ vapours cross sectional area}$$

w_L = 1.5 m/s for a bubble cap tray

$$w_D = \frac{1.1 * 1.5}{\sqrt{0.08}} = 5.8\ \mathrm{m/s}$$
$$G = 3600 * 0.08 * 5.8 * 1.77 = 2956\ \mathrm{kg/h}$$

w_L = 2.5 m/s for a sieve tray

$$w_D = \frac{1.1 * 2.5}{\sqrt{0.08}} = 9.7\ \mathrm{m/s}$$
$$G = 3600 * 0.08 * 9.7 * 1.77 = 4945\ \mathrm{kg/h}$$

The comparable **air velocity** is especially suitable for checking the flow velocity in the holes of sieve trays.

Due to entrainment the upper comparable air velocity in the hole should be a maximum of **w_L = 16 m/s** and because of weeping the lower flow velocity should be **w_L = 8 m/s.**

Calculation of the maximum allowable flow velocity w_{Kmax} in sieve trays, based on the active area of the vapour flow [6] for avoiding entrainment is:

$$w_{\mathrm{K\,max}} = 2.5 * \left(\frac{\phi^2 * \sigma * \Delta\rho * g}{\rho_V^2}\right)^{0.25} (\mathrm{m/s}) \quad w_{\mathrm{hole\,max}} = \frac{w_{\mathrm{K\,max}}}{\phi}\ (\mathrm{m/s})$$

Calculation of the minimum required flow velocity in the hole to avoid weeping is:

$$w_{\mathrm{hole\,min}} = 1.4 * \sqrt{0.37 * d_{\mathrm{hole}} * g * \left(\frac{\rho_L - \rho_V}{\rho_V}\right)^{1.25}}\ (\mathrm{m/s})$$

ϕ = hole fraction of the tray
d_{hole} = hole diameter (m)
σ = surface tension (N/m)
$\Delta\rho = \rho_L - \rho_V$ = density difference between liquid and vapour.

Example 9.1.5: Calculation of the maximum and minimum flow velocity

$$\phi = 0.1 \quad d_{\text{hole}} = 20\ \text{mm} \quad \Delta\rho = 697\ \text{kg/m}^3 \quad \sigma = 0.03 \quad \text{N/m} \ = 30\ \text{dyn/cm}$$

$$w_{\text{K max}} = 2.5 * \left(\frac{0.1^2 * 0.03 * 697 * 9.81}{3^2}\right)^{0.25} = 1.72\ \text{m/s}$$

$$w_{\text{hole max}} = \frac{1.72}{0.1} = 17.2\ \text{m/s}$$

$$w_{\text{hole min}} = 1.4 * \sqrt{0.37 * 0.02 * 9.81 * \left(\frac{700-3}{3}\right)^{1.25}} = 11.3\ \text{m/s}$$

For other hole sizes (mm):	d = 20	d = 10	d = 5	d = 2
w_{holemin} (m/s)	11.3	8	5.7	3.6

Example 9.1.6: Allowable vapour loading *G* (kg/h) in sieve trays

Vapour density $\rho_V = 0.188\,\text{kg/m}^3$
$A_D = 3.14\ \text{m}^2$ = vapour cross section of the column

Sieve tray with 16% free flow area A_{hole} in the holes

$A_{\text{hole}} = 0.16 * 3.14 = 0.5\ \text{m}^2$ = total cross sectional area of the holes

Upper hole velocity w_L = 16 m/s

$$w_D = \frac{1.1 * 16}{\sqrt{0.188}} = 40.6\ \text{m/s}$$
$$G = 3600 * 0.188 * 40.6 * 0.5 = 13739\ \text{kg/h}$$

Lower hole velocity w_L = 8 m/s

$$w_D = \frac{1.1 * 8}{\sqrt{0.188}} = 20.3\ \text{m/s}$$
$$G = 3600 * 0.188 * 20.3 * 0.5 = 6869\ \text{kg/h}.$$

9.1.2 *Required Downcomer Cross Section for the Liquid [1–7]*

The required flow cross section A_F for the outflow of the liquid to the next lower tray results from the given allowable flow velocity w_{Fl} in the liquid downcomer shown in Fig. 9.7.

$$A_F = \frac{V_F}{3600 * w_{FL}} \ (\mathrm{m}^2)$$

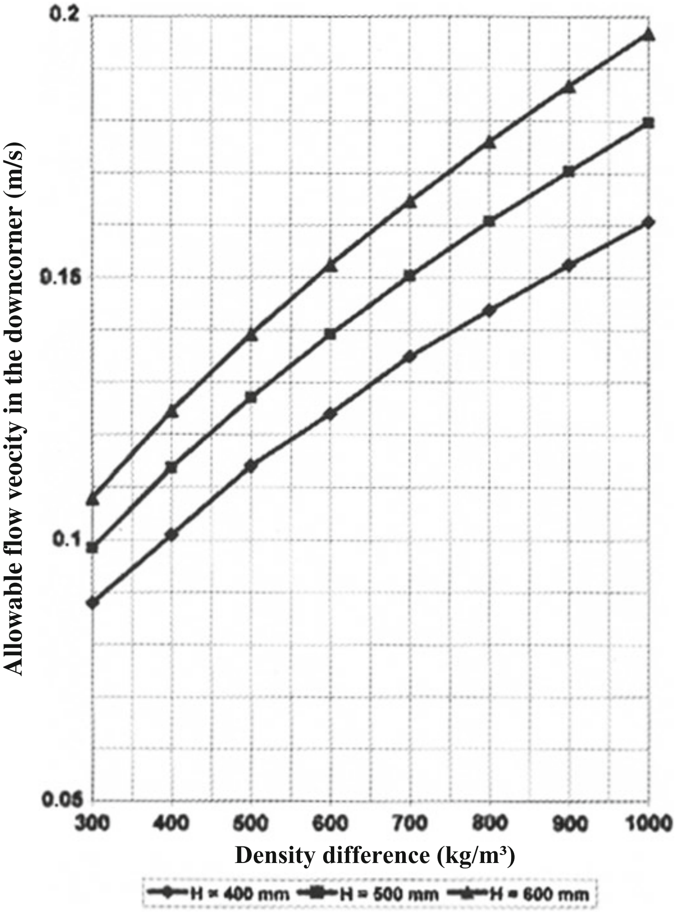


Fig. 9.7 Allowable flow velocity in the downcomer as a function of the tray spacing H and the density difference $\Delta\rho = \rho_L - \rho_V$ for a foaming factor of 1

A_F = required flow cross section for the liquid outflow (m^2)
V_F = liquid loading (m^3/h)
w_{FL} = allowable flow velocity in the downcomer (m/s).

Figure 9.7 shows that the allowable flow velocity in the downcomer increases with increasing density difference $\Delta\rho = \rho_L - \rho_V$ between a gas and a liquid, this is because both phases separate better at larger density differences.

With foaming media the calculated downcomer velocity w_{Fl} must be corrected with a foaming factor.

$$w_{\mathrm{Flcorr}} = \text{ foaming factor } * w_{\mathrm{Fl}} \ (\mathrm{m/s})$$

	Foaming factor
Non-foaming	1
Moderately foaming (oil absorber, amine + glycol regenerator)	0.8–0.9
Freon	0.9
Strongly foaming (absorber for amine + glycole)	0.7–0.75
Stable foamer	0.2

Alternatively, the allowable flow velocity in the downcomer for a foaming factor of one can be calculated:

$$w_{\mathrm{Fl}} = 0.008 * \sqrt{H * \Delta\rho}\,(\mathrm{m/s})$$

H = tray spacing (m)
$\Delta\rho = \rho_L - \rho_V$ (kg/m^3).

Example 9.1.2.1: Calculation of the flow velocity in the downcomer

$$H = 0.4 \text{ m} \quad \Delta\rho = 600 \text{ kg/m}^3 \quad \text{Foaming factor } = 1$$

$$w_{\mathrm{Fl}} = 0.008 * \sqrt{0.4 * 600} = 0.124 \text{ m/s}$$

A larger tray spacing H increases the allowable velocity in the downcomer because there is more time for the phase separation, in addition, the flooding risk is reduced.

Checking the residence time for the phase separation in the downcomer.

The liquid V_S streaming out of the downcomer which is saturated with vapour has a larger volume than the pure liquid V_F, this is because the liquid contains up to about 60% vapour, i.e., gas.

The liquid flow V_S which is saturated with gas streaming down from the downcomer is determined as follows:

$$V_S = \frac{V_F}{0.6} = 1.67 * V_F \ (\mathrm{m^3/h})$$

The residence time in the downcomer should be about 5 s based on the pure liquid flow V_F without dissolved gases, or about 3 s based on the foaming gas containing liquid V_S.

Example 9.1.2.2: Determination of the required downflow cross section and the residence times in the downcomer

$$V_F = 10 \ \mathrm{m^3/h} \quad H = 0.4 \ \mathrm{m} \quad \text{Density difference } \Delta\rho = 400 \ \mathrm{kg/m^3}$$

From Fig. 9.7 we notice that the allowable flow velocity in the downcomer w_{Fl} = 0.101 m/s.

Calculation of the required downflow cross section for the liquid:

$$A_F = \frac{10}{3600 * 0.101} = 0.0275 \ \mathrm{m^2}$$

Calculation of the residence time t_A for the clear liquid V_F without dissolved gases:

$$t_A = \frac{A_F * H}{V_F} = \frac{0.0275 * 0.4}{10/3600} = 3.96 \ \mathrm{s}$$

Calculation of the residence time for the gas-saturated liquid V_S:

$$V_S = 1.67 * 10 = 16.7 \ \mathrm{m^3/h} \quad t_A = \frac{0.0275 * 0.4}{16.7/3600} = 2.37 \ \mathrm{s}$$

In this case, the downcomer is chosen too small and is enlarged to 0.0413 $\mathrm{m^2}$.

After this adjustment the residence time for the clear liquid is 5.94 s and for the vapour saturated liquid it is 3.6 s.

Normally, 10% of the column cross section is chosen for the liquid outflow and 10% for the liquid feed.

This gives the weir length L_W and the segment height H_S as:

$$\text{Weir length } L_W = 0.7267 * D_K$$

$$\text{Segment height } H_S = 0.1565 * D_K.$$

Example 9.1.2.3: Dimensioning of the downcomer, and the weir length L_W and segment Height H_S for A_F = 10% of the column cross section

$$\text{Column diameter } D_K = 1 \ \mathrm{m} \quad \text{Column cross section } A_{tot} = 0.785 \ \mathrm{m^2}$$

$$A_F = 0.1 * 0.785 = 0.0785 \ \mathrm{m^2} \quad A_D = A_{tot} - 2 * A_F = 0.785 - 2 * 0.0785 = 0.628 \ \mathrm{m^2} = 80\%$$

$$\text{Weir length } L_W = 0.7276 * 1 = 0.7276 \ \mathrm{m} \quad \text{Segment height } H_S = 0.157 * 1 = 0.157 \ \mathrm{m}$$

Another aspect of the column design is the allowable **weir loading W_L** and the **Weir overflow height h_{ow}**.
It should be anticipated that $W_L = 0.6 - 15$ l/s m and $h_{ow} = 5$–40 mm.

$$W_L = \frac{V_F * 1000}{3600 * L_W} (\text{l/s m})$$

$$h_{ow} = 2.83 * \left(\frac{V_F}{L_W}\right)^{2/3} (\text{mm})$$

V_F = liquid flow rate (m^3/h)
L_W = weir length (m).

Example 9.1.2.4: Calculation of the weir loading and the weir overflow height

$$L_W = 0.3573 \text{ m} \quad V_F = 10 \text{ m}^3/\text{h}$$

$$W_L = \frac{10 * 1000}{3600 * 0.3573} = 7.77 \left(\frac{1}{\text{sm}}\right)$$

$$h_{ow} = 2.83 * \left(\frac{10}{0.3573}\right)^{2/3} = 26 \text{ mm.}$$

9.1.3 Required Column Diameter D_K

The total column cross sectional area A_{tot} results from the assumption that 10% of the column area for the liquid outflow and the liquid inflow, i.e., in total 20% of the column cross section for the liquid flow, is as follows:

$$A_{tot} = A_D + 2 * A_F = \frac{A_D}{0.8} (\text{m}^2)$$

$$\text{Column diameter } D_K = \sqrt{\frac{4}{\pi} * A_{tot}} (\text{m})$$

Example 9.1.2.5: Design of a tray

$$G = 15{,}500 \text{ kg/h} = 5{,}000 \text{ m}^3/\text{h} \quad \rho_V = 3.1 \text{ kg/m}^3 \quad H = 0.45 \text{ m} \quad A_F = 0.1 * A_{tot}$$

$$L = 14{,}000 \text{ kg/h} = 20 \text{ m}^3/\text{h} = V_F \quad \rho_L = 700 \text{ kg/m}^3 \quad L/G = 0.9 \quad C_{SB} = 0.08$$

$$w_D = 0.8 * C_{SB} * \sqrt{\frac{\rho_{Fl} - \rho_D}{\rho_D}}\ (\mathrm{m/s}) = 0.8 * 0.08 * \sqrt{\frac{700 - 3.1}{3.1}} = 0.96\ \mathrm{m/s}$$

Flow cross section for vapors $A_D = \frac{G(\mathrm{m}^3/\mathrm{h})}{3600 * w_D}(\mathrm{m}^2) = \frac{5000}{3600 * 1.2} = 1.45\ \mathrm{m}^2$

Required total flow cross section $A_{tot} = \frac{A_D}{0.8}(\mathrm{m}^2) = \frac{1.45}{0.8} = 1.8\ \mathrm{m}^2$

Required column diameter $D_K = \sqrt{\frac{4}{\pi} * A_{ges}}(\mathrm{m}) = \sqrt{\frac{4}{\pi} * 1.8} = 1.5\ \mathrm{m}$

Weir length $L_W = 0.7267 * D_K = 0.7267 * 1.5 = 1.1\ \mathrm{m}$

Segment height $H_S = 0.1565 * D_K = 0.1565 * 1.5 = 0.23\ \mathrm{m}$

Downflow cross section $A_F = 0.1 * A_{ges}(\mathrm{m}^2) = 0.1 * 1.8 = 0.18\ \mathrm{m}^2$

Weir loading $W_L = \frac{V_F(m^3/h) * 1000}{3600 * L_W}\left(\frac{l}{s\,m}\right) = \frac{20 * 1000}{3600 * 1.1} = 5.05\ l/s\,m$

Weir overflow height $h_{\ddot{U}W} = 2.83 * \left(\frac{V_F}{L_W}\right)^{2/3}(\mathrm{mm}) = 2.83 * \left(\frac{20}{1.1}\right)^{2/3} = 19.6\ \mathrm{mm}$

Flow velocity in the downcomer $w_{Fl} = \frac{V_F}{3600 * A_F}(\mathrm{m/s}) = \frac{20}{3600 * 0.18} = 0.03\ \mathrm{m/s}$

Residence time in the downcomer $t_A = \frac{A_F * H}{V_F/3600}(\mathrm{s}) = \frac{0.18 * 0.45}{20/3600} = 14.5\ \mathrm{s}.$

9.1.4 Flooding and Weeping in a Tray Column

9.1.4.1 Flooding of a Column (Fig. 9.8)

If the height of the foaming liquid in the downcomer rises to the next tray above the flooding of the column begins.

The essential influencing parameters on the flood conditions are:

- Weir height h_W: 40–80 mm.
- Weir overflow height h_{ow}: 5–40 mm.
- Pressure loss at the tray ΔP_t: 150–300 mm liquid height or 2–3 mbar.
- Liquid gradient on the tray Δ: 5–10 mm liquid height.
- Pressure loss in the inlet slot for the liquid h_D: 2–5 mm liquid height.
- Foaming factor Φ = 0.5–0.6 = 50–60% foaming proportion in the liquid.

Fig. 9.8 Flooding of column trays

$H_D = h_W + h_{ow} + \Delta p_{tray} + \Delta + h_D$ (mm liquid height)

$H_D = 80 + 10 + 150 + 0 + 3 = 243$ mm liquid height

$H_{Dfoam} = H_D / \Phi = 243 / 0.6 = 486$ mm liquid height

Recommended: $H = 2 * H_D = 2 * 243 = 486$ mm

Chosen: $H = 500$ mm

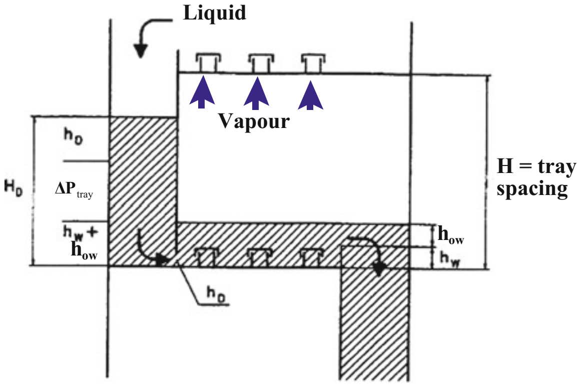


Figure 9.8 shows how the height of the clear liquid H_D in the downcomer is calculated and how a determination is made of the tray spacing.

Generally the tray spacing is chosen as $\boldsymbol{H = 2 * H_D}$.

H_D = height of the clear liquid in the downcomer.
H_{Dfoam} = height of the foam in the downcomer.

In order to calculate H_D the pressure loss of the tray ΔP_{tray} and the pressure loss in the inlet slot h_D are needed.

Calculation of the **pressure loss in the inlet slot**: $h_D = 140 * w_{Slot}^2$
w_{Slot} = flow velocity in the inlet slot (m/s).

Example 9.1.4.1: Determination of the pressure loss in the inlet slot

$L_W = 0.6$ m $\quad H_{slot} = 25$ mm $\quad A_{slot} = L_W * H_{slot} = 0.015\ \text{m}^2 =$ slot area
$V_F = 10\ \text{m}^3/\text{h}$

$$w_{slot} = \frac{10}{3600 * 0.015} = 0.185\ \text{m/s}$$
$$h_D = 140 * w_{slot}^2 = 140 * 0.185^2 = 4.8\ \text{mm liquid height.}$$

9.1.4.2 Weeping

If the vapor flow velocity is too low then weeping of the liquid occurs in sieve trays and valve trays to the next lowest tray.

The tray efficiency falls.

In bubble cap trays with a riser a weeping is not possible.

The required **minimum vapor flow velocity in the holes of a sieve tray** can be calculated as follows:

$$w_{\text{hole min}} = 1.4 * \sqrt{0.37 * d_{\text{hole}} * g * \left(\frac{\rho_{\text{L}} - \rho_{\text{V}}}{\rho_{\text{V}}}\right)^{1.25}}\ (\text{m/s})$$

d_{hole} = hole diameter (m)
$\Delta\rho = \rho_{\text{L}} - \rho_{\text{V}}$ = density difference between the liquid and the vapour.

Alternatively, a similar minimum comparable air velocity of w_{L} = 8–10 m/s in the holes can be assumed.

$$w_{\text{hole min}} = 1.1 * \frac{w_{\text{L}}}{\sqrt{\rho_{\text{V}}}} = \frac{8}{\sqrt{\rho_{\text{V}}}}.$$

Example 9.1.4.1: Determination of the minimum flow velocity in the sieve tray

$$\text{Data}: \rho_{\text{V}} = 3\ \text{kg/m}^3 \quad \rho_{\text{L}} = 700\ \text{kg/m}^3 \quad d_{\text{hole}} = 8\ \text{mm}$$

$$w_{\text{holemin}} = 1.4 * \sqrt{0.37 * 0.008 * 9.81 * \left(\frac{700 - 3}{3}\right)^{1.25}} = 7.2\ \text{m/s}$$

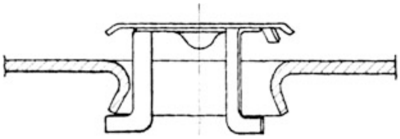
$$w_{\text{holemin}} = 1.1 * \frac{10}{\sqrt{3}} = 6.35\ \text{m/s}$$

The required minimum flow velocity for valve tray columns can be estimated as follows:

V1 valve = flat valve tray:

$$w_{\min} = 0.0167 * H_{\text{Fl}}^{0.615} * \sqrt{\frac{\rho_{\text{L}}}{\rho_{\text{V}}}}\ (\text{m/s})$$

V4 valve = venturi valve tray:



$$w_{\min} = 0.0263 * H_{\mathrm{Fl}}^{0.615} * \sqrt{\frac{\rho_{\mathrm{L}}}{\rho_{\mathrm{V}}}}\ (\mathrm{m/s})$$

$$H_{\mathrm{fl}} = h_{\mathrm{W}} + h_{\mathrm{ow}}(\mathrm{mm\ FS})$$

Example 9.1.4.2: Determination of the minimum flow velocity in valve trays

$$\text{Data: } \rho_{\mathrm{V}} = 3\ \mathrm{kg/m^3} \quad \rho_{\mathrm{L}} = 700\ \mathrm{kg/m^3} \quad H_{\mathrm{fl}} = 45\ \mathrm{mm\ FS}$$

$$V1 - \text{valve: } w_{\min} = 0.0167 * 45^{0.615} * \sqrt{\frac{700}{3}} = 2.6\ \mathrm{m/s}$$

$$V4 - \text{valve: } w_{\min} = 0.0263 * 45^{0.615} * \sqrt{\frac{700}{3}} = 4.1\ \mathrm{m/s}$$

Example 9.1.4.3: Checking of a double-flow valve tray with regard to weeping

Column diameter $D_{\mathrm{K}} = 4.2$ m with $n_{\mathrm{V}} = 1782$ V1 valves with flat arrangement
Weir length: external $2 \times 2 = 4$ m; in the middle $2 \times 3.95 = 7.9$ m
Gas flow: $G = 9.5$ t/h $= 10{,}275\ \mathrm{m^3/h}$ Gas density $\rho_{\mathrm{V}} = 0.9245\ \mathrm{kg/m^3}$
Liquid flow: 40 t/h $= 40\ \mathrm{m^3/h}$ $\rho_{\mathrm{L}} = 1000\ \mathrm{kg/m^3}$

Calculated weir overflow height and weir loadings:

External for $L_{\mathrm{W}} = 4$ m : $h_{\mathrm{ow}} = 12.9$ mm $W_{\mathrm{L}} = 2.7$ l/s m
In the middle for $L_{\mathrm{W}} = 7.9$ m : $h_{\mathrm{ow}} = 8.3$ mm $W_{\mathrm{L}} = 1.4$ l/s m

Outflow velocity in the downcomer:

In the middle: $w = 0.011$ m/s External: $w = 0.015$ m/s

The tray is overdimensioned toward the liquid side.

The normal operating region of a ballast V1 valve is designed for a similar air volume of 20–60 $\mathrm{m^3/h}$.

Conversion of the vapour volume of $G = 10{,}275\ \mathrm{m^3/h}$ to a similar air volume V_L gives:

$$V_{\mathrm{L}} = \frac{G * \sqrt{\frac{\rho_{\mathrm{D}}}{\rho_{\mathrm{L}}}}}{n_{\mathrm{V}}} = \frac{10275 * \sqrt{\frac{0.9245}{1.21}}}{1782} = 5.04\ \mathrm{m^3/h\ per\ valve}$$

An airflow of $5.04\ \mathrm{m^3/h}$ is much too small compared with the required $20\ \mathrm{m^3/h}$ comparable air volume per valve!

Calculation of the minimum velocity for vapour in the valve:

$$w_{\mathrm{Vmin}} = 0.0167 * H_{Fl}^{0.615} * \sqrt{\frac{\rho_{\mathrm{L}}}{\rho_{\mathrm{V}}}} = 0.0167 * 42.9^{0.615} * \sqrt{\frac{1000}{0.9245}} = 5.5\ \mathrm{m/s}$$

$$\text{Alternative calculation: } w_{\mathrm{V\,min}} = 0.158 * \sqrt{\frac{\rho_{\mathrm{L1}}}{\rho_{\mathrm{V}}}} = 0.158 * \sqrt{\frac{1000}{0.9245}} = 5.9\ \mathrm{m/s}$$

Required vapour flow V_V for a valve with $d = 40$ mm:

$$V_{\mathrm{V}} = W_{\mathrm{V\,min}} * A_{\mathrm{Ventil}} * 3600 = 5.9 * 0.0013 * 3600 = 26.7\ \mathrm{m^3/h\ pro\ Ventil}$$

Available vapour flow V_V per valve:

$$V_{\mathrm{V}} = \frac{10275}{1782} = 5.76\,\mathrm{m^3/h\ pro\ Ventil}$$

Conclusion

The flow cross section for the vapour must be reduced by covering of valves.

9.1.5 Pressure Drop Calculations [1–7]

The pressure loss ΔP_{tray} in the cross stream trays is subdivided into the dry pressure loss ΔP_{dry}, when flowing through a cap on a bubble cap tray, a hole in a sieve tray, or a valve on a valve tray, and the liquid pressure loss ΔP_{liq} from the liquid level on the tray.

$$\boldsymbol{\Delta P_{\mathrm{tray}} = \Delta P_{\mathrm{dry}} + \Delta P_{\mathrm{liq}}(\mathrm{mm\ liquid\ height})}$$

Bubble cap trays [3] Calculation of the dry pressure loss when flowing through the riser and the cap:

$$\Delta P_{\text{dry}} = 274 * K * \frac{\rho_V}{\rho_L - \rho_V} * w_K^2 = 274 * K * \frac{\rho_V}{\rho_L - \rho_V} * \left(\frac{V}{f_K}\right)^2 \text{ (mm liquid)}$$

K = pressure drop coefficient

V = vapour loading of the column (m^3/s).

The pressure loss coefficient K depends on the quotient ring cross sectional area between the riser and cap and the riser cross sectional area ($K = f\,(f_R/f_K)$)

f_K = cross sectional area of all risers on the tray (m^2)
f_R = ring cross sectional area of all caps on the tray (m^2)
w_K = flow velocity of the vapour in the riser (m/s)

$$\frac{f_R}{f_K} = 1 \quad \Rightarrow \; K = 0.65 \qquad \frac{f_R}{f_K} = 1.5 \quad \Rightarrow \; K = 0.55$$

The wet pressure loss ΔP_{liq} on a bubble cap tray results from the open slot height h_{slot}, the slot seal or submergence h_T, the weir overflow height h_{ow}, and the liquid gradient ΔF on the tray from inflow to outflow.

$$\Delta P_{\text{liq}} = h_{\text{slotl}} + h_T + h_{\text{ow}} + \Delta F/2 (\text{mm liquid}).$$

h_T = slot seal = vertical distance between slot top edge and weir height h_W (mm liquid)

h_{ow} = weir overflow height (mm liquid)
ΔF = liquid gradient on the tray (mm liquid)
h_{slot} = open slot height (mm liquid)
$V_{\max}$ = maximum allowable vapour loading of the slots (m^3/s)
V = actual vapour loading (m^3/s)

The maximum allowable vapour loading of the bubble cap slots $V_{\max}$ is determined as follows:

$$V_{\max} = K_S * \sqrt{H_{\text{slot}} * \frac{\rho_L - \rho_V}{\rho_V}} * A_{\text{slot}} (\text{m}^3/\text{s})$$

$$\text{Open slot height } h_{\text{slot}} = \frac{V}{V_{\max}} * H_{\text{slot}} \text{ (mm liquid)}$$

A_{slot} = slot cross sectional area of all caps (m^2)

H_{slotl} = slot height (mm)
K_S for triangular slots: 1.2
K_S rectangular slots: 1.51
K_S for trapezoidal slots = f (R_S)
R_S = ratio of the upper slot width a to the bottom slot width b
$R_S = a/b = 6/13.9 = 0.43 \rightarrow K_S = 1.38$

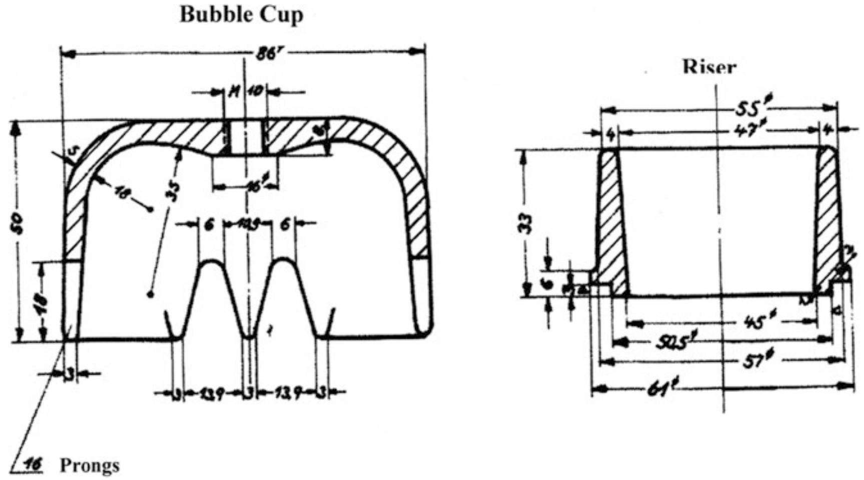


Fig. 9.9 Bubble cup and riser

Example 9.1.5.1: Pressure loss calculation for a bubble cap tray with a diameter of 1.48 m

$$A_{\text{tot}} = 1.72\ \text{m}^2 \quad A_{\text{D}} = 0.8 * 1.72 = 1.37\ \text{m}^2 \quad \rho_{\text{V}} = 3\ \text{kg/m}^3 \quad \rho_{\text{L}} = 700\ \text{kg/m}^3$$

$$R = 9 \quad L/G = 9/10 = 0.9 \quad h_{\text{T}} = 5\ \text{mm} \quad h_{\text{ow}} = 15\ \text{mm} \quad \Delta F = 10\ \text{mm}$$

Vapour loading of the column $V = 0.8\ \text{m}^3/\text{s}$
Bubble cap tray with 95 caps according to Fig. 9.9:

$$16\ \text{slots} \quad \text{Slot height}\ H_{\text{slot}} = 18\ \text{mm} \quad h_{\text{W}} = 30\ \text{mm} \quad K = 0.47$$

$$\text{Slot area}\ A_{\text{slot}} = \frac{6 + 13.9}{2} * 18 * 16 * 95 * 10^{-6} = 0.272\ \text{m}^2$$

$$\text{Riser area}\ f_{\text{K}} = 0.045 * 0.785 * 95 = 0.151\ \text{m}^2$$

$$w_{\text{K}} = \frac{V}{f_K} = \frac{0.8}{0.151} = 5.3\ \text{m/s}$$

$$\Delta P_{\text{dry}} = 274 * K * \frac{\rho_{\text{V}}}{\rho_{\text{L}} - \rho_{\text{V}}} * w_{\text{k}}^2 = 274 * 0.47 * \frac{3}{697} * 5.32^2 = 15.6\ \text{mm liquid}$$

$$\Delta P_{\text{dry}} = 274 * K * \frac{\rho_{\text{V}}}{\rho_{\text{L}} - \rho_{\text{V}}} * \left(\frac{V}{f_{\text{K}}}\right)^2 = 274 * 0.47 * \frac{3}{697} * \left(\frac{0.8}{0.151}\right)^2 = 15.6\ \text{mm liquid}$$

$$V_{\max} = K_S * \sqrt{H_{\text{slot}} * \frac{\rho_L - \rho_V}{\rho_V}} * A_{\text{slot}} = 1.38 * \sqrt{0.018 * \frac{697}{3}} * 0.272 = 0.768\,\text{m}^3/\text{s}$$

$$h_{\text{slot}} = \frac{V}{V_{\max}} * H_{\text{slot}} = \frac{0.8}{0.768} * 18 = 18.8\,\text{mm}$$

$$\Delta P_{\text{liq}} = h_{\text{slot}} + h_T + h_{\text{ow}} + \Delta F/2 = 18.8 + 5 + 15 + 10/2 = 43.8\ \text{mm liquid}$$

$$\boldsymbol{\Delta P_{\text{tray}} = \Delta P_{\text{dry}} + \Delta P_{\text{liq}} = 15.6 + 43.8 = 59.4\,\textbf{mm liquid height} = 4.1\,\textbf{mbar}}$$

Example 9.1.5.2: Pressure loss calculation for a bubble cap tray (Fig. 9.10)

$$\text{Vapour loading } V = 0.685\ \text{m}^3/\text{s} \rightarrow w_{\text{riser}} = 4.54\ \text{m/s}$$
$$\rho_V = 3\ \text{kg/m}^3 \quad \rho_L = 700\ \text{kg/m}^3 \quad h_T = 1\,\text{mm} \quad h_{\text{ow}} = 10\,\text{mm} \quad \Delta F = 8\ \text{mm}$$
$$\text{Slot area } f_{\text{slot}} = 0.272\ \text{m}^2 \quad \text{Riser area } f_K = 0.151\ \text{m}^2$$

$$K = 0.6 \quad K_S = 1.38 \quad \Delta P_{\text{liq}} = 1 + 10 + 8/2 = 15\,\text{mm liquid height}$$

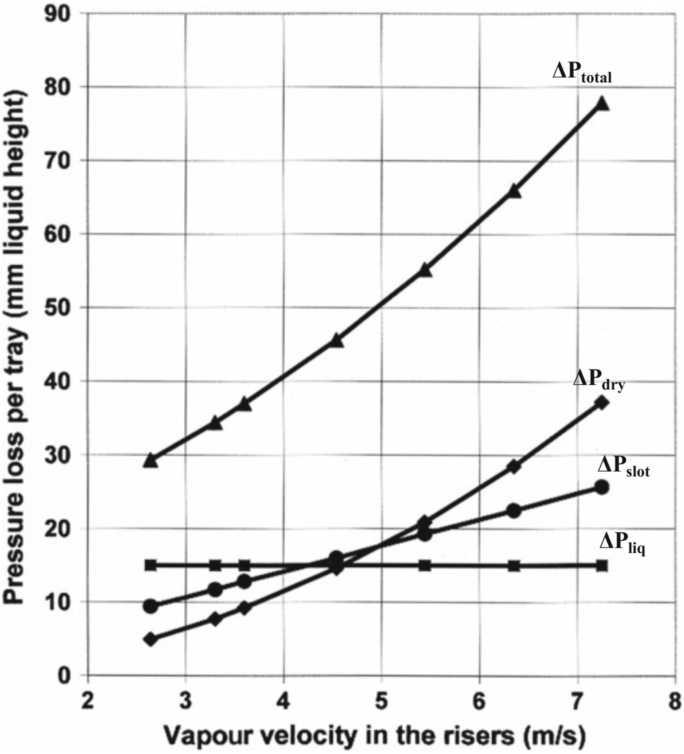


Fig. 9.10 Pressure losses in a bubble cap tray as a function of the flow velocity in the risers

$$\Delta P_{\mathrm{dry}} = 274' * 0.6 * \frac{3}{697} * \left(\frac{0.685}{0.151}\right)^2 = 14.6\ \text{mm liquid height}$$

$$V_{\max} = 1.38 * \sqrt{0.018 * \frac{697}{3} * 0.272} = 0.768\ \text{m/s}$$

$$h_{\mathrm{slot}} = \frac{0.685}{0.768} * 18 = 16\ \text{mm liquid}$$

$$\boldsymbol{\Delta P_{\mathrm{tray}} = 14.6 + 16 + 15 = 45.6\ \textbf{mm liquid height}}$$

Sieve trays

The total pressure loss consists of the dry pressure loss when flowing through the holes and the wet pressure loss through the liquid height on the trays.

Calculation of the **dry pressure loss**:

$$\Delta P_{\mathrm{dry}} = 4.72 * \left(\frac{w_{\mathrm{hole}}}{C_{\mathrm{sieve}}}\right)^2 * \frac{\rho_V}{\rho_L}\ (\text{mm liquid})$$

The pressure loss coefficient C_{Sieve} is dependent on the hole diameter and the tray thickness.

Practical calculations can be performed with $C_{\mathrm{Sieve}} = 0.2$ bis 0.22.

Calculation of the **wet pressure loss** through the liquid level on the tray:

$$\Delta P_{\mathrm{liq}} = h_W + h_{\mathrm{ow}}\ (\text{mm liquid height})$$

Example 9.1.5.3: Pressure loss calculation for a sieve tray

$$w_{\mathrm{hole}} = 6.85\ \text{m/s} \quad h_W = 20\ \text{mm} \quad h_{\mathrm{ow}} = 4.3\text{mm} \quad \vec{\rho}_V = 3\ \text{kg/m}^3$$
$$\rho_L = 700\ \text{kg/m}^3$$

$$\Delta P_{\mathrm{dry}} = 4.72 * \left(\frac{6.85}{0.22}\right)^2 * \frac{3}{700} = 19.6\ \text{mm liquid} \quad \Delta P_{\mathrm{liq}} = 20 + 4.3 = 24.3\ \text{mm liquid}$$

Total Pressure drop $\Delta P_{\mathrm{tray}} = 19.6 + 24.3 = 43.9$ mm liquid $= 3.07$ mbar

Valve Trays

The total pressure loss consists of the dry pressure loss when streaming through the holes and the wet pressure loss through the liquid height on the trays.

The dry pressure loss is different for the flat arranged *V*1 valves and the *V*4 venturi valves.

Calculation of the **dry pressure loss:**

$$\text{Flat valve: } \Delta P_{\text{dry}} = 224 * w_{\text{hole}}^2 * \frac{\rho_V}{\rho_L} \text{ (mm liquid)}$$
$$\text{Venturi valve: } \Delta P_{\text{dry}} = 122 * w_{\text{hole}}^2 * \frac{\rho_V}{\rho_L} \text{ (mm liquid)}$$

Calculation of the **wet pressure loss through** the liquid level on the tray:

$$\Delta P_{\text{liq}} = h_W + h_{\text{ow}} \text{(mm liquid height)}$$

Example 9.1.5.4: Pressure loss calculation for valve trays
Data used here is the same as in Example 9.1.5.3.

$$\Delta P_{\text{liq}} = 24.3 \text{ mm FS}$$

$$\text{Flat valve: } \Delta P_{\text{dry}} = 224 * 6.85^2 * \frac{3}{700} = 45 \text{ mm liquid}$$
$$\Delta P_{\text{tray}} = 45 + 24.3 = 69.3 \text{ mm liquid height} = 4.8 \text{ mbar}$$
$$\text{Venturi valve: } \Delta P_{\text{dry}} = 122 * 6.85^2 * \frac{3}{700} = 24.5 \text{ mm liquid}$$
$$\Delta P_{\text{tray}} = 24.5 + 24.3 = 48.8 \text{ mm liquid height} = 3.4 \text{ mbar}$$

Example 9.1.5.5: Hydraulic tray design for an atmospheric distillation

$D_K = 1.48$ m $A_{\text{tot}} = 1.72$ m^2 $A_D = 0.8 * 1.72 = 1.37$ m^2 $\rho_V = 3$ kg/m^3
$\rho_L = 700$ kg/m^3 $R = 9$

$$\frac{L}{G} = \frac{R}{R+1} = \frac{9}{10} = 0.9$$

$$F_{LV} = 0.9 * \sqrt{\frac{3}{700}} = 0.0589 \quad C_{SB} = 0.039$$
$$w_{\max} = 0.039 * \sqrt{\frac{697}{3}} = 0.59 \text{ m/s}$$
$$G_{\max} = 0.59 * 1.37 = 0.8 \text{ m}^3/\text{s} = 2910 \text{ m}^3/\text{h} = 8730 \text{ kg/h}$$

Bubble cap tray: $f_K = 0.151$ m^2 $h_T = 1$ mm $h_{\text{ow}} = 12$ mm $\Delta = 4$ mm
Sieve tray: hole area $f_{\text{hole}} = 0.1$ m^2 $h_{\text{ow}} = 12$ mm $h_W = 30$ mm
Valve tray: hole area $f_{\text{hole}} = 0.15$ m^2 $h_{\text{ow}} = 12$ mm $h_W = 30$ mm

Column velocity w_D (m/s)	0.4	0.5	0.6	0.7	0.8
Vapour flow rate (m^3/s)	0.548	0.685	0.822	0.959	1.096
Bubble cap tray w_{riser} (m/s)	3.6	4.54	5.44	6.35	7.25
Sieve tray w_{hole} (m/s)	5.48	6.85	8.22	9.59	11
Valve tray w_{hole} (m/s)	3.65	4.56	5.48	6.39	7.3

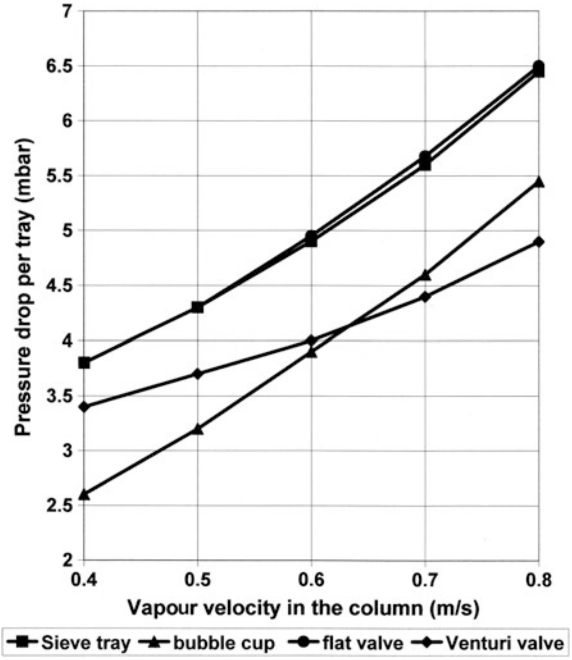


Fig. 9.11 Pressure loss of sieve, valve, and bubble cap trays as a function of the vapour flow velocity in the column

The calculated pressure losses are given in Fig. 9.11.

Example 9.1.5.6: Hydraulic tray design for a vacuum column

$$D_K = 1.48\ \text{m} \quad A_{tot} = 1.72\ \text{m}^2 \quad A_D = 0.8 * 1.72 = 1.37\text{m}^2 \quad \rho_V = 0.55\ \text{kg/m}^3$$

$$\rho_L = 765\ \text{kg/m}^3 \quad \text{R} = 3 \quad L/G = 0.75$$

$$F_{LV} = 0.75 * \sqrt{\frac{0.055}{765}} = 0.006 \quad C_{SB} = 0.064$$

$$w_{max} = 0.064 * \sqrt{\frac{765 - 0.55}{0.055}} = 7.55\ \text{m/s} * 0.85 = 6.4\ \text{m/s}$$

$$G_{max} = 6.4 * 1.37 = 8.8\ \text{m}^3/\text{s}$$

Bubble cap tray : $f_K = 0.151\ \text{m}^2$ $h_T = 1\ \text{mm}$ $h_{ow} = 4.3\ \text{mm}$ $\Delta = 6\ \text{mm}$

Sieve tray : hole area $f_{Loch} = 0.164\ \text{m}^2$ $h_{ow} = 4.3\ \text{mm}$ $h_W = 20\ \text{mm}$

Valve tray : hole area $f_{Loch} = 0.15\ \text{m}^2$ $h_{ow} = 4.3\ \text{mm}$ $h_W = 20\ \text{mm}$

Column velocity w_D (m/s)	6.42	5.47	4.38	2.9
Vapour flow rate (m^3/s)	8.8	7.5	6	4
Bubble cap tray w_{riser} (m/s)	58.3	49.7	39.7	26.5
Sieve tray w_{hole} (m/s)	53.6	45.7	36.5	24.3
Valve tray w_{hole} (m/s)	44	37.5	30	20

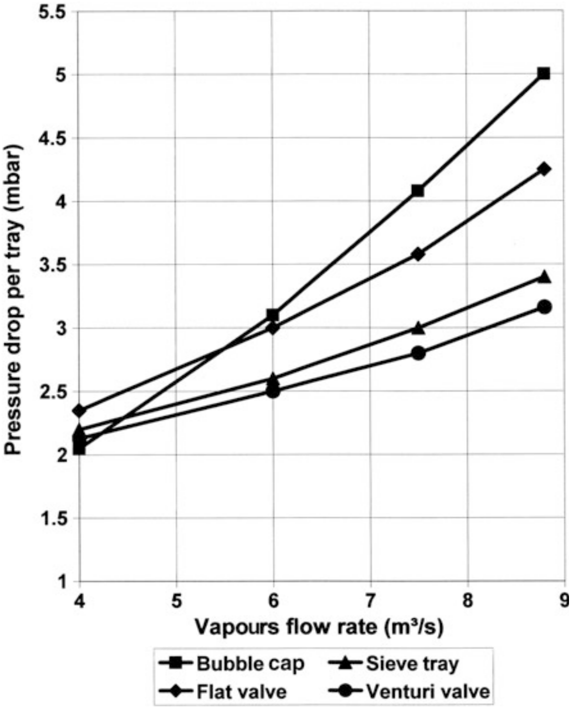


Fig. 9.12 Pressure losses in vacuum distillation with different trays as a function of the vapour loading

The calculated pressure losses are given in Fig. 9.12.

A complete tray calculation should be performed with a computer program because the determination of the pressure loss is somewhat tedious.

The suppliers of distillation trays possess such programs.

9.2 Efficiency of Cross Stream Trays

In Chaps. 3, 4, 5, 6, and 8 it was shown how to determine the required number of theoretical trays N_{theor} for a given separation.

For the conversion to the number of the required practical trays N_{prac} the efficiency E_{T} of the distillation trays is needed.

$$E_{\mathrm{T}} = \frac{N_{\mathrm{theor}}}{N_{\mathrm{prac}}} \qquad N_{\mathrm{prac}} = \frac{N_{\mathrm{theor}}}{E_{\mathrm{T}}}$$

What are the **essential influencing parameters on tray efficiency**?

In Fig. 9.13 from Drickamer–Bradford [8] the strong dependence of tray efficiency on the average molar viscosity of the liquid feed product at average column temperature is shown.

When distilling the viscosities are low and the efficiency is high.

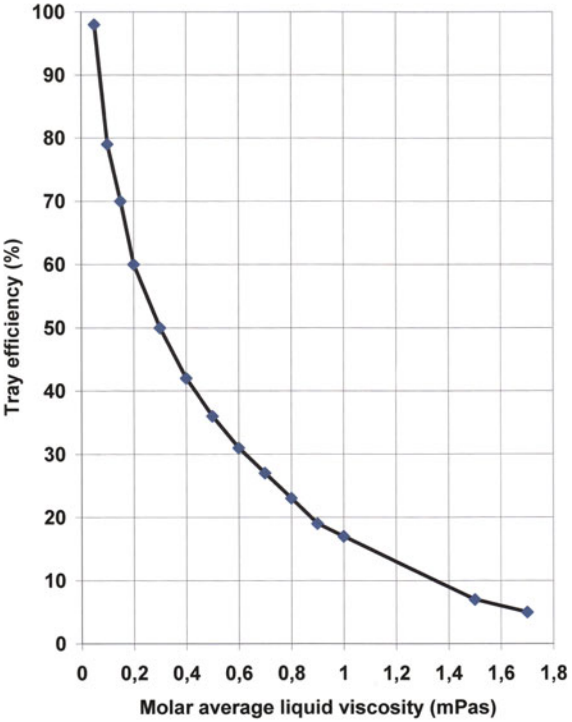


Fig. 9.13 Tray efficiency at an average column temperature as a function of the molar average liquid viscosity according Drickamer–Bradford [8]

When absorbing the viscosity is higher and the tray efficiency is lower.

This relationship is also shown in Fig. 9.14 of Lockhart–Legget [8].

The tray efficiency E_{T} is plotted on the ordinate above the product separation factor α with the viscosity η (mPas) plotted on the abscissa.

The upper line is valid for the distillation and the lower line for the absorption.

On the lower abscissa for the absorption the calculation was performed with a K_2 value for the high boiling washing fluid of $K_2 = 0.1$.

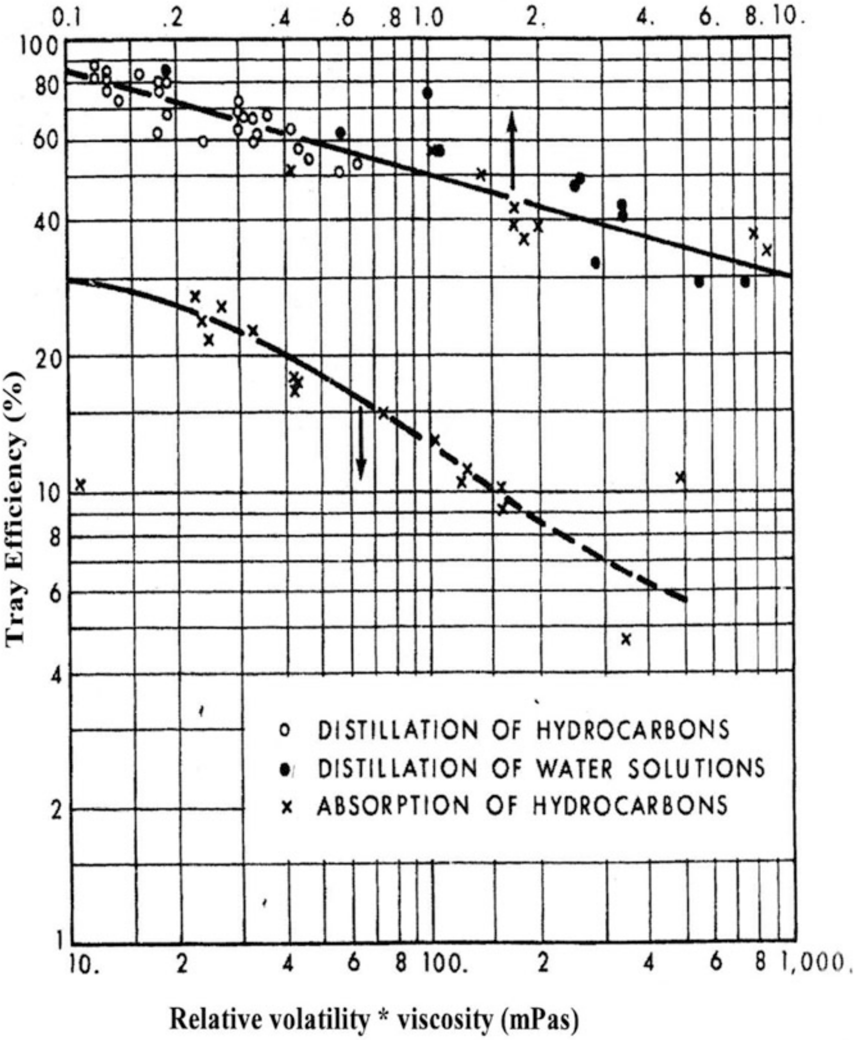


Fig. 9.14 Tray efficiency E_B as a function of $\alpha * \eta$ according Lockhart–Legget [8]

Example 9.2.1: Determination of the tray efficiency from Fig. 9.14
Distillation: $\alpha = 1.2 \quad \eta = 0.2$ mPa $\quad \alpha * \eta = 1.2 * 0.2 = 0.24 \quad E_T = 70\%$

Absorption: $\alpha = \frac{K_1}{K_2} = \frac{K_1}{0.1} = \frac{0.5}{0.1} = 5 \quad \eta = 2$ mPas $\quad \alpha * \eta = 10 \quad E_T = 30\,\%$

The tray efficiency is largely dependent on the dynamic viscosity η and the relative volatility α according to the measurement of Drickamer–Bradford und O'Connel.

The efficiency reduces with increasing separation factor because a larger material quantity, due to the equilibrium, has to be transferred.

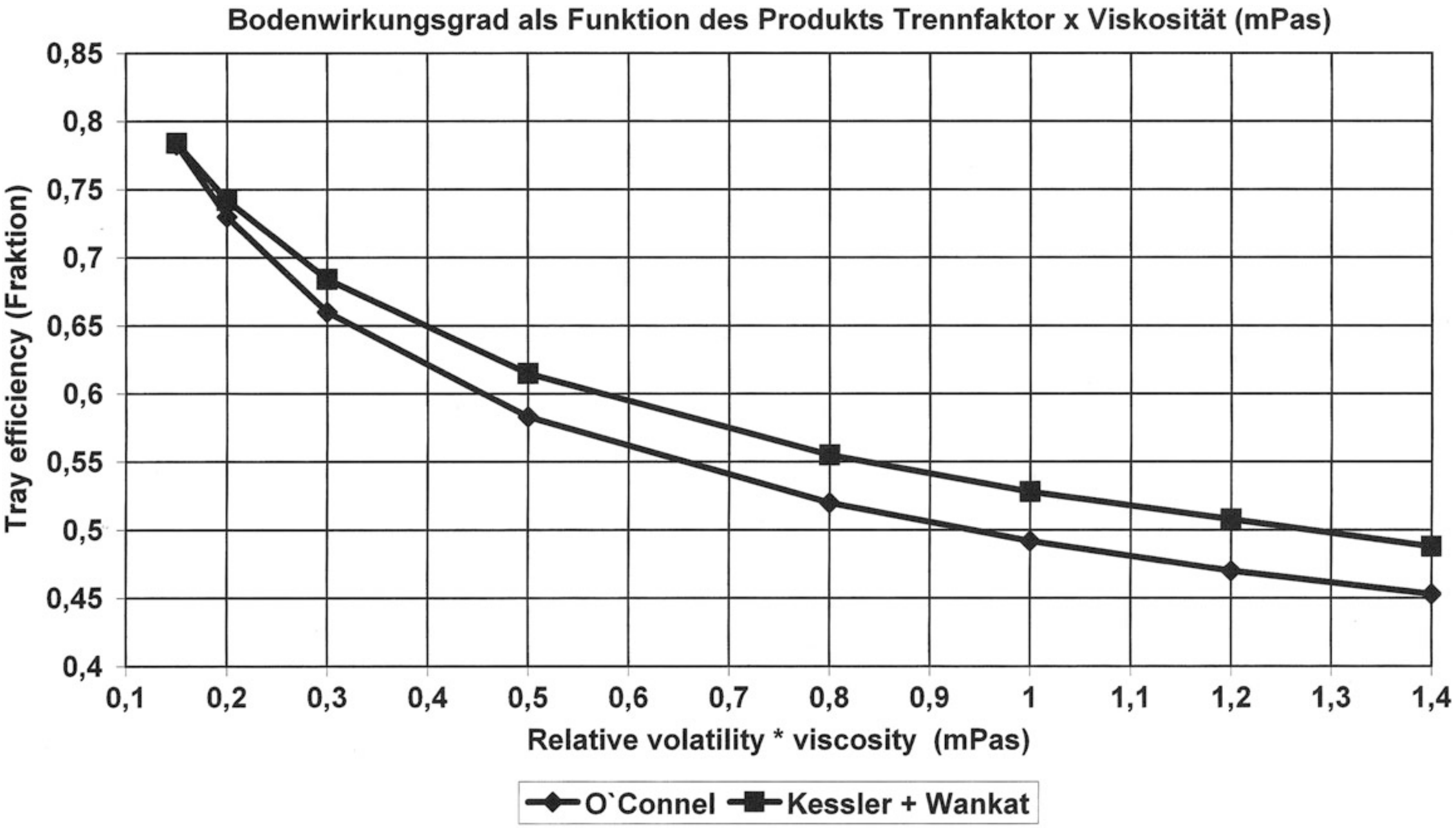


Fig. 9.15 Tray efficiency as a function of the product $\alpha * \eta$

The calculated tray efficiencies, as function of the product of the separation factor * viscosity, using the approximation equations of O'Connel and Kessler and Wankat, are given in Fig. 9.15.

Approximation equation according to O'Connel [1]:

$$E_{\mathrm{T}} = 0.492 * (\eta * \alpha)^{-0.245}$$

Approximation equation according to Kessler and Wankat [2]:

$$E_{\mathrm{T}} = 0.52782 - 0.27511 * \lg(\alpha * \eta) + 0.0449 * (\lg \alpha * \eta)^2$$

The mass transport from gas to liquid phase, and vice versa, occurs by diffusion, e.g., in the gas phase up to the interface and further in the liquid phase.

During absorption, the mass transport occurs mainly from the gas to the liquid phase.

When distilling, transport from the gas phase into the liquid phase, and from the liquid phase into the gas phase, occurs at the same time.

The transport rate is dependent on:

(a) the interface or contact area;
(b) the turbulence of both phases; and
(c) the physical properties of viscosity, surface tension, and volatility.

With specifically chosen column internals—trays and packings—the contact area and the turbulence can be improved.

An alternative method for the determination of the tray efficiency in the distillation was suggested by Bakowski [9–11] (Fig. 9.16).

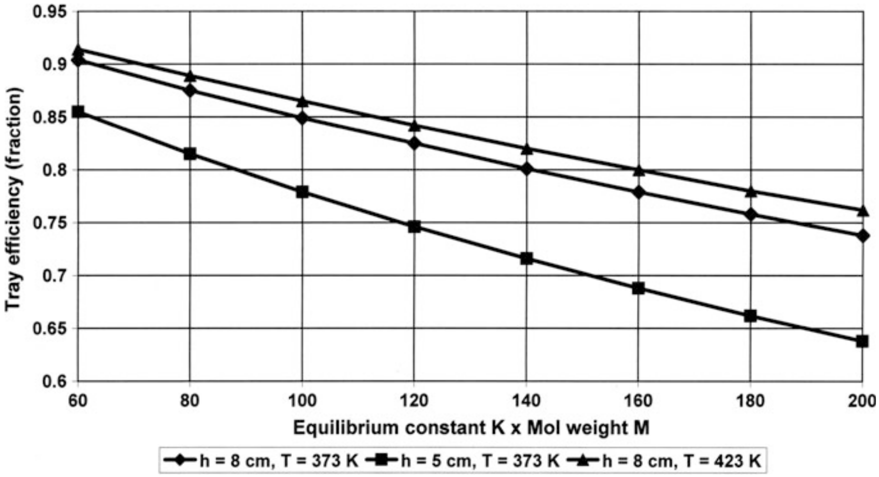


Fig. 9.16 Tray efficiency in distillation as a function of $K * M$

$$E_{\mathrm{T}} = \frac{1}{1 + \frac{3.7 * K * M}{h * \rho * T}}$$

K = y/x = equilibrium constant

M = mol weight
h = liquid height (cm)
T = average column temperature (°K)
ρ = liquid density (g/cm^3)

With increasing mole weight the tray efficiency drops.

Larger molecules are more viscous and diffuse more slowly.

With a lowering liquid height on the tray the efficiency falls because less liquid is available for mass transfer.

With increasing temperature the tray efficiency increases because the viscosity reduces and the diffusion rate increases.

Within the column the efficiency changes because the vapour rates and liquid rates change.

With an increasing V/L ratio the column efficiency increases.

For multi-component mixtures the efficiency is different for different components.

The column efficiency E_{Col} is determined from the tray efficiency E_{T} for a linear operating line as follows:

$$E_{\mathrm{Col}} = \frac{\ln\left[1 + E_{\mathrm{T}} * \left(\frac{K*V}{L} - 1\right)\right]}{\ln\left(\frac{K*V}{L}\right)}$$

K = y/x = equilibrium constant

L = liquid loading (kmol/h)
V = vapour loading (kmol/h)

From Fig. 9.17 it can be seen that the effective column efficiency E_{Col} at V/L ratios >1 is larger than the tray efficiency E_{T} while at a V/L ratio <1 is less than the tray efficiency.

Furthermore, it can be recognized that the light boiling components with higher K values have a better efficiency.

In the rectification section of the column with $V/L > 1$ the efficiency is better than E_{T}.

In the stripping section with $V/L < 1$ the column efficiency is worse than the tray efficiency E_{T}.

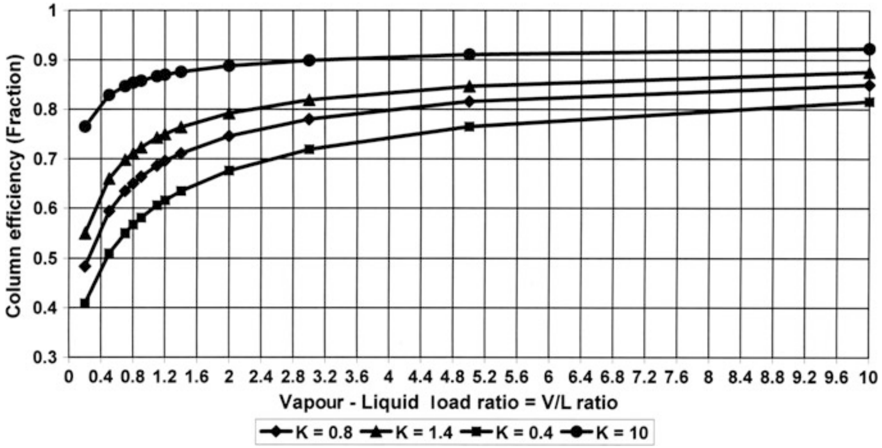


Fig. 9.17 Column efficiency for a tray efficiency E_T = 0.7 for different equilibrium factors as a function of the *V*/*L* ratio

Practical experience gained whilst designing distillation plants for aliphatics, olefins, paraffin hydrocarbons, aromatics, amines, methanol, isopropanol, nitrotoluene, nitrodichlorbenzene, fatty acid, methyl ester, and fatty alcohols the authors consider a *V*/*L* ratio of one is on the safe side with a column efficiency of 70–80% when distilling.

The required separation tasks were always achieved.

Often better product qualities were achieved.

The methods shown for the determination of tray efficiency are only valid for a hydraulically well-designed tray without entrainment of droplets at too high vapour velocities or weeping of liquid at too low vapour loadings.

The deterioration of the tray efficiency by entrainment at low tray spacings and high vapour velocities is calculated as follows:

$$E_{\mathrm{Tcorr}} = E_{\mathrm{T}} * \frac{1}{1 + r * E_{\mathrm{T}}}$$

$$r = \text{Entrainment rate} = \frac{\Delta L}{L}$$

ΔL = entrained liquid rate (kg/h)
L = total flow rate (kg/h)

Example 9.2.2: Deterioration of tray efficiency by entrainment

$$E_{\mathrm{T}} = 0.7 \quad \mathrm{r} = 0.1$$

$$E_{\mathrm{Tcorr}} = 0.7 * \frac{1}{1 + 0.1 * 0.7} = 0.65$$

Tray efficiency deteriorates by the entrainment rate r = 0.1 from 0.7 to 0.65.

Example 9.2.3: Calculation of tray efficiency E_T for α = 1.2 and η = 0.15 mPa

Acc. O'Connel $E_T = 0.492 * (1.2 * 0.15)^{-0.245} = 0.749$

Acc. Wankat/Kessler

$$E_\mathrm{T} = 0.52782 - 0.27511 * \lg(1.2 * 0.15) + 0.0449 * (\lg(1.2 * 0.15))^2 = 0.758$$

Example 9.2.4: Conversion from theoretical to practical trays

$K = 1.2 \quad M = 100 \quad \mathrm{h} = 5\ \mathrm{cm} \quad T = 120\,^\circ\mathrm{C} = 393\,^\circ\mathrm{K} \quad \rho = 0.7\ \mathrm{g/cm^3}$

Number of theoretical trays N_theor = 25

$$E_\mathrm{T} = \frac{1}{1 + \frac{3.7*K*M}{h*\rho*T}} = \frac{1}{1 + \frac{3.7*1.2*100}{5*0.7*393}} = 0.755$$

$$N_\mathrm{prac} = \frac{N_\mathrm{theor}}{E_\mathrm{T}} = \frac{25}{0.755} = 33.$$

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Chapter 10
Fluid Dynamic Design of Random Packings and Structured Packings and the Determination of the HTU/HETP Values

In random packing and structured packing columns the material exchange occurs between the upwards streaming gas or vapour and the downwards streaming liquid in a countercurrent system.

Allowable vapour and liquid loadings and pressure losses have to be determined.

Moreover, it is important to be able to determine which packing height, for a calculated number of transfer units NTU or theoretical stages NT, is required.

10.1 Random Packed Columns

The most important parameters for this design are listed here:

HTU value = required packing height for a mass transfer unit NTU
HETP value = required packing height for a theoretical stage NT
Flooding factor = percentage capacity utilization
Pressure loss of vapour or gas when streaming through the column (mbar/m packing)
Required minimum sprinkling rate (m^3/m^2h)
Miscellaneous: support grids, distributors, collectors, and installability.

Design guidelines for random packed columns

Ratio of column diameter/packing diameter $\approx 10:1$
Gas loading factor $F = w * \sqrt{\rho} = 2 - 2.5$
w = gases flow velocity (m/s)
ρ = gas density (kg/m^3)
Liquid loading: 4–80 m^3/m^2 h
Recommended redistribution after 4-m packing height
Free-stream cross section of the distributor: >50% of the column cross section

M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_10

Free-stream cross section of the support grid: 80% of the column cross section
Pressure loss ~ 1–4 mbar/m, depending on the loading and type of packing.

A good liquid distribution is very important for efficiency [1]:

The authors recommend 100–200 feeding points per m^2 with a uniform distribution over the entire column cross section. The number of required droplet points increases with increasing specific surface area of packing.

A good gas distribution at the inlet to the column improves effectiveness.

For a uniform gas distribution over the column cross section a minimum pressure loss is required.

By installing modern high-performance packings in technical columns the following advantages are achievable:

High separation efficiency
Lower pressure loss
High throughput performance

The requirement in order to gain these advantages is a uniform gas and liquid distribution in the column.

Specifically, you do not want large bottlenecks to occur at support grids or liquid distributors for gas streaming (Fig. 10.1).

Dimensioning of a liquid distributor with the equation for the gravity outflow is as follows

Liquid throughput V_L

$$V_L = 7639.62 * n * d_i^2 * \sqrt{h}\,(\mathrm{m}^3/\mathrm{h})$$

Required number of discharge tubes n

$$n = \frac{V_L}{7639.62 * d_i^2 * \sqrt{h}}$$

Required liquid height h

$$h = \left(\frac{V_L}{7639.62 * d_i^2 * n}\right)^2 (\mathrm{m})$$

V_L = liquid throughput through the hole distributor (m^3/h)
d_i = inner diameter of the discharge pipes (m)
h = head of the liquid above the discharge pipes (m)
n = number of discharge pipes with di

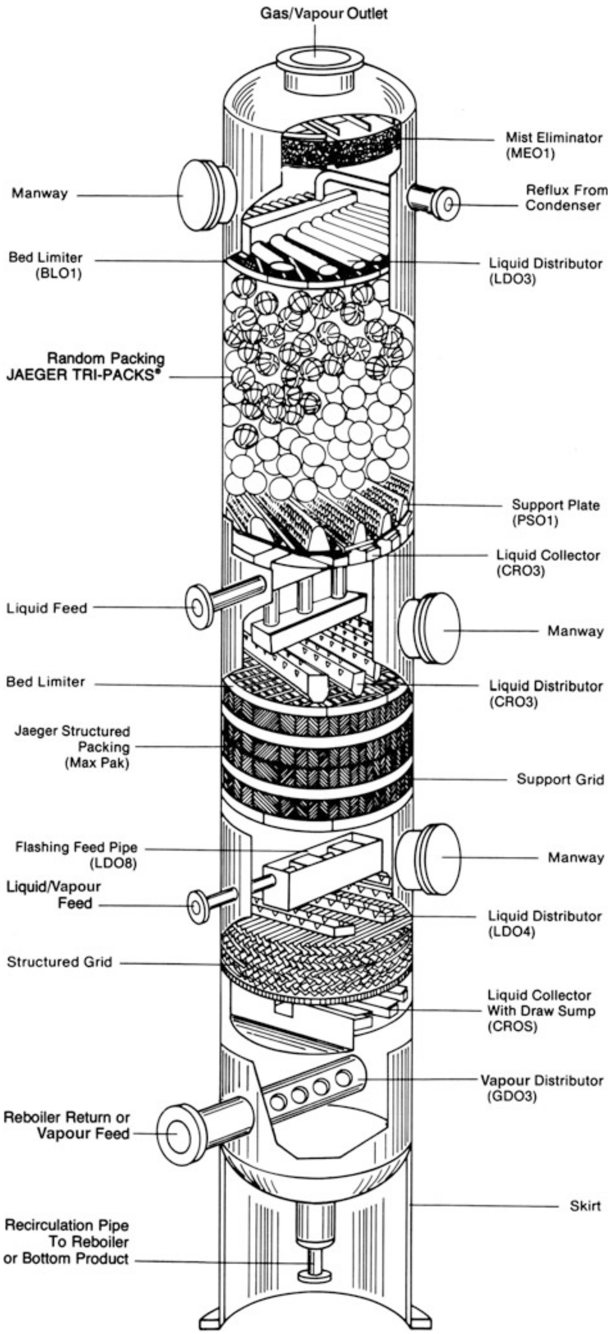


Fig. 10.1 Random packed column with internals according to Raschig and Jaeger

Example 10.1.1: Design of a hole distributor

$$V_{\mathrm{L}} = 2\,\mathrm{m}^3/\mathrm{h} \quad d_i = 6.3\,\mathrm{mm} \quad h = 170\,\mathrm{mm}$$

$$n = \frac{2}{7639.62 * 0.0063^2 * \sqrt{0.17}} = 16\,\text{discharge tubes}$$

$$h = \left(\frac{2}{7639.62 * 0.0063^2 * 16}\right)^2 = 0.17\,\mathrm{m}$$

For other liquid rates you will have other heads above the outflow pipes:

Liquid flow (m^3/h)	Heads (mm liquid height)
2	170
1.6	109
1.0	42.5
0.8	27.2

In Fig. 10.2 a hole distributor is shown.

Remark: If the head h is chosen too small a non-uniform liquid distribution over the column cross section may occur.

Requirement for gas distribution:

In order to prevent the free jet of incoming gas, with a half angle of 12°, spreading and directly hitting the support grid with the stream, you need to ensure there is sufficient space H between the inlet nozzle and the support grid.

Horizontal inlet nozzle (Fig. 10.3):

When the free jet hits the opposite wall the flow velocity w_{Str} should be lowered to 15% of the nozzle inlet velocity w_{in}.

Therefore, the required flow path x results as follows:

$$\frac{w_{\mathrm{in}}}{w_{\mathrm{Str}}} = 0.15 = \frac{3 * d}{x} \qquad x = \frac{3 * d}{0.15} = 20 * d$$

d = nozzle diameter (m)
D = column diameter (m)
w_{in} = nozzle inlet velocity (m/s)
w_{Str} = free jet-flow velocity (m/s)
x = required flow length (m)

At a distance x = 100 * d a free jet separates.

This free flow length is mostly not used in practical columns.

Therefore, a pre-distributor is installed, according to Fig. 10.4.

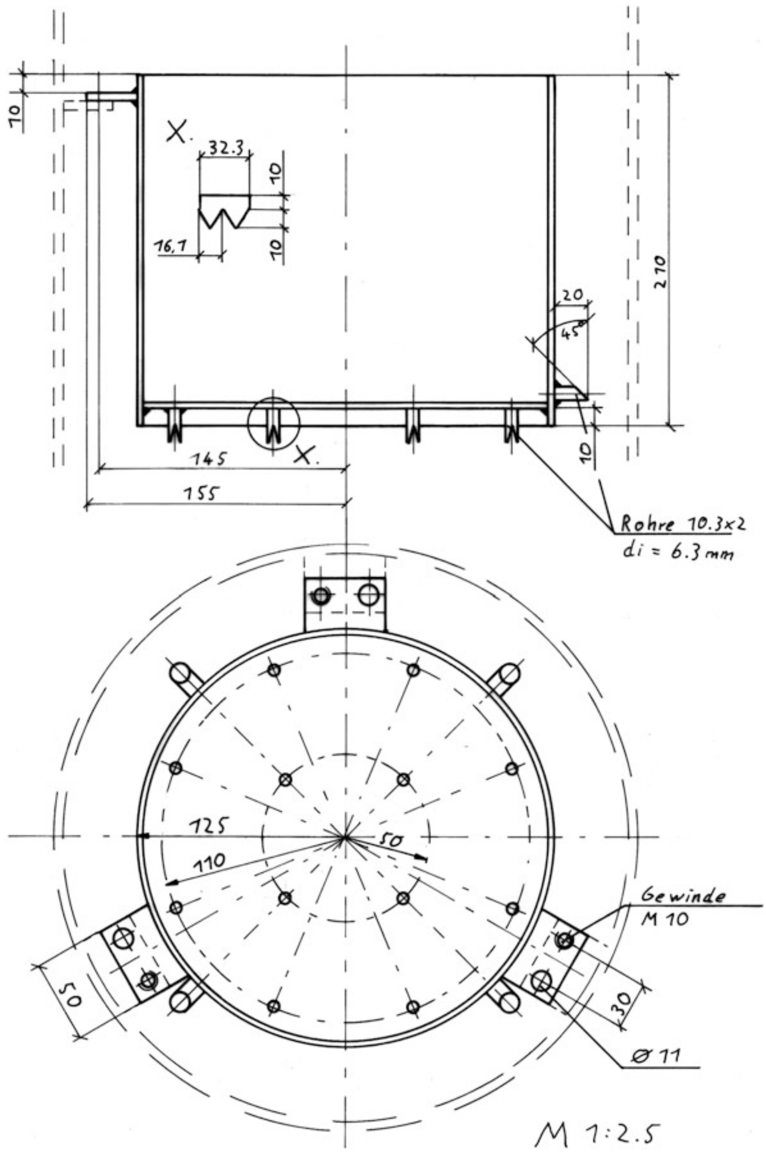


Fig. 10.2 Hole distributor for a random packed column

Vertical gas inlet nozzle (Fig. 10.5):
The gas inlet stream expands as a free jet with a half angle of 12° in the column.

The free jet should expand over the column diameter D before hitting the support grid.

Fig. 10.3 Horizontal gas inlet

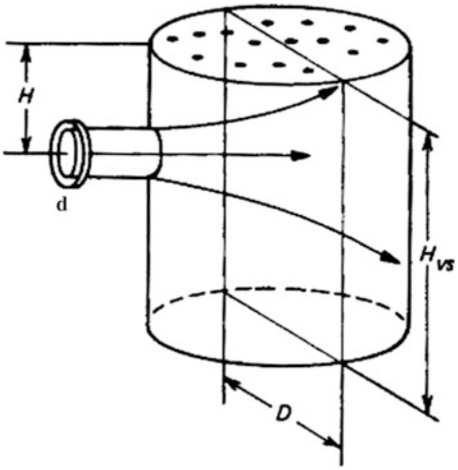
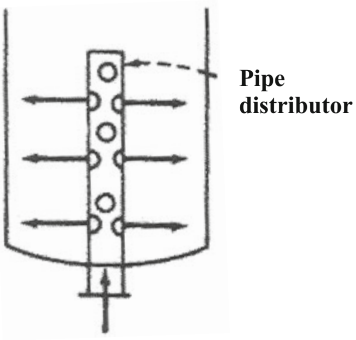


Fig. 10.4 Pipe distributor



The required height H for the free jet expansion results as follows:

$$H = \frac{D/2}{tg\,12^\circ} = \frac{D}{2 * 0.213} = 2.35 * D\,(\mathrm{m})$$

By installing a gas pre-distributor the required height H is reduced (Fig. 10.6).

10.1.1 Calculation Methods for the Pressure Loss in Random Packings [2–10]

The pressure loss in random packings is dependent on the gas and liquid loading.

With increasing gas velocity the pressure loss rises as it does with increasing liquid loading.

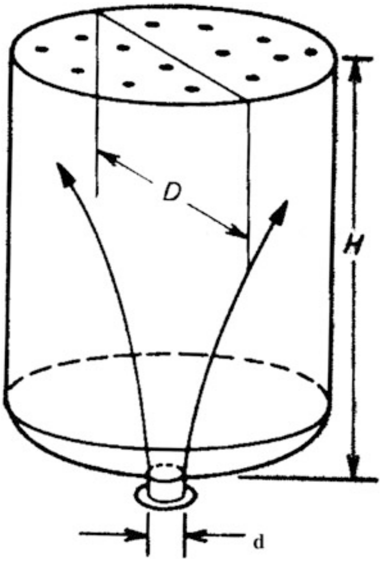


Fig. 10.5 Vertical gas inlet

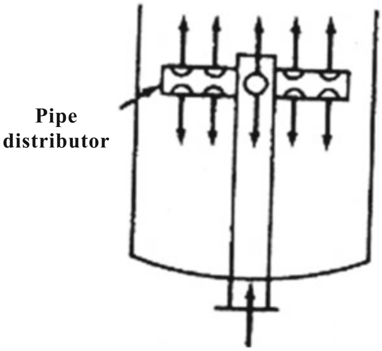


Fig. 10.6 Pipe distributor

A series of models for the pressure loss calculation exists which are listed in the literature.

The different models give different results.

The authors recommend the use of a calculation program delivered by the packing supplier.

In Fig. 10.7 the calculated pressure losses, as a function of the gas flow velocity using different models for Pall rings sized at 50 mm, are shown.

It can be seen that with an increasing flow velocity the pressure loss rises significantly and at higher liquid loading (70 m^3/m^2 h) a higher pressure loss occurs.

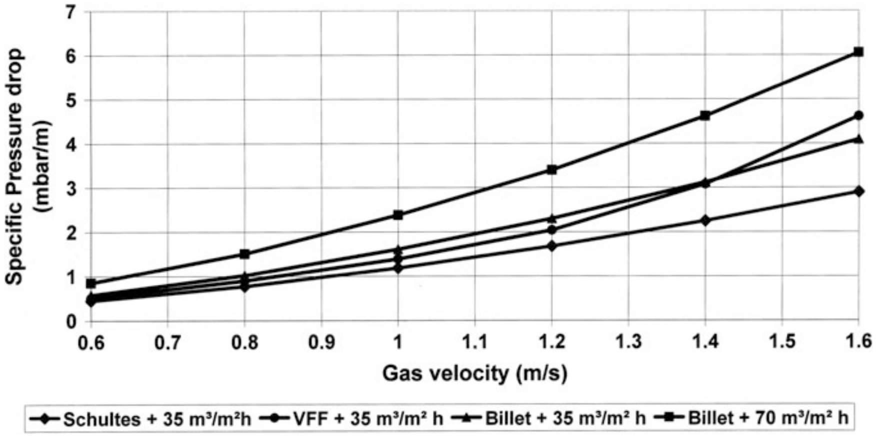


Fig. 10.7 Pressure losses of Pall rings according to different models in the cold wash of air containing gasoline vapour with cold gasoline at −20 °C

In Fig. 10.8 the pressure losses of different metallic random packings for the water/air system at atmospheric pressure are plotted as a function of the gas velocity.

Result:

For different packings very different pressure losses result.

The curves for VSP 40 and VSP 25 show that the pressure loss for smaller random packings is higher.

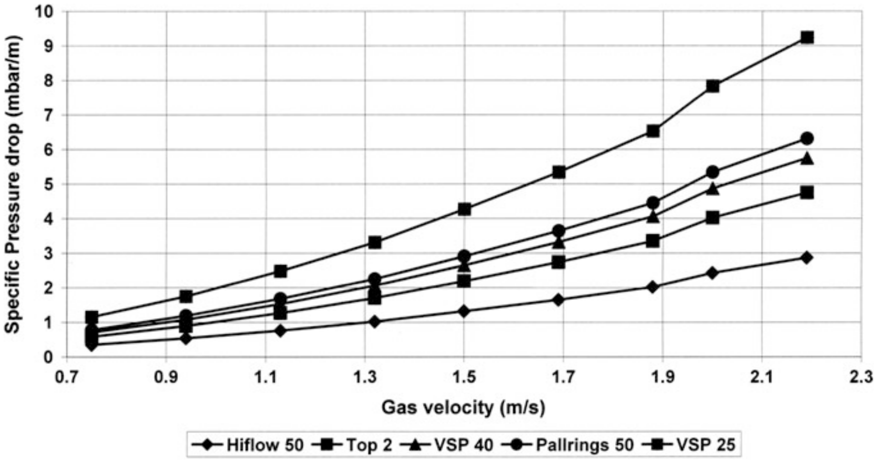


Fig. 10.8 Pressure losses of different metallic random packings for a water/air system as a function of the gas velocity in the column

Calculation procedure for pressure loss determination according to Billet and Schultes [3]

Calculation of the dry pressure loss:

$$\text{Partikel diameter}\, d_{\mathrm{P}} = 6 * \frac{1-\varepsilon}{a}\ (\mathrm{m})$$

$$\text{Wall Factor}\, \frac{1}{K} = 1 + \frac{2}{3} * \frac{1}{1-\varepsilon} * \frac{d_{\mathrm{P}}}{D_{\mathrm{K}}}$$

$$\text{Gas Reynolds number}\, Re_{\mathrm{G}} = \frac{w_{\mathrm{G}} * d_{\mathrm{P}}}{(1-\varepsilon) * \nu_{\mathrm{G}}} * K$$

$$\text{Calculation Parameter}\, \Psi_{\mathrm{G}} = C_{\mathrm{P}} * \left(\frac{64}{Re_{\mathrm{G}}} + \frac{1.8}{Re_{\mathrm{G}}^{0.08}}\right)$$

$$\text{Gas Loading Factor}\, F = w_{\mathrm{G}} * \sqrt{\rho_{\mathrm{G}}}$$

$$\text{Dry Pressure loss}\left(\frac{\Delta P}{H}\right)_{\mathrm{dry}} = \Psi_{\mathrm{G}} * \frac{a}{\varepsilon^3} * \frac{F}{2} * \frac{1}{K}\ (\mathrm{Pa/m})$$

Calculation of the pressure loss of sprinkled random packings:

$$\text{Holdup of the packing}\, h_{\mathrm{L}} = \left(\frac{12 * \eta_{\mathrm{L}} * u_{\mathrm{L}} * a^2}{g * \rho_{\mathrm{L}}}\right)^{1/3}$$

$$\text{Reynold number of the liquid}\, Re_{\mathrm{L}} = \frac{u_{\mathrm{L}} * \rho_{\mathrm{L}}}{a * \eta_{\mathrm{L}}}$$

$$\text{Calculation Factor}\, f_{\mathrm{S}} = \exp\left(\frac{Re_{\mathrm{L}}}{200}\right)$$

$$\text{Calculation Parameter}\, \Psi_{\mathrm{L}} = \Psi_{\mathrm{G}} * f_{\mathrm{S}} * \left(\frac{\varepsilon - h_{\mathrm{L}}}{\varepsilon}\right)^{1.5}$$

$$\left(\frac{\Delta P}{H}\right)_{\mathrm{wet}} = \Psi^2 * \frac{a}{(\varepsilon - h_{\mathrm{L}})^3} * \frac{F^2}{2} * \frac{1}{K}\,(\mathrm{Pa/m})$$

a = packing surface area ($\mathrm{m^2/m^3}$)
C_{P} = packing characteristic number
ε = porosity of the packing
ρ_{G} = gas density ($\mathrm{kg/m^3}$)
D_{K} = column diameter (m)
ρ_{L} = liquid density ($\mathrm{kg/m^3}$)
w_{G} = gas velocity (m/s)
ν_{G} = gas viscosity ($\mathrm{m^2/s}$)
u_{L} = liquid velocity (m/s)
η_{L} = liquid viscosity (Pa)

Example 10.1.1.1: Pressure loss calculation for 50-mm Pall rings according to Billet and Schultes

$$a = 112.6\,\mathrm{m^2/m^3} \quad \varepsilon = 0.951 \quad C_P = 0.763 \quad D_K = 0.5\,\mathrm{m}$$

$$\eta_L = 1\,\mathrm{mPa} \quad \nu_G = 15\,\mathrm{mm^2/s} \quad \rho_G = 1.5\,\mathrm{kg/m^3} \quad \rho_L = 780\,\mathrm{kg/m^3}$$

Liquid loading (m^3/m^2h)	6.87	6.87	6.87	13.74	13.74
Gas velocity (m/s)	0.6	1	1.4	1.4	1.6
d_P (m)	0.00261	0.00261	0.00261	0.00261	0.00261
$1/K$	1.071	1.071	1.071	1.071	1.071
Re_G	1990	3317	4643	4643	5206
ψ_G	0.7725	0.7327	0.7095	0.7095	0.7
F	0.735	1.22	1.71	1.71	1.96
u_L (m/s)	0.00972	0.00972	0.00972	0.0194	0.0194
h_L	0.0578	0.0578	0.0578	0.0728	0.0728
Re_L	67.3	67.3	67.3	134.6	134.6
f_S	1.4	1.4	1.4	1.96	1.96
ψ_L	0.984	0.9339	0.9042	1.234	1.219
Δp_{tdry} (mbar/m)	0.292	0.77	1.46	1.46	1.88
Δp_{wet} (mbar/m)	0.449	1.18	2.25	3.23	4.16

Figure 10.9 shows the result of a column calculation for a water wash for the removal of ethanol from exhaust air using the Raschig Program.

10.1.2 Calculation of the HTU and HETP Values [8–14]

The HTU value is the required packing height for a mass transfer unit NTU.

The required total packing height for a separation results from the product: NTU * HTU.

The different models used to calculate HTU values are listed in the literature.

The following data are used in the calculation of the HTU values

Equilibrium constant $K = y/x$
Gas loading (kmol/h)
Liquid loading (kmol/h)
Schmidt number
Packing characteristic numbers

The required packing heights for the gas side mass transfer HTU_G, and the liquid side mass transfer HTU_L, are determined separately.

Figure 10.10 gives the HTU values calculated according to two models.

The required heights for the gas side mass transfer HTU_G values decrease with increasing liquid loading.

Fig. 10.9 Calculation of a water wash for exhaust air containing ethanol using the Raschig program [7]

Gas stream: Air with Ethanol vapors	
Feed stream	8000 kg/h
Gas density	1,2 kg/m^3
Mol weight	29
Viskosity	0,018 mPas
Inlet concentration	5000 mg/m^3
Outlet concentration	100 mg/m^3
Temperature	30 °C
Liqid Stream: Water	
Volume stream	5 m^3/h
Liqid density	1000 kg/m^3
Mol weight	18
Viskosity	1 mPas
Surface tension	72 mN/m
Inlet concentration	0,0 mg/m^3
Outlet concentration	6533 mg/l
Temperature	22 °C
Absorbend	Ethanol
Mol weight	46
Henry constant	480 * 10^{-3}
Stripping Factor	0,477
Diffusion coefficient Gas	1,27 * 10^{-5} m^2/s
Diffusion coefficient Liquid	1,23 * 10^{-9} m^2/s
Column diameter	906 mm
Sprinkling rate	7,8 m^3/m^{2}h
Flood factor	60 %
Pressure Drop	2,4 mbar/m packing
NTU$_{OL}$	3
HTU$_{OL}$	1,7 m
NT	4,4
HETP	1,16 m
Packing height	5,1 m
Total Pressure Loss	12,2 mbar
Chosen	15 mbar

The required heights for the liquid side mass transfer HTU$_L$ values increase with increasing liquid loading.

The following material introduces some calculation models used to determine HTU values.

HTU-Calculation acc. Billet/Mackowiak

Gas Loading Factor $F = w_G * \sqrt{\rho_G}$

Mass Transfer Coefficient in the gas phase

$$\beta_G * a_{ph} = C * F^n * u_L^q * D_G^{0.67}(1/s)$$

$$HTU_G = \frac{w_G}{\beta_G * a_{ph}}(m)$$

$$\beta_L * a_{ph} = C_0 * u_L^n * D_L(1/s)$$

$$HTU_L = \frac{u_L}{\beta_L * a_{ph}}(m)$$

Stripping factor $S = K * \frac{G}{L}$

$$HTU_{OG} = HTU_G + S * HTU_L$$

$$HETP = HTU_{OG} * \frac{\ln S}{S - 1}$$

Required Packing data: $\boldsymbol{C}$, $\boldsymbol{C_0}$ **and the exponents** $\boldsymbol{m}$, $\boldsymbol{n}$, $\boldsymbol{q}$

HTU-Calculation acc. Fair/Bolles:

$$HTU_G = \frac{\Psi * \left(\frac{\nu_G}{D_G}\right)^{0.5} * \left(\frac{D_K}{0.305}\right)^m * \left(\frac{L_{Full}}{3.05}\right) * 0.305}{\left[\frac{L}{4.88} * (\eta_L * 1000)^{0.16} * \left(\frac{1000}{\rho_L}\right)^{-1.25} * \left(\frac{\sigma_L}{0.0728}\right)^{-0.8}\right]^n}(m)$$

$$L = u_L * 3600 * \rho_L$$

$$HTU_L = \Phi * C_{fl} * \left(\frac{L_{Full}}{3.05}\right)^{0.15} * \left(\frac{\nu_L}{D_L}\right)^{0.5} * 0.305(m)$$

Required Packing Data: $\boldsymbol{\Phi}$, $\boldsymbol{\Psi}$, ε, $\boldsymbol{d}$, $\boldsymbol{C_{fl}}$, $\boldsymbol{m}$, $\boldsymbol{n}$

HTU-Calculation acc. Onda:

$$\frac{a_{ph}}{a} = 1 - \exp\left[-1.45 * \left(\frac{\sigma_c}{\sigma}\right)^{0.75} * \left(\frac{u_L}{a * \nu_L}\right)^{0.1} * \left(\frac{u_L^2 * a}{g}\right)^{-0.05} * \left(\frac{u_L^2 * \rho_L}{\sigma_L * a}\right)^{0.2}\right]$$

$$\beta_G * a_{PH} = 5.23 * \left(\frac{D_G}{da}\right) * \left(\frac{\nu_G}{D_G}\right)^{0.33} * \left(\frac{w_G}{a * \nu_G}\right)^{0.7} * \frac{1}{da}$$

$$HTU_G = \frac{w_G}{\beta_G * a_{Ph}}(m)$$

$$\beta_L = 0.051 * \left(\frac{D_L}{da}\right) * \left(\frac{da^3 * g}{\nu_L^2}\right)^{0.33} * \left(\frac{u_L}{a * \nu_L}\right)^{0.67} * \left(\frac{a_{Ph}}{a}\right)^{-0.67} * \left(\frac{\nu_L}{D_L}\right)^{0.5} * (a * da)^{0.4}$$

$$\beta_L * a_{Ph} = \beta_L * \left(\frac{a_{Ph}}{a}\right) * a$$

$$HTU_L = \frac{u_L}{\beta_L^* a_{Ph}}(m)$$

Required packing data: *da*, ε, *a* and the critical surface tension

a = packing surface (m^2/m^3)
a_{Ph} = phase contact area (m^2/m^3)
D_G = gas diffusion coefficient (m^2/s)
D_L = liquid diffusion coefficient (m^2/s)
D_K = column diameter (m)
da = packing diameter (m)
G = gas loading (kmol/h)
$K = y/x$ = equilibrium constant
L = liquid loading (kmol/h)
u_L = liquid velocity (m/s)
w_G = gas velocity (m/s)
η_L = dynamic liquid viscosity (Pa)
ε = porosity of the packing (fraction)
ν_G = kinematic gas viscosity (m^2/s)
ρ_G = gas density (kg/m^3)
ρ_L = liquid density (kg/m^3)
σ_L = surface tension (N/m).

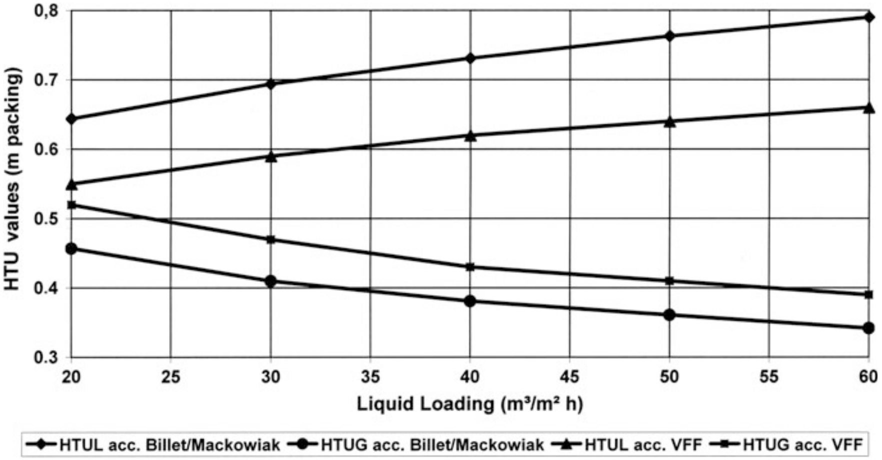


Fig. 10.10 Required heights for the gas side, and liquid side, mass transfer as a function of liquid loading

Example 10.1.2.1: Calculation of the HTU and the HETP Values for Metal 50-mm PALL Rings

Physical Data:

$\rho_G = 1.54\,\mathrm{kg/m^3}$ $\rho_L = 780\,\mathrm{kg/m^3}$ $\nu_G = 7 \times 10^{-6}\,\mathrm{m^2/s}$ $\nu_L = 1 \times 10^{-6}\,\mathrm{m^2/s}$
$D_G = 7 \times 10^{-6}\,\mathrm{m^2/s}$ $D_L = 1 \times 10^{-9}\,\mathrm{m^2/s}$ $\sigma_L = 0.03\,\mathrm{N/m}$
$D_K = 0.5\,\mathrm{m}$ $W_G = 0.6\,\mathrm{m/s}$ $u_L = 35\,\mathrm{m^3/m^2h} = 0.00972\,\mathrm{m^3/m^2s} = 0.00972\,\mathrm{m/s}$
$G = 22.5\,\mathrm{kmol/h}$ $L = 72.4\,\mathrm{kmol/h}$ $K = 0.45$

Calculation acc. Billet/Mackowiak for metal pallrings 50 mm:

Packing Data:

$$\mathrm{da} = 0.05\,\mathrm{m} \qquad \mathrm{a} = 112.6\,\mathrm{m}^2 \qquad € = 0951$$

$$C = 1.904 \times 10^4 \qquad m = 0.815 \qquad n = 0.77 \qquad q = \mathbf{0.26} \qquad C_0 = \mathbf{1.88 \times 10^4}$$

$$F = 0.6 * \sqrt{1.54} = 0.7446$$

$$\beta_G * a_{Ph} = 1.904 \times 10^4 * 0.7746^{0.77} * 0.00972^{0.26} * \left(7 \times 10^{-6}\right)^{0.67} = 1.61/\mathrm{s}$$

$$\mathrm{HTU_G} = \frac{0.6}{1.6} = 0.375\,\mathrm{m}$$

$$\beta_L * a_{Ph} = 1.88 \times 10^4 * 0.00972^{0.815} \times \left(10^{-9}\right)^{0.5} = 0.0136$$

$$\mathrm{HTU_L} = \frac{0.00972}{0.0136} = 0.71\,\mathrm{m}$$

$$S = 0.45 * \frac{22.5}{72.4} = 0.1398$$

$$\mathrm{HTU_{OG}} = 0.375 + 0.1398 * 0.71 = 0.475\,\mathrm{m}$$

$$\mathrm{HETP} = 0.475 * \frac{\ln 0.1398}{0.1398 - 1} = 1.08\,\mathrm{m}$$

Calculation acc. Fair/Bolles for metal pallrings 50 mm:

Packing Data:

$$da = 0.05\,\mathrm{m} \qquad L_{\mathrm{full}} = 3\,\mathrm{m} \qquad \Psi = 140 \qquad \Phi = 0.06 \qquad C_{\mathrm{fl}} = 1$$

$$m = 1.24 \qquad n = 0.6$$

$$\mathrm{L} = 0.00972 * 3600 * 780 = 27{,}294\,\mathrm{kg/h}$$

$$\mathrm{HTU_G} = \frac{140 * \left(\frac{7\times10^{-6}}{7\times10^{-6}}\right)^{0.5} * \left(\frac{0.5}{0.305}\right)^{1.24} * \left(\frac{3}{3.05}\right)^{1/3} * 0.305}{\left[\frac{27294}{4.88} * (0.78 \times 10^{-3} * 1000)^{0.16} * \left(\frac{1000}{780}\right)^{-1.25} * \left(\frac{0.03}{0.0728}\right)^{-0.8}\right]^{0.6}} = 0.356\,\mathrm{m}$$

$$\mathrm{HTU_L} = 0.09 * 1.0 * \left(\frac{3}{3.05}\right)^{0.15} * \left(\frac{10^{-6}}{10^{-9}}\right)^{0.5} * 0.305 = 0.866\,\mathrm{m}$$

$$\mathrm{HTU_{OG}} = 0.356 + 0.1398 * 0.866 = 0.477\,\mathrm{m}$$

$$\mathrm{HETP} = 0.477 * \frac{\ln 0.1398}{0.1398 - 1} = 1.09\,\mathrm{m}$$

Calculation acc. Onda for metal Pallrings 50 mm:

Packing Data

da = 0.05 m € = 0.951 a = 112.6 $\mathrm{m^2/m^3}$ $\sigma_c = 0.072\,\mathrm{N/m}$

$$\frac{a_{\mathrm{ph}}}{a} = 1 - \exp\left[-1.45 * \left(\frac{0.072}{0.03}\right)^{0.75} * \left(\frac{0.00972}{112.6 \times 10^{-6}}\right)^{0.1} * \left(\frac{0.00972 * 112.6}{9.81}\right)^{-0.05} * \left(\frac{0.00972 * 780}{0.03 * 112.6}\right)^{0.2}\right]$$

$$\frac{a_{\mathrm{Ph}}}{a} = 0.9426$$

$$\beta_{\mathrm{G}} = 5.23 * \left(\frac{7 \times 10^{-6}}{0.05}\right) * \left(\frac{7 \times 10^{-6}}{7 \times 10^{-6}}\right)^{0.33} * \left(\frac{0.6}{112.6 * 7 \times 10^{-6}}\right)^{0.7} * \frac{1}{0.05} = 1.523$$

$$\mathrm{HTU_G} = \frac{0.6}{1.523} = 0.394\,\mathrm{m}$$

$$\beta_{\mathrm{L}} = 0.0051 * \left(\frac{10^{-9}}{0.05}\right) * \left(\frac{0.05^2 * 9.81}{(10^{-6})^2}\right)^{0.33} * \left(\frac{0.00972}{112.6 \times 10^{-6}}\right)^{0.67} * (0.9426)^{-0.67} * \left(\frac{10^{-6}}{10^{-9}}\right)^{0.5} * (112.6 * 0.05)^{0.5} = 0.001326$$

$$\beta_{\mathrm{L}} * a_{\mathrm{Ph}} = 0.0001326 * 0.9426 * 112.6 = 0.0141$$

$$\mathrm{HTU_L} = \frac{0.00972}{0.0141} = 0.689\,\mathrm{m}$$

$$\mathrm{HTU_{OG}} = 0.394 + 0.1398 * 0.689 = 0.49\,\mathrm{m}$$

$$\mathrm{HETP} = 0.49 * \frac{\ln 0.1398}{0.1398 - 1} = 1.12\,\mathrm{m}$$

The total height $\mathrm{HTU_{OG}}$ or $\mathrm{HTU_{Ol}}$ is determined, from both $\mathrm{HTU_G}$ for the gas side and $\mathrm{HTU_L}$ for the liquid side, whilst considering the gas side and liquid side mass transfer resistances.

$$\mathrm{HTU_{OG}} = \mathrm{HTU_G} + \frac{m * G}{L} * \mathrm{HTU_L}\ (\mathrm{m}) \tag{10.1}$$

$$\mathrm{HTU_{OL}} = \mathrm{HTU_L} + \frac{L}{m * G} * \mathrm{HTU_G}\ (\mathrm{m}) \tag{10.2}$$

The packing height for a theoretical stage is called the HETP value.

The HETP values can be calculated from the $\mathrm{HTU_{OG}}$ or the $\mathrm{HTU_{OL}}$ value.

$$\mathrm{HETP} = \frac{\ln S}{S - 1} * \mathrm{HTU_{OG}}\ (\mathrm{m})$$

$$\mathrm{HETP} = \frac{S * \ln S}{S - 1} * \mathrm{HTU_{OL}}\ (\mathrm{m})$$

$$S = \frac{m * G}{L}$$

G = gas loading (kmol/h)
L = liquid loading (kmol/h)
$m = y/x$ = slope of the equilibrium line

From the Eqs. (10.1) **and** (10.2) **the following can be derived**:
If the slope of the equation line m is small, for instance in **absorbing**, then the $\mathrm{HTU_G}$ determines to a great extent the $\mathrm{HTU_{OG}}$ value.

The material transport is controlled by gas phase resistance.

If the slope of the equilibrium line m is high, for instance in **stripping**, then the $\mathrm{HTU_L}$ value determines the height of $\mathrm{HTU_{OL}}$.

The liquid phase resistance controls the material transfer.

Figure 10.11 plots the $\mathrm{HTU_{OG}}$ values that are calculated according to different models depending on the gas flow velocity in the column.

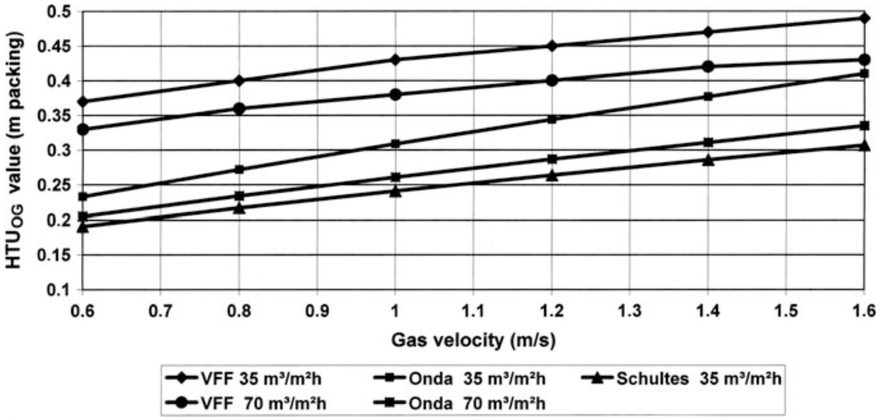


Fig. 10.11 $\mathrm{HTU_{OG}}$ values according to different models for 50-mm pall rings depending on the gas velocity in the column

Example 10.1.2.1: Calculation of $\mathrm{HTU_{OG}}$, $\mathrm{HTU_{OL}}$, and the HETP values.

$$G = 34\,\mathrm{kmol/h} \qquad L = 500\,\mathrm{kmol/h} \qquad \mathrm{HTU_G} = 0.5\,\mathrm{m} \qquad \mathrm{HTU_L} = 0.3\,\mathrm{m}$$

Calculation for the gas side with *m* = 0.3:

$$\begin{aligned} S &= 0.3 * \frac{34}{500} = 0.0204 \\ \mathrm{HTU_{OG}} &= 0.5 + 0.0204 * 0.3 = 0.506\,\mathrm{m} \\ \mathrm{HETP} &= 0.506 * \frac{\ln 0.0204}{0.0204 - 1} = 2.01\,\mathrm{m} \end{aligned}$$

Calculation for the liquid side with *m* = 100

$$\begin{aligned} S &= 100 * \frac{34}{500} = 6.8 \\ \mathrm{HTU_{OL}} &= 0.3 + \frac{1}{6.8} * 0.5 = 0.37\,\mathrm{m} \\ \mathrm{HETP} &= 0.37 * \frac{6.8 * \ln 6.8}{6.8 - 1} = 0.83\,\mathrm{m} \end{aligned}$$

From the calculated values of $\mathrm{HTU_G}$ and $\mathrm{HTU_L}$ the distribution of the mass transfer resistance on the gas and liquid phases can be determined.

$$R_{\mathrm{DF}} = \frac{\mathrm{HTU_G}}{S * \mathrm{HTU_L}}$$

$\mathrm{R_{DF}} > 1$ → the gas phase resistance determines the mass transfer
$\mathrm{R_{DF}} < 1$ → the liquid phase resistance controls the mass transfer.

Example 10.1.2.2: Which resistance determines the mass transfer?

(a) $\mathbf{HTU_G = 0.5\,m} \qquad \mathbf{HTU_L = 0.3\,m} \qquad S = \mathbf{0.0204} \qquad R_{\mathbf{DF}} = \mathbf{81.7}$

The gas side mass transfer is the determining factor.

The resistance for the mass transfer lies in the gas phase if in the absorption the gases are reasonably soluble and are of minor m values or if in the chemical wash the reactions are irreversibly fast.

Examples: NH_3 in H_2O, SO_2 in H_2O, SO_2 in alkali, HCl in H_2O, and H_2S in H_2O.

(b) $\mathbf{HTU_G = 0.5\,m} \qquad \mathbf{HTU_L = 0.3\,m} \qquad \mathbf{S = 6.8} \qquad \mathbf{R_{DF} = 0.245}$

The liquid phase resistance is the determining factor.

With poor soluble gases with large m values or slow reversible reactions the main resistance lies in the liquid phase.

Examples: CO_2 in H_2O, CO_2 in NaOH, Cl_2 in H_2O, O_2 in H_2O, and H_2 in H_2O.

The HTU values given in Figs. 10.10 and 10.11 were determined on the following basis data for a cold gasoline wash.

Gas data: air with gasoline vapour

Gas density $\rho_G = 1.54\,\mathrm{kg/m^3}$ $M = 29$
Gas viscosity v_G = 7 mm^2/s
Gas diffusion coefficient $D_G = 7 \times 10^{-6}\ m^2/s$
Schmidt number Sc_G = 1
Slope of equilibrium line m = 0.45

Liquid data: cold liquid gasoline

Liquid density $\rho_L = 780\,\mathrm{kg/m^3}$ $M = 74$
Liquid viscosity v_L = 1 mm^2/s
Liquid diffusion coefficient $D_L = 1 \times 10^{-9}$
Surface tension σ_L = 0.03 N/m
Schmidt number Sc_L = 1000

Table 10.1–10.4 contains the HTU and HETP values calculated using different models as a function of the liquid loading of the packings listed for a gas flow velocity of 0.75 m/s (G = 28.2 kmol/h).

The HTU_L values increase with an increasing liquid loading of 41.4–144.9 kmol/h.

The $HTU_{OV} = HTU_{OG}$ values drop with increasing liquid loading u_L.

According to Schultes, Fair and Bolles, and Billet and Mackowiak the HETP values fall with increasing liquid loading.

According to Onda the HETP values rise along with the liquid loading.

The deviations between the results according to the different models are substantial.

With a lower m value the differences become even larger, for instance, for m = 0.1:

	According to Schultes (m)	According to Onda (m)
HTU_{OG}	0.215–0.124	0.458–0.437
HETP	0.62–0.499	1.32–1.75

The HETP values converted from the HTU values are given in Fig. 10.12.

HETP = required packing height for a theoretical stage.

Table 10.1 Calculation according to Schultes [12]

u_L (m^3/m^2 h)	20	30	40	50	60	70
HTU_L (m)	0.381	0.425	0.459	0.486	0.513	0.533
HTU_V (m)	0.189	0.161	0.143	0.130	0.122	0.114
HTU_{OV} (m)	0.306	0.248	0.213	0.190	0.174	0.161
HETP (m)	0.521	0.495	0.472	0.454	0.442	0.430

Table 10.2 Calculation according to Billet and Mackowiak [8]

u_L (m^3/m^2 h)	20	30	40	50	60	70
HTU_L (m)	0.644	0.694	0.731	0.763	0.790	0.810
HTU_V (m)	0.457	0.410	0.381	0.361	0.342	0.329
HTU_{OV} (m)	0.655	0.552	0.493	0.455	0.423	0.400
HETP (m)	1.12	1.10	1.093	1.087	1.08	1.07

Table 10.3 Calculation according to Fair and Bolles [10]

u_L(m^3/m^2 h)	20	30	40	50	60	70
HTU_L (m)	0.770	0.866	0.938	1.01	1.06	1.11
HTU_V (m)	0.344	0.269	0.227	0.198	0.178	0.162
HTU_{OV} (m)	0.452	0.390	0.358	0.339	0.326	0.317
HETP (m)	1.03	0.892	0.819	0.775	0.746	0.725

Table 10.4 Calculation according to Onda [9]

u_L (m^3/m^2 h)	20	30	40	50	60	70
HTU_L (m)	0.545	0.613	0.712	0.720	0.761	0.800
HTU_V (m)	0.421	0.421	0.421	0.421	0.421	0.421
HTU_{OV} (m)	0.588	0.546	0.530	0.510	0.499	0.491
HETP (m)	1.00	1.09	1.17	1.22	1.27	1.31

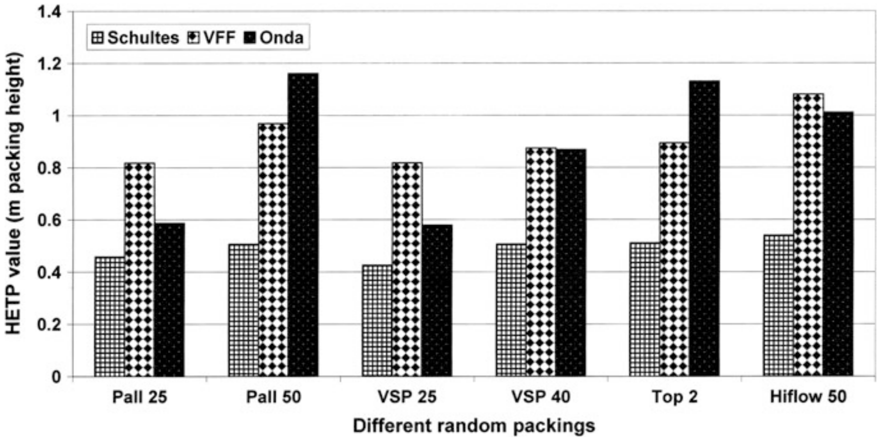


Fig. 10.12 Calculated HETP values according to different models for a cold gasoline wash

Clearly, different HETP values result from the calculations using the different models.

Figure 10.13 gives the HTU_{OG} values which are calculated according to five models as function of the liquid loading.

With increasing liquid loading HTU_{OG} values drop.

Figure 10.14 shows the influence of the gas flow velocity at two different liquid loadings.

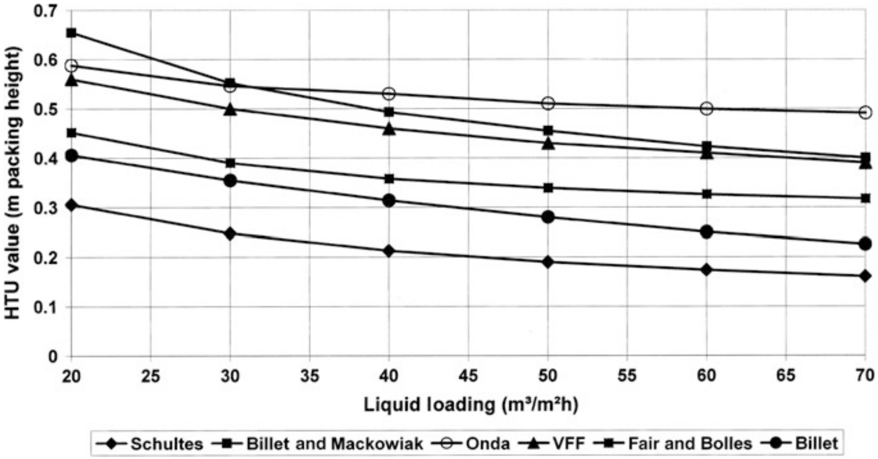


Fig. 10.13 HTU_{OG} values according to different models as a function of the liquid loading

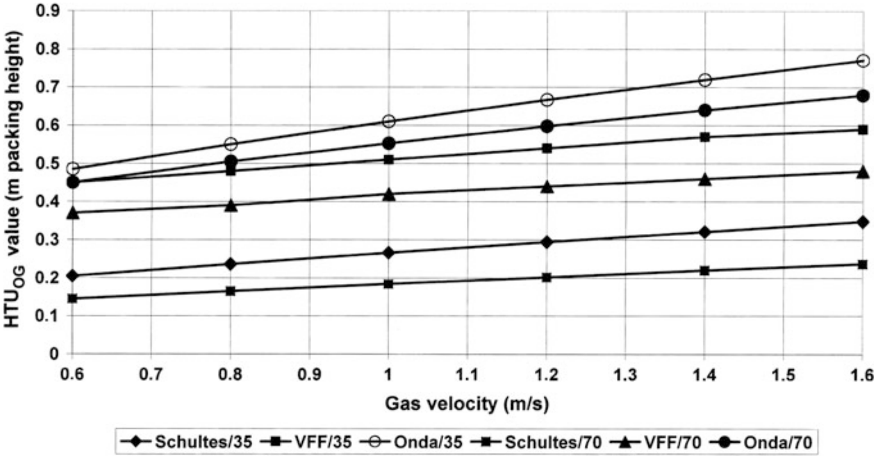


Fig. 10.14 HTU_{OG} values according to different models with different liquid loadings as a function of the gas velocity in the column

With increasing gas velocity the HTU_{OG} values rise whereas with higher liquid loading the values reduce.

Figures 10.15 and 10.16 show the results of an optimization study for a steam stripper for stripping out high boiling aromatic hydrocarbons from a waste water stream.

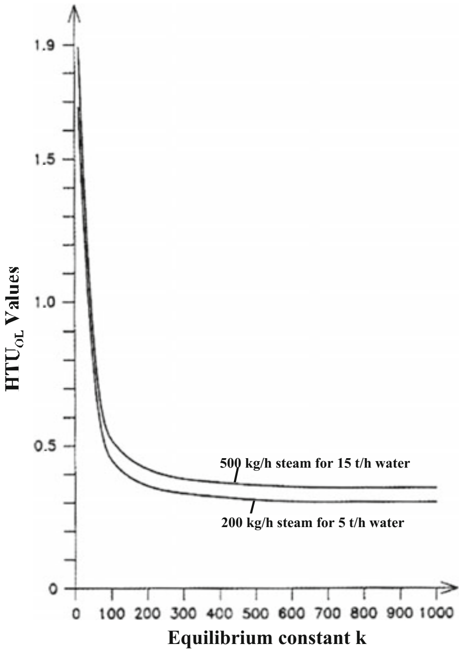
Figure 10.15 shows that the HTU_{OL} values drop with increasing equilibrium constant *K*.

Figure 10.16 shows the influence of the stripping steam rate and the liquid loading on the

HTU_{OG}, the HTU_{OL}, and the HETP values.

- The HTU_{OL} value falls with increasing stripping steam rate and the HTU_{OG} value rises.
- With a liquid loading of 15 t/h the HTU_{OG} value is lower than at 10 t/h.
- The HTU_{OL} values are lower at a lower liquid rate.
- At a higher liquid loading of 15 t/h the HETP value is a little lower than at 10 t/h.

Fig. 10.15 HTU_{OL} values as a function of the equilibrium factor *K*



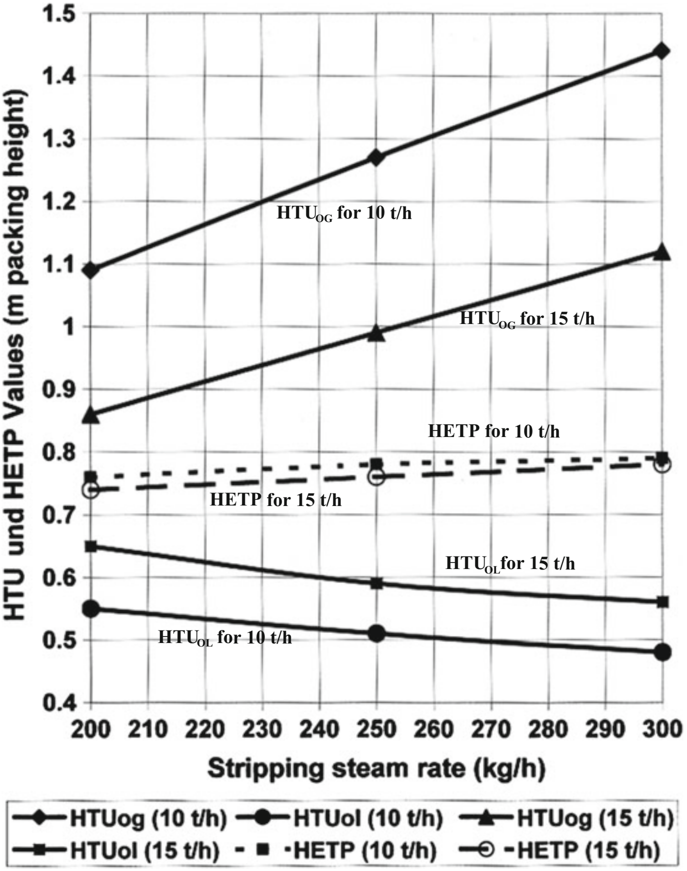


Fig. 10.16 HTU and HETP values as a function of the stripping steam rate for 10 t/h and 15 t/h liquid loadings

A most important parameter in the determination of the HTU values is the Schmidt number *Sc* which is defined as the quotient of the kinematic viscosity and the diffusion coefficient.

Using the Schmidt number allows the HTU values to be converted to comparable conditions.

$$Sc = \frac{\nu}{D} = \frac{\eta}{\rho * D}$$

$$\text{Gas side: } Sc_{\mathrm{G}} = \frac{\nu_{\mathrm{G}}}{D_{\mathrm{G}}} = \frac{\eta_{\mathrm{G}}}{\rho_{\mathrm{G}} * D_{\mathrm{G}}}$$

$$\text{Liquid side } Sc_{\mathrm{L}} = \frac{\nu_{\mathrm{L}}}{D_{\mathrm{L}}} = \frac{\eta_{\mathrm{L}}}{\rho_{\mathrm{L}} * D_{\mathrm{L}}}$$

For other components with other physical data the HTU values can be converted using the Schmidt numbers for the gas and the liquid side.

$$\mathrm{HTU_{G2}} = \mathrm{HTU_{G1}} * \sqrt{\frac{Sc_{\mathrm{G2}}}{Sc_{\mathrm{G1}}}}\,(\mathrm{m})$$

$$\mathrm{HTU_{L2}} = \mathrm{HTU_{L1}} * \sqrt{\frac{Sc_{\mathrm{L2}}}{Sc_{\mathrm{L1}}}}\,(\mathrm{m})$$

D = diffusion coefficient ($\mathrm{m^2/s}$)
D_{G} = gas side diffusion coefficient ($\mathrm{m^2/s}$)
D_{L} = liquid side diffusion coefficient ($\mathrm{m^2/s}$)
Sc_{G1} = gas side Schmidt number for the known $\mathrm{HTUG_1}$ value
Sc_{G2} = schmidt number of the new component on the gas side
Sc_{L1} = liquid side Schmidt number for the known $\mathrm{HTUL_1}$ value
Sc_{L2} = Schmidt number of the new component on the liquid side
η = dynamic viscosity (Pa)
v = kinematic viscosity ($\mathrm{m^2/s}$)
ρ = density ($\mathrm{kg/m^3}$)

In the following text some Schmidt numbers for absorptions in water are listed:

	Temp. (°C)	v_{G} (10^{-6} $\mathrm{m^2/s}$)	D_{G} (10^{-6} $\mathrm{m^2/s}$)	Sc_{G}	v_{L} (10^{-6} $\mathrm{m^2/s}$)	D_{L} (10^{-9} $\mathrm{m^2/s}$)	Sc_{L}
Ammonia–air/water	20	15.1	23.8	0.633	1.03	1.72	598
Acetone–air/water	27	15.6	10.8	1.44	0.86	1.18	728
Methanol–air/water	27	15.6	16.5	0.95	0.86	1.44	597

Example 10.1.2.3: Conversion of the HTU values using the Schmidt number

(a) **Gas side conversion**:

$$\mathrm{HTU_{G1}} = 0.5\,\mathrm{m} \qquad Sc_{\mathrm{G1}} = 1$$

Data of the new component:

$$v_{\mathrm{G2}} = 2.0 \times 10^{-6}\,\mathrm{m^2/s} \qquad D_{\mathrm{G2}} = 4.7 \times 10^{-6}\,\mathrm{m^2/s}$$

$$Sc_{G2} = \frac{v_{\mathrm{G2}}}{D_{\mathrm{G2}}} = \frac{2 \times 10^{-6}}{4.7 \times 10^{-6}} = 0.425$$

$$\mathrm{HTU_{G2}} = 0.5 * \sqrt{\frac{0.425}{1}} = 0.326\ \mathrm{m}$$

(b) **Liquid side conversion**:

$$\mathrm{HTU}_{\mathrm{L1}} = 0.4 \qquad Sc_{\mathrm{L1}} = 1000$$

Data of the new component:

$$v_{\mathrm{L2}} = 0.7 \times 10^{-6}\,\mathrm{m}^2/\mathrm{s} \qquad D_{\mathrm{L2}} = 5 \times 10^{-9}\,\mathrm{m}^2/\mathrm{s}$$

$$Sc_{\mathrm{L2}} = \frac{0.7 \times 10^{-6}}{3 \times 10^{-9}} = 233$$

$$\mathrm{HTU}_{\mathrm{L2}} = 0.4 * \sqrt{\frac{233}{1000}} = 0.19\,\mathrm{m}$$

(c) **Calculation of the $\mathrm{HTU}_{\mathrm{OG}}$ values and the HETP values for $S = 0.2$**:

$$\begin{aligned}
\mathrm{HTUO}_{\mathrm{OG1}} &= \mathrm{HTU}_{\mathrm{G1}} + S * \mathrm{HTU}_{\mathrm{L1}} = 0.5 + 0.2 * 0.4 = 0.58\,\mathrm{m} \\
\mathrm{HTUO}_{\mathrm{OG2}} &= \mathrm{HTU}_{\mathrm{G2}} + S * \mathrm{HTU}_{\mathrm{L2}} = 0.326 + 0.2 * 0.19 = 0.36\,\mathrm{m} \\
\mathrm{HETP}_1 &= \mathrm{HTU}_{\mathrm{OG1}} * \frac{\ln S}{S-1} = 0.58 * \frac{\ln 0.2}{0.2-1} = 1.17\,\mathrm{m} \\
\mathrm{HETP}_2 &= \mathrm{HTU}_{\mathrm{OG2}} * \frac{\ln S}{S-1} = 0.36 * \frac{\ln 0.2}{0.2-1} = 0.72\,\mathrm{m}
\end{aligned}$$

Diffusion coefficients (cm^2/s) and Schmidt number of some vapour in air at 25 °C:

Gas	CO_2	Methanol	Propanol	Benzene	Toluene	Chlorobenzene	Chlorotoluene
D_G	0.164	0.159	0.1	0.088	0.084	0.073	0.065
Sc_G	0.94	0.97	1.55	1.76	1.84	2.12	2.38

Figures 10.17 and 10.18 shows the Schmidt numbers of some components in gases and liquids.

Figure 10.19 plots the diffusion coefficients according to the different models for diffusion in gases at 1 bar [15].

The diffusion coefficient rises with rising temperature (Fig. 10.20) and decreasing pressure (Fig. 10.21).

Figure 10.22 shows the diffusion coefficients in liquids as a function of the temperature calculated using different models [16].

The diffusion coefficients for diffusion in liquids rise with increasing temperature and decreasing viscosity (Fig. 10.23).

The dynamic viscosity of gases and vapour rises with temperature (Fig. 10.24).

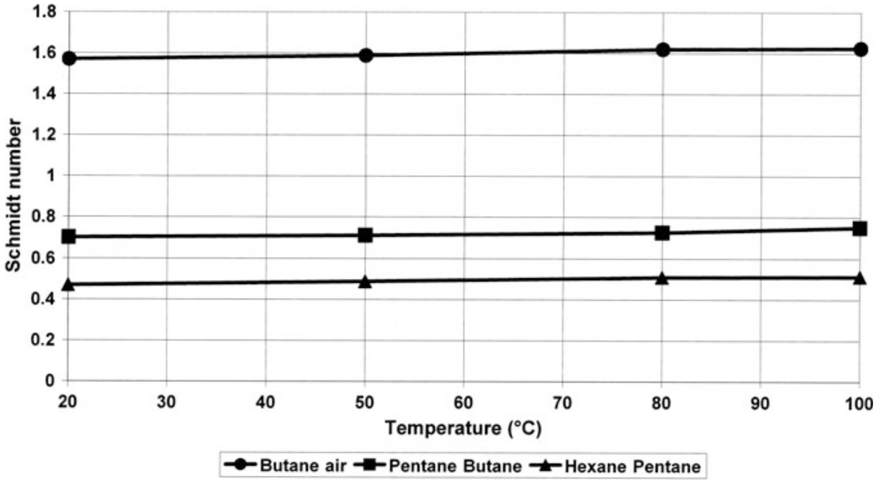


Fig. 10.17 Schmidt numbers for diffusion in gases as a function of temperature

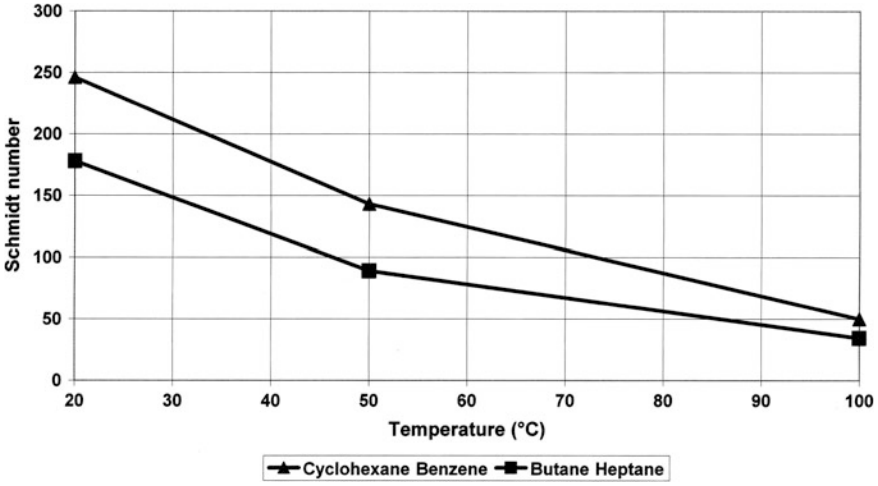


Fig. 10.18 Schmidt numbers for diffusion in liquids as a function of temperature

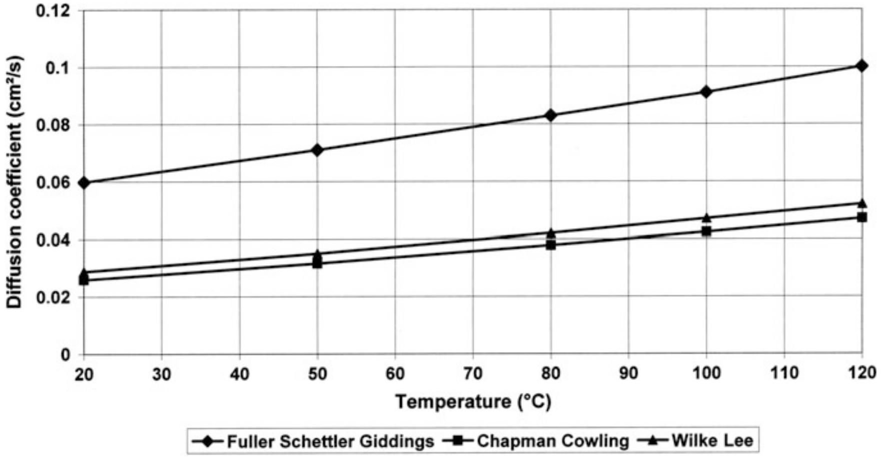


Fig. 10.19 Diffusion coefficients for the diffusion of ethane in hexane vapour according to different models as a function of temperature

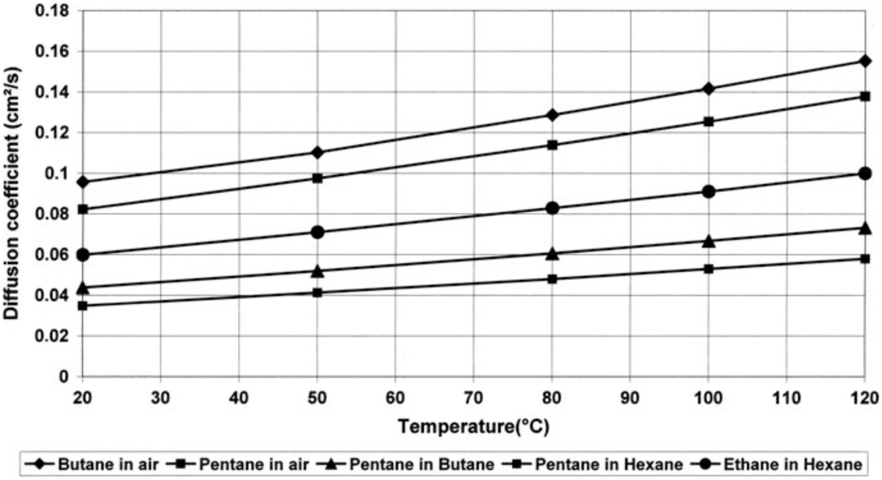


Fig. 10.20 Diffusion coefficients of gases according to Fuller as a function of temperature

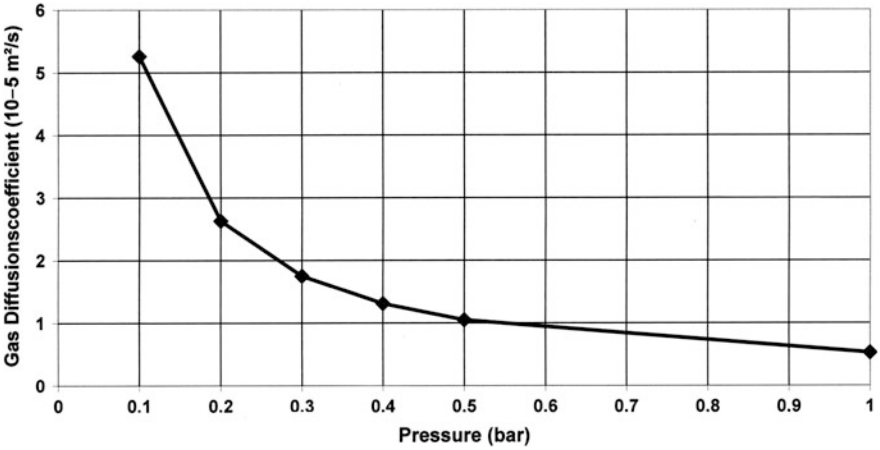


Fig. 10.21 Diffusion coefficient of butane in pentane at 50 °C as a function of pressure

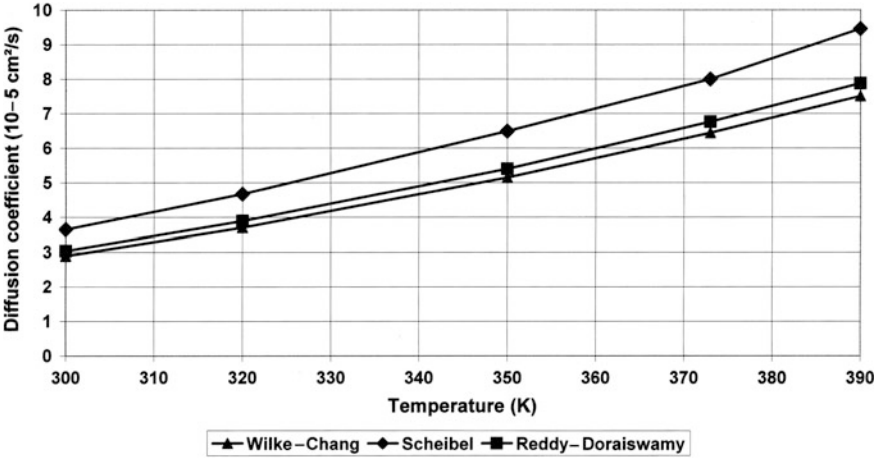


Fig. 10.22 Diffusion coefficient of liquid cyclohexane in benzene using different models at different temperatures

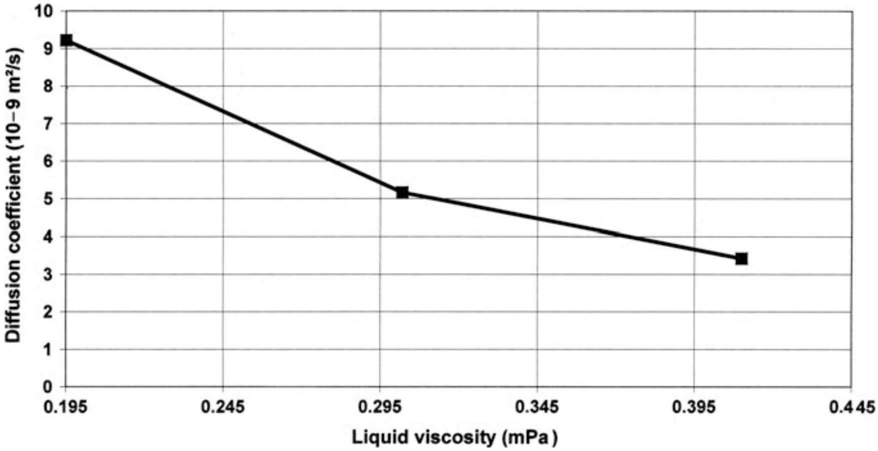


Fig. 10.23 Diffusion coefficients of butane in liquid heptane as a function of liquid viscosity

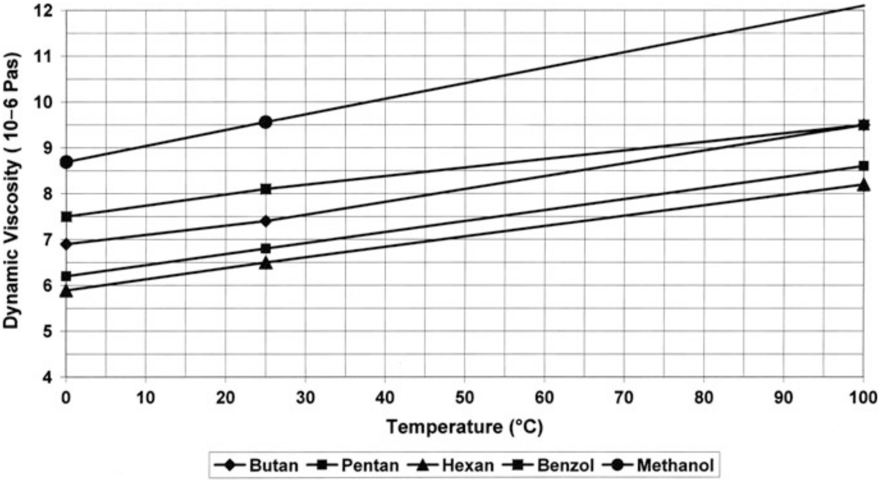


Fig. 10.24 Dynamic viscosity of some vapour as a function of temperature

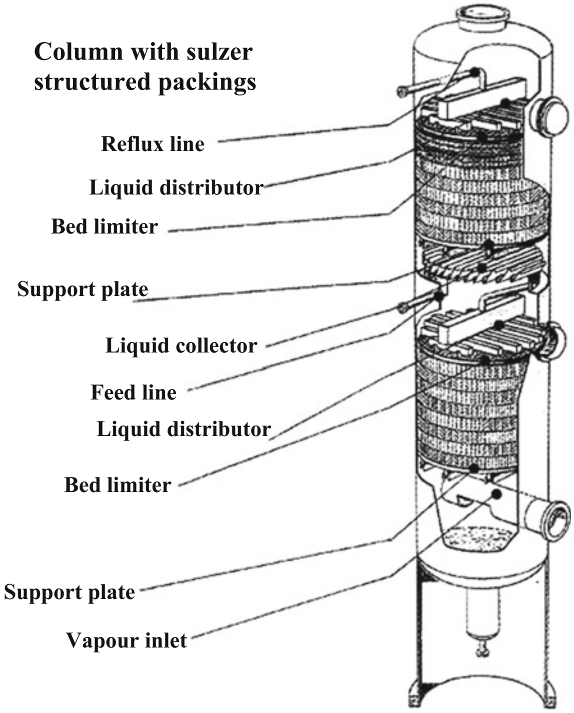


Fig. 10.25 Structured, packed column with internals

10.2 Columns with Structured Packing

Figure 10.25 shows a structured, packed column by the "Sulzer" Company.

Advantages of the structured packing:

Lower pressure losses.
Higher separation efficiencies than with trays.
Larger throughput capacity than with trays.
Wider operation range than with trays.
Lower liquid content, meaning lower "hold up".

The most important design criteria are:

HETP values (m packing height per theoretical stage).
Pressure losses (mbar/m packing height).
Flood loading (% capacity utilization).
Spray rate (m^3 liquid/m^2 h).

Design guideline for structured packings:

Gas loading factor $F = 2$–2.5.
Liquid loading: 1–100 m^3/m^2h.
Liquid distribution: 100–200 droplet points per m^2.
Free streaming cross section at the distributors: >50% of the column cross section.
Free streaming cross section at the support grids: 80% of the column cross section.
Maximum packing height: 15–20 theoretical stages.
Redistribution in metal sheet structured packings after 4–5 m.
Redistribution in wire gauze packings after 5–7 m.
Construction height of a collector–distributor: depending on the column diameter.

Theoretical stages: approximately five theoretical stages in wire gauze packings;

Approximately 2.5 theoretical stages in sheet metal structured packings.

Gas distribution: by a pre-distribution, for instance in a chimney tray [1].

A poor liquid distribution and a non-uniform gas flow influence strongly, i.e., hinder, the separation efficiency.

The HETP values and the pressure losses are dependent on the gas and the liquid loading and the physical data.

Disadvantages of structured packings:

High tolerance requirements and high costs.
Less suitable for dirty feed products.
Less suitable for multi-phase liquids.
Less suitable for columns with several side draws.
Ignition danger for explosive air–solvent mixtures on hot wire mesh.

Selection criteria:

- For vacuum distillation in which a high number of trays and a lower pressure loss is required an expensive fabric structured packing should be chosen.
- For large throughput capacities and low pressure losses a sheet metal structured packing can be used.
- For high liquid loadings in the stripping section random packings are very suitable because the film thickness is smaller than on the sheet metal structured packing.

In individual cases the design is based on the diagrams delivered by the vendor, including the separation efficiency for test mixtures and the pressure loss curves.

Furthermore there are suppliers (Montz, Raschig, Sulzer) of calculation programs for hydraulic designs.

“Anstaupacking” is now under development in which two different package sizes are installed [17] for the improvement of separation effectiveness.

In the smaller package the liquid is accumulated and a bubble layer is created.

Such optimization trials restrict flexibility.

Often however it is reasonable to vary the package sizes in the column if the hydraulic conditions are very different, for instance in the rectification and stripping sections.

Example 10.2.1: Separation of a binary mixture in a packed column
The required separation is specified in the following mass balance.

Component	Feed F		Distillate D		Bottoms draw B	
	(kmol/h)	(molfr.)	(kmol/h)	(molfr.)	(kmol/h)	(molfr.)
Light comp.	50	0.5	49.45	0.999	0.55	0.01
Heavy comp.	50	0.5	0.05	0.001	49.95	0.99
	100	1.0	49.5	1.000	50.5	1.00

Relative volatility $\alpha = 1.2$
Minimum reflux ratio:

$R_{\min} = 9.98$ at a liquid feed with bubble point temperature
$R_{\min} = 11$ at a vapour feed with dew point temperature

Required number of theoretical stages at different reflux:

	Liquid feed			Vapour feed		
$R/R_{\min}$	N_V	N_S	N_{tot}	N_V	N_S	N_{tot}
1.4	63.6	43.1	106.8	61.7	42	103.7
1.6	58.1	39.2	97.3	56.8	38.2	95
1.8	54.7	36.9	91.6	53.6	35.8	89.4
2.0	52.2	35.2	87.4	51.4	34.2	85.6
2.2	50.4	34	84.4	49.7	33	82.7
2.4	49	33	82	48.4	32.1	80.5

Column loading	Liquid feed	Vapour feed
Reflux ratio R	20	22
Distillate D (kmol/h)	49.5	49.5
Vapour flow V_V (kmol/h)	1040	1140
Liquid L_V (kmol/h)	990	1090
Vapour flow V_S (kmol/h)	1040	1040
Liquid L_S (kmol/h)	1090	1090
Bottoms draw B (kmol/h)	50.5	50.5

V_V = vapour flow in the rectification section (kmol/h)
N_S = stripping trays
L_V = liquid flow in the rectification section (kmol/h)
N_V = rectification trays
V_S = vapour flow in the stripping section (kmol/h)
L_S = liquid flow in the stripping section (kmol/h)

Example 10.2.2: Column design for the liquid feed at bubble point temperature

Rectification section:

$$\rho_{\mathrm{D}} = 3.2\,\mathrm{kg/m^3} \qquad \rho_{\mathrm{L}} = 760\,\mathrm{kg/m^3} \qquad M = 100\,\mathrm{kg/kmol}$$

$$V_{\mathrm{V}} = 1040\,\mathrm{kmol/h} = 1040 * 100 = 104{,}000\,\mathrm{kg/h} = \frac{104{,}000\,\mathrm{m^3/h}}{3.2\,\mathrm{kg/m^3}} = 32{,}500\,\mathrm{m^3/h}$$

$$L_{\mathrm{V}} = 990\,\mathrm{kmol/h} = 990 * 100 = 99{,}000\,\mathrm{kg/h} = \frac{99{,}000}{760} = 130.3\,\mathrm{m^3/h}$$

Calculation of the required column diameter D_{req} for $F = 2.2$:

$$F = w_{\mathrm{D}} * \sqrt{\rho_{\mathrm{D}}} = 2.2 \qquad w_{\mathrm{D}} = \frac{2.2}{\sqrt{3.2}} = 1.22\,\mathrm{m/s}$$

$$A = \frac{V_{\mathrm{V}}(\mathrm{m^3/h})}{3600 * w_{\mathrm{D}}(\mathrm{m/s})} = \frac{32{,}500}{3600 * 1.22} = 7.4\,\mathrm{m^2}$$

$$D_{\mathrm{req}} = \sqrt{A * \frac{4}{\pi}} = \sqrt{7.4 * \frac{4}{\pi}} = 3.06\,\mathrm{m}$$

Checking the liquid loading B_{L} of the structured packing:

$$B_{\mathrm{L}} = \frac{L_{\mathrm{V}}(\mathrm{m^3/h})}{A(\mathrm{m^2})} = \frac{130.3}{7.4} = 17.6\,\mathrm{m^3/m^2h}$$

Stripping section:

$$\rho_{\mathbf{D}} = 3.3\,\mathrm{kg/m^3} \qquad \rho_{\mathrm{L}} = 770\,\mathrm{kg/m^3} \qquad M = 120\,\mathrm{kg/kmol}$$

$$V_{\mathrm{S}} = 1040\,\mathrm{kmol/h} = 1040 * 120 = 124{,}800\,\mathrm{kg/h} = \frac{124{,}800\,\mathrm{m^3/h}}{3.3\,\mathrm{kg/m^3}} = 37{,}818\,\mathrm{m^3/h}$$

$$L_{\mathrm{S}} = 1090\,\mathrm{kmol/h} = 1090 * 120 = 130{,}000\,\mathrm{kg/h} = \frac{130{,}000}{770} = 169.9\,\mathrm{m^3/h}$$

Calculation of the required column diameter D_{req} for $F = 2.2$:

$$F = w_{\mathrm{D}} * \sqrt{\rho_{\mathrm{D}}} = 2.2 \qquad w_D = \frac{2.2}{\sqrt{3.3}} = 1.21\,\mathrm{m/s}$$

$$A = \frac{V_{\mathrm{V}}(\mathrm{m^3/h})}{3600 * w_{\mathrm{D}}(\mathrm{m/s})} = \frac{37{,}818}{3600 * 1.21} = 8.68\,\mathrm{m^2}$$

$$D_{\mathrm{req}} = \sqrt{A * \frac{4}{\pi}} = \sqrt{8.68 * \frac{4}{\pi}} = 3.3\,\mathrm{m}$$

Checking the liquid loading B_L of the structured packing:

$$B_{\mathrm{L}} = \frac{L_{\mathrm{S}}(\mathrm{m}^3/\mathrm{h})}{A(\mathrm{m}^2)} = \frac{169.9}{8.68} = 19.6\,\mathrm{m}^3/\mathrm{m}^2\mathrm{h}$$

Conclusion: the stripping section requires a larger diameter than for the rectification section.

Example 10.2.3: Column design for the vapour feed at dew point temperature
For a vapour feed to the column the vapour and liquid loadings in the rectification section are larger than for the liquid feed.

$$V_{\mathrm{L}} = 1140\,\mathrm{kmol/h} = 1140 * 100 = 114{,}000\,\mathrm{kg/h} = \frac{114{,}000\,\mathrm{m}^3/\mathrm{h}}{3.2\,\mathrm{kg/m}^3} = 35{,}625\,\mathrm{m}^3/\mathrm{h}$$

$$L_{\mathrm{V}} = 1090\,\mathrm{kmol/h} = 1090 * 100 = 109{,}000\,\mathrm{kg/h} = \frac{109{,}000}{760} = 142.4\,\mathrm{m}^3/\mathrm{h}$$

Calculation of the required column diameter D_{req} for $F = 2.2$:

$$F = w_{\mathrm{D}} * \sqrt{\rho_{\mathrm{D}}} = 2.2 \qquad w_D = \frac{2.2}{\sqrt{3.2}} = 1.22\,\mathrm{m/s}$$

$$A = \frac{V_{\mathrm{V}}(\mathrm{m}^3/\mathrm{h})}{3600 * w_{\mathrm{D}}(\mathrm{m/s})} = \frac{35{,}625}{3600 * 1.22} = 8.11\,\mathrm{m}^2$$

$$D_{\mathrm{req}} = \sqrt{A * \frac{4}{\pi}} = \sqrt{8.11 * \frac{4}{\pi}} = 3.21\,\mathrm{m}$$

Summary: For a vapour feed a larger column diameter is required in the rectification section than for the liquid feed.

If different packings are used then different required column diameters and different required packing heights for the trays result.

Rectification:

$N_V = 52$ theoretical stages

Packing	D_{req} (m)	H_{req} (m)	F value	HETP	ΔP (mbar/m)
250 Y	3.2	20.8	2.2	2.5	1.9 (39.5 mbar)
250 X	2.8	26	2.7	2	1.6 (41.6 mbar)
350 Y	3.45	14.9	1.7	3.5	1.9 (28.3 mbar)
350 X	3.03	19.3	2.2	2.7	2 (38.6 mbar)
500 Y	3.78	13	1.4	4	2.1 (27.3 mbar)
500 X	3.32	17.3	1.9	3	2 (34.6 mbar)
BX	3.3	13	1.9	4	2.3 (29.9 mbar)

Stripping section:

$N_S = 35$ theoretical stages

Packing	D_{req} (m)	H_{req} (m)	F value	HETP	ΔP (mbar/m)
250 Y	3.34	14	2	2.5	2.1 (29.4 mbar)
250 X	2.9	17.5	2.7	2	1.8 (31.5 mbar)
350 Y	3.64	10	1.7	3.5	1.9 (19.0 mbar)
350 X	3.17	13	2.2	2.7	2 (26.0 mbar)
500 Y	4	8.75	1.4	4	2.1 (18.4 mbar)
500 X	3.5	11.7	1.8	3	2 (23.4 mbar)
BX	3.5	8.7	1.8	4	2.3 (20.0 mbar)

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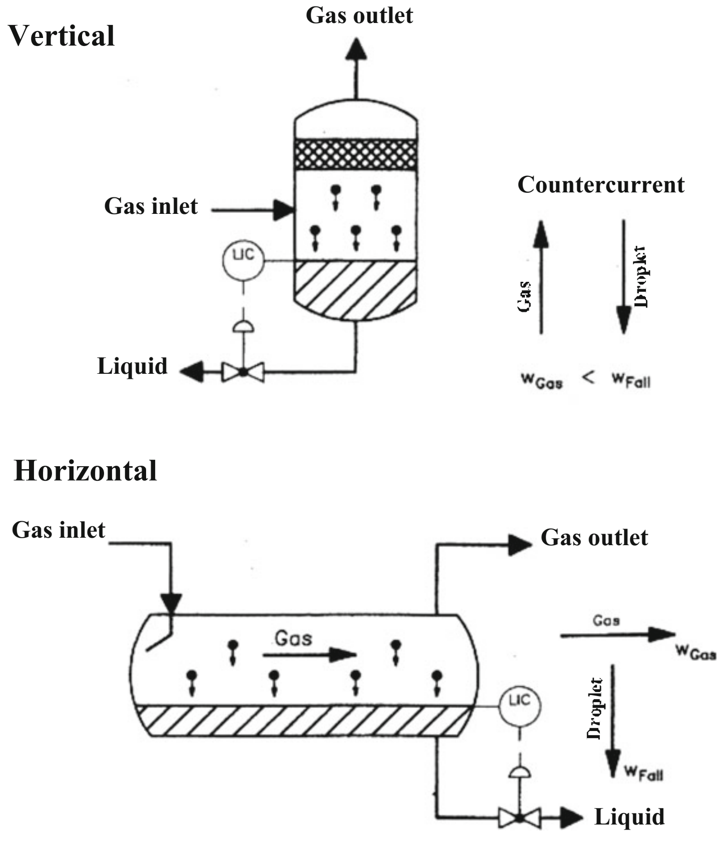
Chapter 11
Demister Design



M. Nitsche and R. Gbadamosi, *Practical Column Design Guide*,
DOI 10.1007/978-3-319-51688-2_11

11.1 Why Use Demisters?

- To reducing material losses in absorbers, evaporators, and distillation columns, e.g., for reducing glycol or amine losses in natural gas treatment.
- To improve product quality in distillation plants because contamination by entrained droplets is eliminated.
- To avoiding corrosion in the downstream process units through corrosive liquid droplets.
- To protect compressors against liquid droplets.
- To reducing droplet emissions.
- To relieve vacuum pumps.

11.2 Droplet Separation in Gravity, Wire Mesh, and Lamella Separators

For droplet separation both vertical and horizontal separators can be used.

In **vertically streamed separators the fall velocity w_{Fall}** of the droplets must be larger than the upwards directed **gas stream velocity w_{G}**.

$$w_{\mathrm{Fall}} > w_{\mathrm{G}}$$

In this type of design 50–75% droplet fall velocity is used.

$$w_{\mathrm{G}} = 0.5\,\mathrm{bis}\,0.75 * w_{\mathrm{Fall}}$$

In **horizontally streamed separators** the **fall** or **settling time t_{Fall}** for a falling height h must be smaller than the **residence time of the streaming gases t_{res}** in the separator.

$$t_{\mathrm{Fall}} = \frac{h}{w_{\mathrm{Fall}}} \leq t_{\mathrm{res}} = \frac{L}{w_{\mathrm{G}}}$$

h = gas height above the liquid in the separator (m)
L = separator length (m)
w_{Fall} = fall velocity of droplets (m/s)
w_{G} = flow velocity of the gas in the separator

To improve droplet separation at higher gas flow velocities separation aids are used.

The different types of demisters are listed in the following text with limiting droplet size and pressure drop included.

Up to the limiting droplet diameter all droplets are completely separated.

Separator type	Limit droplet (μm)	Pressure loss (mbar)
Gravity	300–400	<1
Wire mesh	5–10	1–2
Vertical lamella separator	30–40	1
Horizontal lamella separator	10–30	2–10
Microfibre	1–3	5–50
Spin vane separator	50–100	6–15
Zyclon	30–50	10–50

With the exception of microfibre separators the droplets are removed from the gas stream by mechanically operating separators, for instance by gravitational and centrifugal force or inertia.

The different separator mechanisms are shown in Fig. 11.1.

In the following text the most important parameters for separation rate A are discussed.

Inertia separators

Sluggish droplets do not follow the gas stream around the barriers but rather they cross the gas stream and hit the wires of the wire mesh separator or the wall of a lamella separator. This enlarges the droplets. Larger droplets fall faster and are separated more easily.

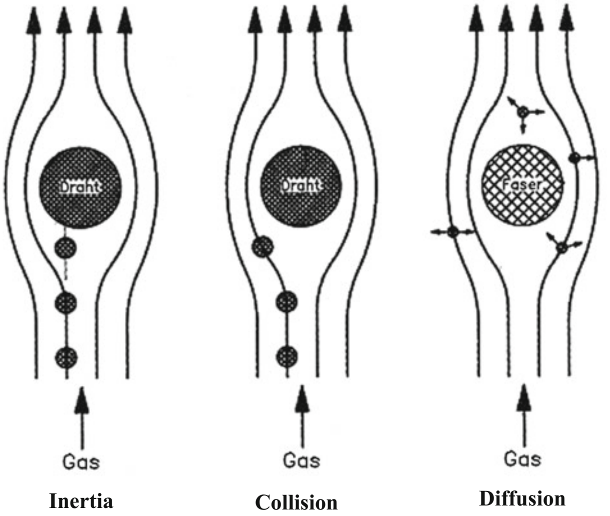
$$A = f\left(\frac{K * \varrho_{\text{fl}} * w_{\text{G}} * d^2}{18 * \eta_{\text{G}} * d_{\text{F}}}\right)$$

A = separator efficiency
d = droplet diameter
d_F = wire or fibre diameter
K = Cunningham factor (>15 μ = 1)
w_G = gas flow velocity
η_G = gas viscosity
ϱ_{Fl} = liquid density.

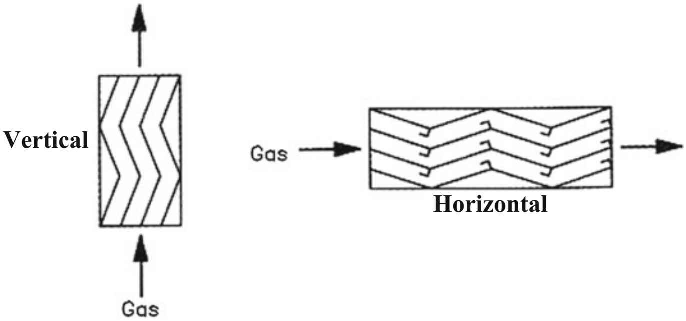
Droplet separation improves with increasing flow velocity, increasing droplet diameter, and decreasing wire or fibre diameter.

A **minimum velocity** is required in order to activate the inertia effect.

On the other hand a **maximum velocity** must not be exceeded in order to avoid the re-entrainment of the constructed, large droplets.



Wire mesh and fibre separators



Lamella separators

Fig. 11.1 Separator mechanisms in demisters

Separation by contact and collision for large droplets

When flowing through narrow tunnels the droplets come into contact with the surface area of the wires, fibres, or lamella plates and remain attached to them.

The separation rate A is dependent on the quotient droplet diameter d to fibre diameter d_F.

$$A = f\left(\frac{d}{d_F}\right)$$

Larger droplets and thinner wires or fibres improve the separation.

Separation by diffusion for small droplets

Due to the larger diffusion velocity of the minimum droplets across the flow direction a better contact with the fibres occurs.

The separation rate A is dependent on the ratio d/d_F and the gas flow velocity.

$$A = f\left(\frac{d}{w_G * d_F}\right)$$

The separation improves with decreasing flow velocity and decreasing fibre diameter.

Demister construction types

Wire mesh packets from wires with 0.1–0.28 mm diameters are mostly used.

The packages have a depth of 100–300 mm.

The **wire mesh demister** is an impingement separator. When streaming through the wire mesh the gas must stream around a number of thin wires.

The heavy droplets cannot escape due to the inertia and they hit the wires. The droplets build a film and flow downwards as large droplets.

The wire mesh demister is especially suitable for separation of small droplets in the region of 5–10 μm.

In **vertically streamed** separators the allowable flow velocity is lower due to the countercurrent flow of gas and liquid rather than with the horizontally streamed wire meshes.

Lamella separators are advantageous for larger liquid loadings and in cases of fouling risk.

Additionally, the gas throughput capacity is essentially higher than in wire mesh separators which tend to flood at high liquid loadings and flow veloctites.

Droplet separation occurs by inertia because the droplets do not follow the gas stream, instead they hit the plates when streaming through the wavy, zigzag lamella packages.

In the vertically arranged lamella package the liquid runs off in the opposite direction to the gas, in other words countercurrent downwards.

In the horizontally streamed lamella packages the liquid is collected with "hook plates" and directed downwards.

Therefore, the gas capacity for a horizontal arrangement is greater because the likelihood of re-entrainments is less.

Microfibre separators, with fibre diameters <0.02 mm, are used as diffusion or inertia separators.

Due to the thinness of the fibres the small droplets are better separated in inertia separators to droplet sizes of 1 μm.

In these separators gas and liquid streams horizontally through the fibre filter.

Vertically upward streaming is avoided. This is because due to the large specific surface area in these separators flooding can easily occur.

In their use as inertia separators, higher flow velocities are required or are more allowable than with diffusion separators.

Cylindrical inertia separators: 1–2 m/s
Cylindrical diffusion separators: 0.05–0.2 m/s
Fibre mat, inertia separators: 2–3 m/s

With diffusion separators only low flow velocities are allowed, so large flow cross sections must be installed.

11.2.1 Allowable Gas Flow Velocities

The allowable flow velocities w_{allow} in demisters are calculated as follows:

$$w_{\mathrm{allow}} = K * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.1}$$

The design velocity w_{des} should lie at 75%: $w_{\mathrm{des}} = 0.75 * w_{\mathrm{allow}}$

The minimum flow velocity lies at 30%: $w_{\mathrm{min}} = 0.3 * w_{\mathrm{allow}}$

In the following text the equations for the determination of the allowable flow velocity in different separators are listed [1–4].

Vertical gravity separator without internals, $K \approx$ 0.033–0.05:

$$w_{\mathrm{allow}} = 0.04 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.1a}$$

Vertical separator with wire mesh demister:

$$w_{\mathrm{allow}} = 0.106 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.1b}$$

Other K values are valid for other conditions:
In vacuum ⇒ $K = 0.03–0.06$
For plastic demister ⇒ $K = 0.065$

Horizontal separator with wire mesh, $K \approx$ 0.12–0.15:

$$w_{\mathrm{allow}} = 0.15 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.1c}$$

Horizontal gravity separator without internals, K = 0.108–0.122:

$$w_{\mathrm{allow}} = 0.12 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.1d}$$

The calculated flow velocity is valid for the free gas cross section above the liquid.

Vertically streamed lamella separator, K = 0.1–0.12:

$$w_{\text{allow}} = 0.12 * \sqrt{\frac{\varrho_{\text{Fl}}}{\varrho_{\text{G}}} - 1} \quad (\text{m/s}) \tag{11.1e}$$

Horizontally streamed lamella separator, K = 0.1–0.2:

$$w_{\text{allow}} = 0.02 * \sqrt{\frac{\varrho_{\text{Fl}}}{\varrho_{\text{G}}} - 1} \quad (\text{m/s}) \tag{11.1f}$$

Microfibre, inertia separator, $K \approx$ 0.04–0.07:

$$w_{\text{allow}} = 0.06 * \sqrt{\frac{\varrho_{\text{Fl}}}{\varrho_{\text{G}}} - 1} \quad (\text{m/s}) \tag{11.1g}$$

Microfibre, fog separator for micro-droplets, K = 0.003–0.006.

$$w_{\text{allow}} = 0.006 * \sqrt{\frac{\varrho_{\text{Fl}}}{\varrho_{\text{G}}} - 1} \quad (\text{m/s}) \tag{11.1h}$$

Example 11.2.1.1: Calculation of the allowable flow velocities in different separators at 1 bar.

Liquid density ρ_{Fl} = 995 kg/m^3

Gas density ρ_{G} = 1.2 kg/m^3

Vertical gravity separator (Eq. 11.1a):

$$w_{\text{allow}} = 0.04 * \sqrt{\frac{995}{1.2} - 1} = 0.04 * 28.78 = 1.15\,\text{m/s}$$

Vertical separator with wire mesh (Eq. 11.1b):

$$w_{\text{allow}} = 0.106 * \sqrt{\frac{995}{1.2} - 1} = 3.05\,\text{m/s}$$

Horizontal gravity separator (Eq. 11.1d):

$$w_{\text{allow}} = 0.12 * \sqrt{\frac{995}{1.2} - 1} = 3.45\,\text{m/s}$$

Horizontally streamed lamella separator (Eq. 11.1f):

$$w_{\text{allow}} = 0.2 * \sqrt{\frac{995}{1.2} - 1} = 5.75\,\text{m/s}$$

Microfibre, fog separator (Eq. 11.1h):

$$w_{\mathrm{allow}} = 0.006 * \sqrt{\frac{995}{1.2} - 1} = 0.17\,\mathrm{m/s}$$

Example 11.2.1.2: Calculation of the allowable flow velocity at a lower gas density in a vacuum

$$\rho_{\mathrm{Fl}} = 995\,\mathrm{kg/m^3} \quad \rho_{\mathrm{G}} = 0.1\,\mathrm{kg/m^3}$$

Vertical gravity separator (Eq. 11.1a):

$$w_{\mathrm{allow}} = 0.04 * \sqrt{\frac{995}{0.1} - 1} = 3.98\,\mathrm{m/s}$$

Vertical separator with wire mesh (Eq. 11.1b):

$$w_{\mathrm{allow}} = 0.06 * \sqrt{\frac{995}{0.1} - 1} = 5.98\,\mathrm{m/s}$$

Conclusion

- Horizontal gravity separators permit higher gas flow velocities.
- Installation of a separator aids the gas capacity causing droplet separation to be improved.

11.2.2 Liquid Capacity

The separator must have a liquid capacity which is chosen to match the problem definition.

The required liquid capacity depends on the required **residence time**, for instance for degassing, and depends on the quality of the installed **level control.**

The control valve must open fast when larger liquid rates occur impulsively.

The k_{V} value of the valve must not be reduced by fouling or flash evaporation in the valve.

In the design of the control valve both geometry and an expansion factor have to be considered.

Required **minimum residence times**:

1–2 min for normal conditions

5–10 min for foaming materials

>15 min for liquid separations

In horizontal separators the residence time is longer, and the liquid surface area is larger, so that a better degasing occurs.

Errors caused by insufficient liquid withdrawal:

- Flooding of the gas inlet nozzle in vertical separators
- Gas cross sectional narrowing in horizontal separators.

11.3 Vertical Demisters

With vertical separators the droplet fall velocity must be higher than the upwards directed flow velocity of the gases.

In Fig. 11.2 the calculated allowable flow velocities in a vacuum, as a function of the gas density, are shown according to Eq. (11.1a) with $K = 0.035$ for gravity separators and Eq. (11.1b) with $K = 0.06$ for separators with a demister.

Additionally, the fall velocities for the droplet sizes 400, 500, 700, and 800 μ as a function of the gas density, are plotted.

The calculation of the droplet fall velocity is covered in the Appendix at the end of this chapter.

From the curves in Fig. 11.2 the following knowledge can be derived:

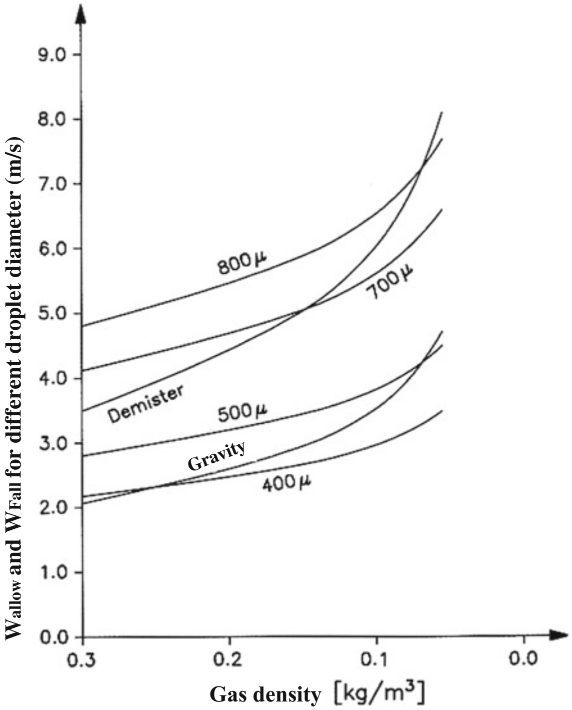


Fig. 11.2 Droplet fall velocities for four droplet sizes and allowable flow velocities in vertical demisters

- With decreasing gas density the fall velocity and the allowable flow velocity in the separator rises.
- In the design of gravity separators according to Eq. (11.1a) only droplets from a diameter of 400–500 µm are precipitated.
  Smaller droplets have a lower fall velocity and are entrained by the gas stream.
- With a wire mesh demister considerably higher flow velocities are allowed because the droplets are enlarged by the coalescence effect of the wires.
  A better droplet separation is achieved, and lower flow cross section or smaller separator diameter is needed.
- A comparison of the allowable gas flow velocity for a demister, with the fall velocities for different droplet sizes, shows that by using a demister the droplets are enlarged to a diameter of approximately 700–800 µm.

Liquid loading of vertical demisters

Vertical demisters are used for low liquid loading and short allowable liquid residence times t_{res}, of 1–2 min.

$$t_{\mathrm{res}} = \frac{D^2 * \pi/4 * h_{\mathrm{Fl}}}{V_{\mathrm{Fl}}} \ (\mathrm{h}) \tag{11.2}$$

D = separator diameter (m)
h_{Fl} = liquid height (m)
V_{Fl} = liquid loading (m^3/h).

11.4 Horizontal Demisters

Horizontal demisters are preferably used if **higher liquid loadings** or sudden liquid strokes occur.

For the droplet separation the residence time t_{res} of the gas in the separator must be longer than the required falling time t_{Fall} of the droplets for a falling height h.

$$t_{\mathrm{Fall}} = \frac{h}{w_{\mathrm{Fall}}} \le t_{\mathrm{res}} = \frac{L}{w_{\mathrm{G}}} \le \frac{L}{w_{\mathrm{allow}}} \tag{11.3}$$

$$w_{\mathrm{G}} = \frac{V_{\mathrm{G}}}{f_{\mathrm{G}} * D^2 * \pi/4 * 3600} \tag{11.4}$$

D = demister diameter (m)
L = demister length (m)
h = gas height in the demister (m)
f_G = cross section part for the gas flow = F_G/F_{ges}
F_G = cross section for gas flow (m^2)
F_{ges} = total cross sectional area of the demister (m^2)
V_G = gas loading (m^3/h)
w_G = gas flow velocity (m/s)
w_{allow} = allowable flow velocity (m/s).

Example 11.4.1: Checking of a horizontal demister

$$D = 1\,\mathrm{m} \quad L = 3\,\mathrm{m} \quad h = 0.5\,\mathrm{m} \quad V_G = 4.000\,\mathrm{m}^3/\mathrm{h}$$

$$\text{Liquid density } \varrho_{Fl} = 995\ \mathrm{kg/m^3} \quad f_G = 0.5$$

$$\text{Gas density } \varrho_G = 1.2\ \mathrm{kg/m^3} \quad \text{Gas viscosity } \eta = 18 * 10^{-6}\ \mathrm{Pa}$$

It is important to check whether the residence time is sufficient.

Available flow velocity w_G:

$$w_G = \frac{4000}{0.5 * 1^2 * 0.785 * 3600} = 2.83\,\mathrm{m/s}$$

Allowable flow velocity w_{zul} according to Eq. (11.1d) for a horizontal gravity demister:

$$w_{allow} = 0.12 * \sqrt{\frac{995}{1.2}} = 3.45\,\mathrm{m/s}$$

The existing flow velocity w_G is less than the allowable velocity w_{allow}.

Checking the residence time for L = 3 m.

First the droplet fall velocity must be calculated (see Appendix at the end of this chapter).

w_{Fall} = 0.3 m/s for droplets with $d_{droplet}$ = 100 μm

$$t_{Fall} = \frac{h}{w_{Fall}} = \frac{0.5}{0.3} = 1.68\,\mathrm{s}$$

$$t_{res} = \frac{L}{w_G} = \frac{3}{2.83} = 1.06\,\mathrm{s}$$

The residence time t_{res} is less than the required falling time t_{Fall}.

The demister is enlarged from $L = 3$ m to $L = 5$ m in order to extend the residence time.

$$L = 5\,\text{m}$$

$$t_{\text{res}} = \frac{5}{2.83} = 1.77\,\text{s}$$

$t_{\text{res}} > t_{\text{Fall}}$ The residence time is longer than the required falling time.

Figure 11.3 **shows** the falling or required settling periods for droplet sizes 100, 200, 300, 400, and 500 μm as function of the given droplet falling height in the demister.

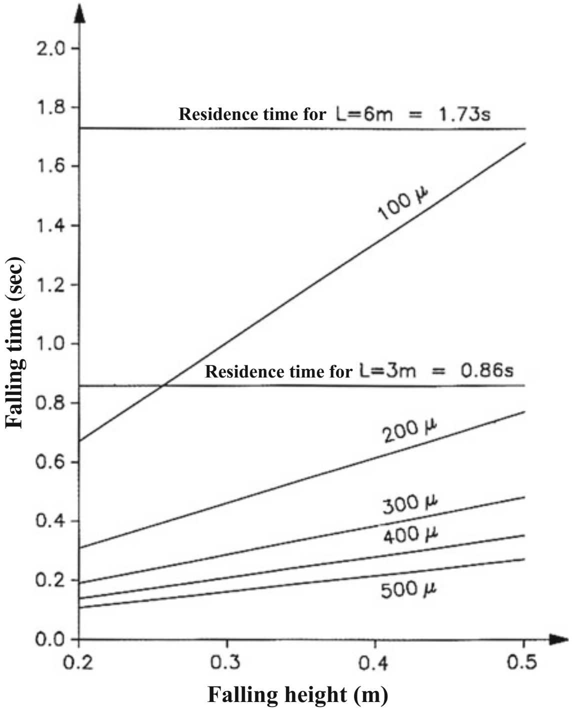
Conclusion:

The required settling periods of the droplets increases with decreasing droplet diameter and increasing falling height.

Additionally, the residence times t_{res} for demister lengths $L = 3$ m and $L = 6$ m are plotted in Fig. 11.3.

The residence times were determined via the allowable flow velocity w_{allow} according to Eq. (11.1d).

Fig. 11.3 Droplet fall periods in a horizontal demister as a function of the falling height



This makes it clear that in the design, according to Eq. (11.1d), droplets > 100 µm are separated if the separator is 6 m long.

For **shorter demisters** the allowable flow velocity must be corrected according to the respective length of the demister.

$$w_{\mathrm{allow}} = \frac{L}{6} * 0.12 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \quad (\mathrm{m/s}) \tag{11.5}$$

Liquid loading

Horizontal demisters are preferably used for higher liquid loadings.

In the dimensioning the required residence time of the liquid t_{res} in the demister has to be considered.

$$t_{\mathrm{res}} = \frac{f_{\mathrm{L}} * D^2 * L * \pi/4}{V_{\mathrm{L}}} \ (\mathrm{h}) \tag{11.6}$$

D = demister diameter (m)
L = demister length (m)
f_{L} = cross sectional part of the liquid stream
V_{L} = liquid loading (m^3/h)

Example 11.4.2: Calculation of the liquid residence time in a demister

$$V_{\mathrm{L}} = 8\,\mathrm{m}^3/\mathrm{h} \quad L = 4\,\mathrm{m} \quad D = 1\,\mathrm{m} \quad f_{\mathrm{L}} = 0.5$$
$$t_{\mathrm{res}} = \frac{0.5 * 1^2 * 4 * 0.785}{8} = 0.196\,\mathrm{h} = 11.8\,\mathrm{min}$$

In the dimensioning of the demister two criteria have to be considered: sufficient **droplet separation** and required **liquid residence time**.

Therefore, both required diameters $\boldsymbol{D_{\mathrm{G}}}$ **for the gas flow** and $\boldsymbol{D_{\mathrm{fl}}}$ **for the liquid capacity** have to be determined.

Starting with the length to diameter ratio L: D = 3 the first estimates of the required dimensions can be estimated according to the following equations.

Required diameter $\boldsymbol{D_{\mathrm{G}}}$ for the gas capacity

$$\begin{gathered} D_{\mathrm{G}} = \left[\frac{V_{\mathrm{G}}}{f_G * 3600 * w_{\mathrm{allow}} * \pi/4}\right]^{1/2} \\ w_{\mathrm{allow}} = \frac{L}{6} * 0.12 * \sqrt{\frac{\varrho_{\mathrm{Fl}}}{\varrho_{\mathrm{G}}} - 1} \end{gathered} \tag{11.7}$$

Required diameter D_{Fl} for the liquid capacity

$$D_{Fl} = \left[\frac{t_{res} * V_L}{f_L * 3 * \pi/4}\right]^{1/3} \tag{11.8}$$

Example 11.4.3: Calculation of the diameter

$$\begin{array}{llll} V_L = 4\,\mathrm{m}^3/\mathrm{h} & t_{res} = 5\,\mathrm{min.} & f_L = 0.5 & \frac{L}{D} = 3 \\ \varrho_{Fl} = 995\,\mathrm{kg/m}^3 & \varrho_G = 1.2\,\mathrm{kg/m}^3 & \mathrm{f}_G = 0.5 & \\ V_G = 1000\,\mathrm{m}^3/\mathrm{h} & w_{zul} = 1.72\,\mathrm{m/s}\ \mathrm{for}\ L = 3\,\mathrm{m} & & \end{array}$$

$$D_G = \left(\frac{1000}{0.50 * 3600 * 1.72 * 0.785}\right)^{1/2} = 0.64\,\mathrm{m}$$

$$D_{Fl} = \left(\frac{5/60 * 4}{0.5 * 3 * 0.785}\right)^{1/3} = 0.656\,\mathrm{m}$$

The determining factor is the liquid capacity →$D = \mathbf{0.656\,m}$.

For the assumed ratio *L*/*D* = 3 the demister length results as follows:

$$\boldsymbol{L = 3 * D = 3 * 0.656 = 2\,\mathrm{m}}.$$

However, the assumed flow velocity of 1.72 m/s is valid for *L* = 3 m.

Using Eq. (11.5) the allowable gas velocity for *L* = 2 m can be determined.

$$w_{allow} = f_G * \frac{L}{3} * \sqrt{\frac{\rho_{Fl}}{\rho_G} - 1} = 0.5 * \frac{2}{3} * \sqrt{\frac{995}{1.2} - 1} = 1.15\ \mathrm{m/s}$$

Due to the lower allowable gas velocity of w_{allow} = 1.15 m/s the diameter increases according to Eq. (11.7):

$$D_G = \left(\frac{1000}{0.5 * 3600 * 1.15 * 0.785}\right)^{1/2} = 0.78\,\mathrm{m}$$

Instead of the expensive diameter enlargement the demister length is increased to *L* = 3 m.

Design: $D = 0.7\,\mathrm{m} \quad L = 3\,\mathrm{m}$.

Cross check calculation

$$w_{\mathrm{G}} = \frac{1000}{0.5 * 3600 * 0.7^2 * 0.785} = 1.44\,\mathrm{m/s}$$
$$\mathrm{w}_{\mathrm{allow}} = 1.72\,\mathrm{m/s} \mathit{for}\, L = 3\,\mathrm{m} \quad \Rightarrow w_{\mathrm{G}} < w_{\mathrm{allow}}$$

Checking the residence time:

$$t_{\mathrm{res}} = \frac{0.5 * 0.7^2 * 0.785 * 3}{4} = 0.144\,\mathrm{h} = 8.65\,\mathrm{min}$$
$$w_{\mathrm{Fl}} = \frac{V_L}{0.5 * D^2 * \pi/4} = \frac{4}{0.5 * 0.7^2 * 0.785} = 20.8\,\mathrm{m/h}$$
$$t_{\mathrm{res}} = \frac{L}{w_{Fl}} = \frac{3}{20.8} = 0.144\,\mathrm{h} = 8.65\,\mathrm{min}$$

The design is OK!

11.5 Selection Criteria and Dimensioning

Recommended design at atmospheric pressure:

Vertical gravity demister: $K = 0.04$ or 75% of the droplet falling velocity.
Horizontal gravity demister: $K = 0.10$.
Vertical wire mesh demister: $K = 0.106$.
Vertical lamella demister: $K = 0.12$.
Horizontal lamella demister: $K = 0.2$.
Horizontal wire mesh demister: $K = 0.15$.

Example 11.5.1: Design of a demister for $V_{\mathrm{G}} = 1000\ \mathrm{m^3/h}$

$$\varrho_{\mathrm{G}} = 1.2\ \mathrm{kg/m^3} \quad \varrho_{\mathrm{Fl}} = 995\ \mathrm{kg/m^3} \quad \eta_{\mathrm{G}} = 18 * 10^{-6}\ \mathrm{Pa}$$

Vertical demister

(a) Gravity demister:

$$w_{\mathrm{allow}} = 0.04 * \sqrt{\frac{995 - 1.2}{1.2}} = 1.15\,\mathrm{m/s}$$
$$w_{\mathrm{des}} = 0.75 * 1.15 = 0.86\,\mathrm{m/s} \rightarrow D = 0.64\,\mathrm{m}$$

(b) Design for 75% of the falling velocity of a 100 μ droplet:

$$w_{\text{Fall}} = 0.297\text{m/s}(\text{see Appendix at the end of this chapter})$$
$$w_{\text{des}} = 0.75 * 0.297\,\text{m/s} = 0.22\,\text{m/s} \rightarrow D = 1.26\,\text{m}$$

(c) Design for 75% of the falling velocity of a 200 μ droplet:
w_{Fall} = 0.65 m/s (see Appendix at the end of this chapter)

$$w_{\text{des}} = 0.75 * 0.65 = 0.487\,\text{m/s} \rightarrow D = 0.85\,\text{m}$$

(d) Wire mesh demister:

$$w_{\text{allow}} = 0.106 * 28.77 = 3.05\ \text{m/s}$$
$$w_{\text{des}} = 0.75 * 3.05 = 2.28\,\text{m/s} \quad \rightarrow D = 0.4\,\text{m}$$

(e) Vertical lamella demister:

$$w_{\text{allow}} = 0.12 * 28.77 = 3.45\,\text{m/s}$$
$$w_{\text{des}} = 0.75 * 3.45 = 2.6\,\text{m/s} \quad \rightarrow D = 0.37\,\text{m}$$

Horizontal demister

(a) Gravity demister:

$$w_{\text{allow}} = 0.1 * 28.77 = 2.87\,\text{m/s}$$
$$w_{\text{des}} = 0.75 * 2.87 = 2.16\,\text{m/s}$$
$$f_{\text{G}} = 0.5(50\%\ \text{gas cross section}) \quad \rightarrow D = 0.57\,\text{m}$$

(b) Horizontal lamella demister:

$$w_{\text{allow}} = 0.2 * 28.77 = 5.77\ \text{m/s}$$
$$w_{\text{des}} = 0.75 * 5.77 = 4.3\,\text{m/s}$$
$$f_{\text{G}} = 0.5(50\%\,\text{gas cross section}) \quad \rightarrow D = 0.4\,\text{m}$$

(c) Horizontal wire mesh demister:

$$w_{\text{allow}} = 0.15 * 28.77 = 4.31\,\text{m/s}$$
$$w_{\text{des}} = 0.75 * 4.31 = 3.32\,\text{m/s}$$
$$f_{\text{G}} = 0.5 \quad \rightarrow D = 0.46\,\text{m}$$

(d) Cross check of the settling time for a gravity demister:

$$w_{\mathrm{Fall}} = 0.165 * 0.75 = 0,123\,\mathrm{m/s}\ \text{for a}\ 60\,\mu\mathrm{m}\ \text{droplet}$$

$$D = 0.6\,\mathrm{m} \quad \text{Falling height}\ h = 0.3\,\mathrm{m} \quad w_{\mathrm{allow}} = 2.16\ \mathrm{m/s}$$

$$t_{\mathrm{Fall}} = \frac{h}{t_{\mathrm{Fall}}} = \frac{0.3}{0.123} = 2.43\ \mathrm{s} \quad t_{\mathrm{res}} = \frac{L}{w_{\mathrm{zul}}} = \frac{6}{2.16} = 2.77\ \mathrm{s}$$

$$t_{\mathrm{res}} > t_{\mathrm{Fall}} \rightarrow \text{droplets} > 60\,\mu\mathrm{m}\ \text{will be separated!}$$

Remark

In the design of **horizontal demisters the flow cross section for the liquid flow section must be subtracted from the total flow cross section.**

Advantages of the gravity demisters

- No plugging and flooding danger.
- No demister installation costs.

Disadvantages of the gravity demisters

- Small droplets are not separated.
- In vertical demisters the allowable flow velocity is essentially lower than in demisters with wire mesh or lamella internals.
- Due to the low allowable flow velocity the demisters must have larger diameters.
- In pressure vessels the required wall thickness rises proportionally to the diameter.
- Thicker walls make the equipment significantly more expensive because of the disproportionate weight increase.

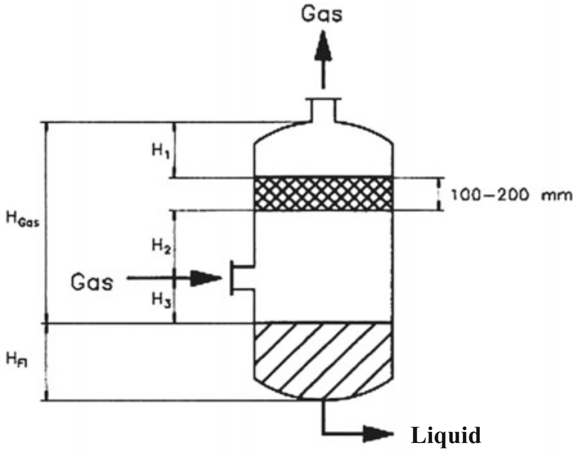
Advantages of separator aids

- In vertical separators less than 50% of the flow cross sectional area is needed with a remarkably improved droplet separation. The required smaller separator diameter reduces the costs of the equipment, especially at higher pressures.
- In horizontal separators the gas capacity increases insignificantly in vertical installations, however, the small droplets are separated. With horizontally arranged lamella separators higher gas velocities are allowed.

Dimensioning of demisters [5]

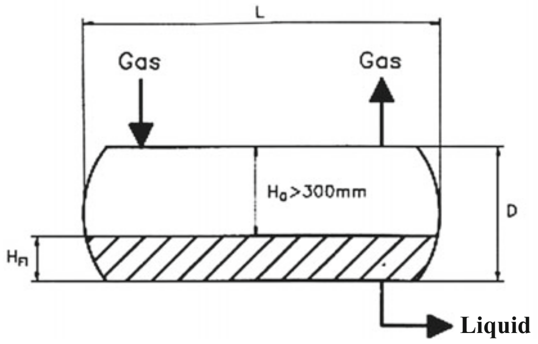
Figure 11.4 shows what happens in the dimensioning of demisters in addition to the calculated required flow cross sections.

Fig. 11.4 Dimensioning of demisters



$H_1 \sim 0.4 * D$ (min. 300 mm)
$H_2 \sim 0.7 * D$ (min. 300 mm)
$H_3 \sim 0.3 * D$ (min. 300 mm)
$H_{Gas} \sim 1.4 * D$
$H_{Fl} \sim 0.3 - 1$ m

Dimensioning of a vertical separator

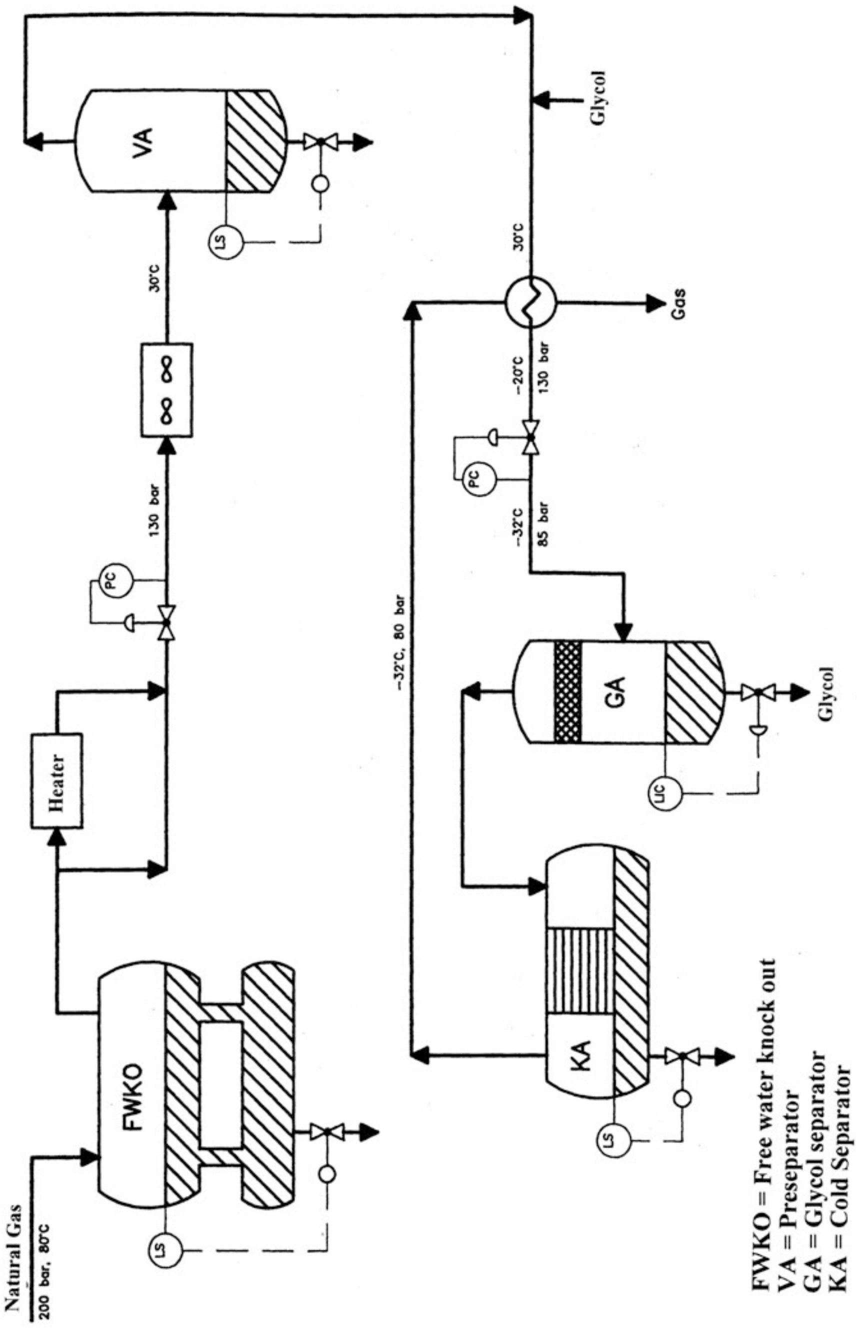


Dimensioning of a horizontal separator

11.6 Droplet Separation at High Pressures [6]

A typical application for demisters operating in the high-pressure sector is the separation of glycol droplets from natural gas at pressures of 80–200 bar.

A **flow diagram of an LTS unit** with cooling by Joule–Thomson release, for the condensation of higher boiling hydrocarbons and water, is shown in Fig. 11.5.



FWKO = Free water knock out
VA = Preseparator
GA = Glycol separator
KA = Cold Separator

Fig. 11.5 LTS plant for natural gas dehydration

In order to avoid pluggages of hydrate formation glycol is dosed and is recovered using demisters.

Often the separated liquid consisting of water, glycol, and hydrocarbons causes problems due to foaming and formation of emulsions, leading to residence times of 20–30 min being required for the liquid.

The droplet fall velocities at pressures of 40–100 bar are listed in Table 11.1. The falling velocities are calculated for the following physical data.

$$\varrho_G = 0.8\ \mathrm{kg/m_N^3} \quad \varrho_{Fl} = 850\ \mathrm{kg/m^3} \quad \eta_G = 15 * 10^{-6}\ \mathrm{Pa}$$

Table 11.1 Droplet fall velocities at different pressures

Droplet size (μm)	Falling velocities (m/s) at different pressures			
	(40 bar)	(60 bar)	(80 bar)	(100 bar)
40	0.0391	0.0343	0.0312	0.0289
60	0.0622	0.0546	0.0497	0.0459
100	0.1110	0.0979	0.089	0.0824
200	0.246	0.216	0.197	0.182
300	0.391	0.344	0.312	0.289

The dimensioning of separators often is carried out with the so-called “practical formula”, for instance according to Campbell’s “Gas Conditioning” [6] for gas throughput.

Vertical separators:

$$Q = 135.6 * D^2 * \frac{P}{P_N} * \frac{1}{z} * \frac{273}{T} * \sqrt{\frac{\varrho_{Fl} - \varrho_G}{\varrho_G}}\,(\mathrm{m^3/h}) \tag{11.9}$$

Horizontal separators:

$$Q = 304.5 * D^2 * \frac{P}{P_N} * \frac{1}{z} * \frac{273}{T} * \sqrt{\frac{\varrho_{Fl} - \varrho_G}{\varrho_G}}\,(\mathrm{m^3/h}) \tag{11.10}$$

Q = gas capacity (m_N^3/h)
P = operating pressure (bar)
P_N = normal pressure = 1013 bar
z = compressibility
D = separator diameter (m)

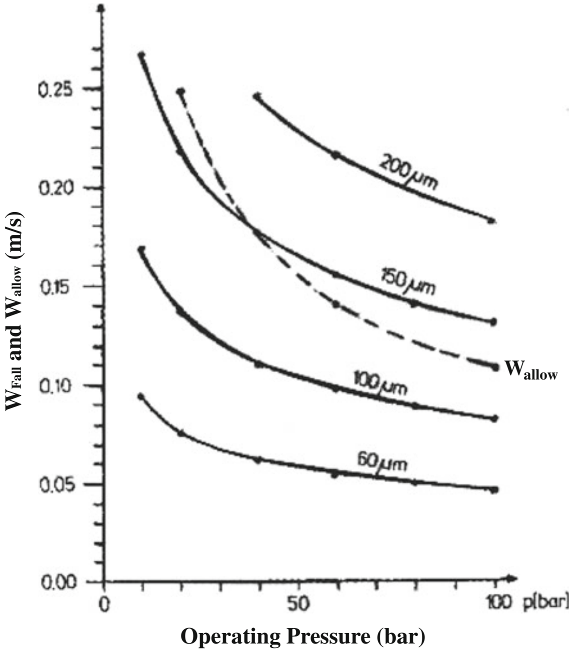


Fig. 11.6 Droplet falling velocity and allowable flow velocity as a function of the pressure in vertical separators

Vertical separators

Figure 11.6 shows the falling velocities of droplets with 60, 100, 150, and 200 µm diameters as a function of pressure.

→**With increasing pressure the falling velocity of the droplets becomes smaller!**

In the same Fig. 11.6 the calculated allowable flow velocities w_{allow} for gravity separators without demisters are drawn, calculated according Eq. (11.1) with K = 0.0335.

Conclusion: In this design only droplets >150 µm are separated.

Horizontal separators

The criterion for the droplet separation is a sufficient residence time for the gas so that the droplets can settle down when flowing through the separator.

Figure 11.7 shows the required residence times for droplet sizes 20, 40, 60, and 100 µm for different falling heights at 80 bar.

In addition, the effective residence time t_{eff} when streaming through a 6 m long separator is drawn in in Fig. 11.7 whereby the allowable flow velocity, according to Eq. (11.1) with K = 0.108, has been calculated.

Conclusion: Only droplets > 60 μm in a 6 m long horizontal separator are separated!

In comparison to the vertical separator the gas capacity of the horizontal separator is on the free gas cross sectional area higher.

Also, the droplet separation in a horizontal separator is better.

This shows the following comparison.

P = 80 bar	Vertical separator	Horizontal separator
w_{allow} (m/s)	0.121	0.392
Limiting droplet (μm)	150	60

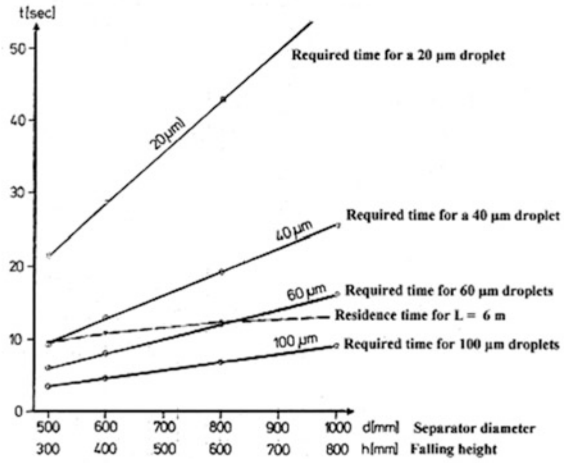


Fig. 11.7 The required residence time for different droplet sizes as a function of the falling heights in horizontal separators

In horizontal separators the falling height can be considerably shortened by the installation of parallel plates.

Thereby, the required falling time is reduced and the separation is improved.

$$t_{\text{Fall}} = \frac{h}{w_{\text{Fall}}}$$

$$\text{h} = \text{falling height (m)}$$

The required plate spacing h_{req} is calculated from the available residence time t_{avail} as follows:

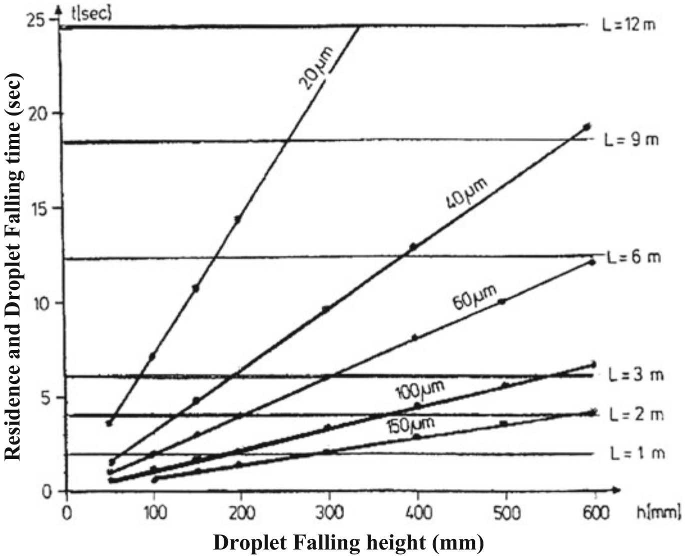


Fig. 11.8 Required residence times for different droplet sizes and separator lengths as a function of the falling height

$$h_{\mathrm{req}} = t_{\mathrm{avail}} * w_{\mathrm{Fall}}\ (\mathrm{m})$$

Figure 11.8 shows the residence times in a horizontal separator with 800 mm diameter and f_G = 0.804 for different separation lengths.

Additionally, the required droplet falling times for droplet sizes 20, 40, 60, 100 and 150 μm, as a function of the falling height h, are drawn in Fig. 11.8.

Using this figure the required falling height can be determined.

For instance, by installation of horizontal separation plates with h = 200 mm the separator length can be shortened from 6 to 3 m.

Thereby, the limiting droplet size of 60 μm is reduced to 40 μm so that a better droplet separation is achieved.

Recommended design at higher pressures.

Vertical separator

Gravity: K = 0.03 until 0.05 or 75% of the droplet falling velocity.
With wire mesh: K = 0.06.
With lamella separator: K = 0.10.

Horizontal separator

Gravity: K = 0.108.
With lamella separator: K = 0.15.

Example 11.6.1: Design of a demister for 100,000 m_N^3/h natural gas at 100 bar

$$V_{\text{operation}} = 435.75\ \text{m}^3/\text{h} \quad \varrho_G = 95.24\ \text{kg/m}^3 \quad \varrho_{Fl} = 800\ \text{kg/m}^3$$

Vertical separator

(a) Gravity separator without internals:

$$w_{\text{allow}} = 0.03 * \sqrt{\frac{800 - 95.24}{95.24}} = 0.0816\,\text{m/s}$$
$$w_{\text{des}} = 0.75 * 0.0816 = 0.0612\ \text{m/s} \quad \rightarrow D = 1.59\,\text{m}$$

(b) Design for 75% of the falling velocity of a 100 μ droplet:
First of all the falling velocities are calculated (see Appendix at the end of this chapter).

Droplet size (μm)	Droplet falling velocity (m/s)
50	0.0323
80	0.0553
90	0.0633
100	0.0714
115	0.0838
120	0.0880
150	0.1135
200	0.1570

$$w_{\text{Fall}} = 0.0714\ \text{m/s}$$
$$w_{\text{des}} = 0.75 * 0.0714 = 0.0536\ \text{m/s} \quad \rightarrow D = 1.7\ \text{m}$$

(c) Wire mesh separator:

$$w_{\text{allow}} = 0.06 * 2.722 = 0.163\ \text{m/s}$$
$$w_{\text{des}} = 0.75 * 0.163 = 0.122\ \text{m/s} \quad \rightarrow D = 1.12\,\text{m}$$

(d) Lamella separator:

$$w_{\text{allow}} = 0.1 * 2.722 = 0.272\ \text{m/s}$$
$$w_{\text{des}} = 0.75 * 0.272 = 0.204\ \text{m/s} \quad \rightarrow D = 0.87\,\text{m}$$

Horizontal separator with f_G = 50% gas cross section

(a) Gravity separator:

$$w_{\text{allow}} = 0.108 * 2.722 = 0.2938\,\text{m/s} \quad w_{\text{des}} = 0.75 * 0.2938 = 0.22\,\text{m/s}$$

$$f_G = 0.5(50\%\,\text{gas cross section}) \quad \rightarrow D = 1.18\,\text{m}$$

Checking:

$$F_{\text{ges}} = 1.1\,\text{m}^2 \quad F_G = 0.55\,\text{m}^2 \quad F_{\text{FL}} = 0.55\,\text{m}^2$$

$$w_G = \frac{435.75}{0.55 * 3600} = 0.22\,\text{m/s}\,\text{Gas velocity}$$

(b) Horizontal lamella separator:

$$w_{\text{allow}} = 0.15 * 2.722 = 0.408\ \text{m/s} \quad w_{\text{des}} = 0.75 * 0.408 = 0.306\ \text{m/s}$$
$$f_G = 0.5 \rightarrow D = 1\,\text{m}$$

(c) Check of the settling time for a gravity separator:

$$w_{\text{Fall}} = 0.0323\ \text{m/s}\,\text{for}\,50\,\mu\text{m}\,\text{droplet} \quad w_{\text{des}} = 0.75 * 0.0323 = 0.0242$$
$$h = 0.6\ \text{m}$$
$$t_{\text{Fall}} = \frac{0.6}{0.0242} = 24.8\,\text{s}$$
$$t_{\text{res}} = \frac{L}{w_G} = \frac{6}{0.22} = 27.3\,\text{s}$$

The residence time is sufficient for the settling of a 50 μ droplet!

(d) Reduction of the settling time by installation of parallel plates with h = 200 mm:

$$h = 0.2\,\text{m} \quad t_{\text{Fall}} = 0.2/0.0242 = 8.26\,\text{s}\,(50\,\mu\text{m}\,\text{droplet})$$

Allowable flow velocity at L = 3 m:

$$w_G = \frac{L}{t_{\text{Fall}}} = \frac{3}{8.26} = 0.36\,\text{m/s}$$
$$f_G = 0.5 \quad \rightarrow D = 0.66\,\text{m}$$

As a consequence of installation of a parallel plate package the diameter can be reduced from 1.2 to 0.7 m and the length from 6 to 4 m!

11.7 Fog Separation in Fibre Filters or by Droplet Enlargement

Fog is a disperse distribution of small liquid droplets in a gas phase.

The droplet sizes lie in the range 0.1–5 μm. These small droplets cannot be separated with normal wire mesh separators from the gas stream because the inertia principle does not hold due to their lack of mass.

The small droplets occur during the shock-cooling of gases with condensation in the gas phase or with chemical reactions in the gas phase to products whose dew points are exceeded, for instance, sulfuric, phosphoric, and nitric acid.

Fog formation occurs during condensation of vapour containing inert gas at large temperature differences between the cooling medium and the inert gas–vapour mixture, for instance, when cooling solvent containing exhaust gas streams with vaporizing liquid nitrogen.

The danger of fog formation increases with [7]:

- Lower cooling medium temperature.
- Increasing inlet partial pressure.
- Decreasing diffusion velocity or increasing mole weight.
- Increasing temperature conductivity.

11.7.1 Fog Separation in Fibre Filters

For the separation of very small droplets on fibres Brownian particle movement is utilized, the back and forth movement of fine components by diffusion.

The diffusion velocity increases with decreasing particle size.

A small particle of 0.1 μm diameter moves 15 times as much as a 5 μm particle.

By strong diffusion the probability that the small droplets collide with a fibre rises.

In order to give the particles sufficient time to diffuse to the fibres only small flow velocities of **5–20 cm/s** are allowed in diffusion separators.

The calculation of the allowable flow velocities follows, according to Sect. 11.2.1, Eq. (11.1h).

With increasing flow velocity and increasing fibre diameter the droplet separation deteriorates according to the diffusion principle.

When correctly designed, droplets up to 0.5 μm are separated.

Usually fibre filters in candle form are used as a diffusion separator (Fig. 11.9).

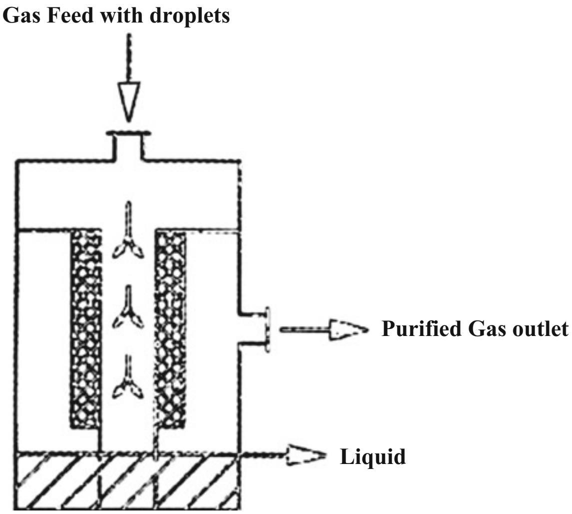


Fig. 11.9 Fog separation in fibre filters

When streaming through the microfibre tissues the separated liquid droplets in the fibre package agglomerate and run out downwards.

11.7.2 Droplet Enlargement by Condensation

Very small droplets with diameters <0.5 μm must first of all be enlarged in order to effect a separation.

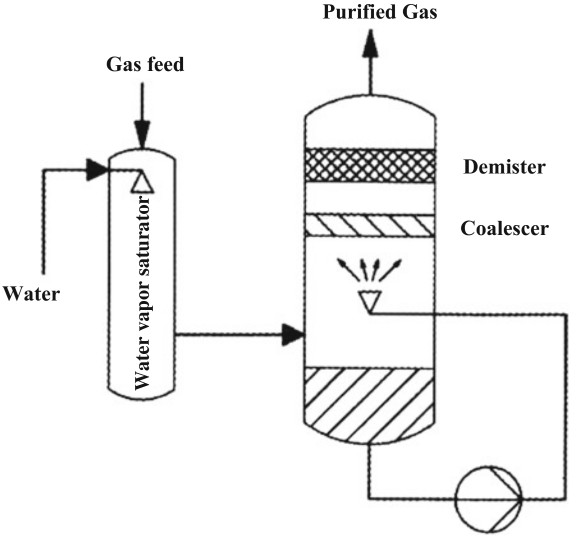


Fig. 11.10 Droplet enlargement by condensation

The process is shown in Fig. 11.10.

First, the raw gas stream is saturated with water vapour, for instance in a preceding column.

The thinest water droplets are then injected into this wet saturated gas stream which are unstably vaporized due to their high water vapour pressure at their bent surface areas.

Thereby, zones form with oversaturated water vapour.

As soon as a fog droplet passes through the wet saturated zone, water vapour condenses on the droplet and enlarges the diameter.

Next, the droplets which are enlarged by condensation stream through a coalescence film and come out with droplet diameters >6 μm.

For the coalescence of small droplets wire mesh or fibre tissue is used, operated under flooding conditions, meaning the droplets are entrained.

The droplets which are enlarged by condensation and coalescence are separated from the gas stream using wire mesh and fibre filters.

Appendix: Calculation of the Falling Velocity of Droplets in Air or Gas

First, the Archimedes number Ar, according to Formulas 11.11 and 11.11a, is calculated and therefore by using Eqs. (11.12a) and (11.12c) the Reynolds number Re is determined.

The falling velocity for the different Reynolds number regions is calculated with Formula 11.13a to 11.13c. Alternatively, the falling velocity can be calculated using the Eq. 11.13d for Re >1.

1. **Archimedes number *Ar***

$$Ar = \frac{d^3 \cdot g \cdot \rho_G(\rho_{Fl} - \rho_G)}{\eta_G^2} \tag{11.11}$$

$$Ar = \frac{Re^2 \cdot (\rho_{Fl} - \rho_G)}{Fr \cdot \rho_G} \tag{11.11a}$$

Fr = Froude number

2. **Reynolds number *Re***

$$Re = \frac{w_{Fall} \cdot d \cdot \rho_G}{\eta_G} \tag{11.12}$$

Because the falling velocity is unknown the Reynolds number has to be determined using the Archimedes number. The following relationships are valid for different regions:

$$Ar < 3.6 \quad Re = \frac{Ar}{18} \tag{11.12a}$$

$$3.6 < Ar < 83000 \quad Re = \left(\frac{Ar}{13.9}\right)^{1/1.4} \tag{11.12b}$$

$$Ar > 83000 \quad Re = 1.73 * \sqrt{Ar} \tag{11.12c}$$

3. **Falling velocity w_{Fall}**

$$w_{\mathrm{Fall}} = \frac{Re \cdot \eta_{\mathrm{G}}}{d \cdot \rho_{\mathrm{G}}} \quad (\mathrm{m/s}) \tag{11.13}$$

3.1 **For the region *Re* < 0.2 Stoke's Law is valid**

$$w_{\mathrm{Fall}} = \frac{d^2(\rho_{Fl} - \rho_G) \cdot g}{18 \cdot \eta_G} \quad (\mathrm{m/s}) \tag{11.13a}$$

3.2. **In the region *Re* = 500 to *Re* = 150,000 the relationships of Newton are valid**

$$w_{\mathrm{Fall}} = 5.48 \cdot \sqrt{\frac{d \cdot (\rho_{\mathrm{Fl}} - \rho_{\mathrm{G}})}{\rho_{\mathrm{G}}}} \quad (\mathrm{m/s}) \tag{11.13b}$$

3.3. **In the intermediate region 0.2 < *Re* < 500 the following equation is valid**

$$w_{\mathrm{Fall}} = \sqrt{\frac{4}{3} . \frac{d}{c} . \frac{g.(\rho_{Fl} - \rho_G)}{\rho_{\mathrm{G}}}} \quad (\mathrm{m/s}) \qquad C = 18.5/Re^{0.6} \tag{11.13c}$$

3.4. **Alternatively, for *Re* > 1**

$$w_{\mathrm{Fall}} = \frac{0.153 \cdot g^{0.71} \cdot d^{1.143} \cdot (\rho_{\mathrm{fl}} - \rho_{\mathrm{G}})^{0.714}}{\rho_{\mathrm{G}}^{0.286} \cdot \eta^{0.429}} \quad (\mathrm{m/s}) \tag{11.13d}$$

d = droplet diameter (m)
g = acceleration of gravity (9.81 m^2/s)
η_{G} = gas viscosity (mPa)
ϱ_{G} = gas density (kg/m^3)
ϱ_{G} = liquid density (kg/m^3)

Example 1 $\boldsymbol{d = 0.1\,\mathrm{mm} \quad \rho_G = 1.2\,\mathrm{kg/m^3} \quad \eta_G = 0.015\,\mathrm{mPa} \quad \rho_{Fl} = 1.000\,\mathrm{kg/m^3}}$
Checking of the falling velocity using Eq. (11.13c):

$$w_{\mathrm{Fall}} = \sqrt{\frac{4}{3} \cdot \frac{0.1 \cdot 10^{-3}}{10.48} \cdot \frac{9.81 \cdot (1000 - 1.2)}{1.2}} = 0.32\,\mathrm{m/s}$$

$$C = 18.5/2.575^{0.6} = 10.48$$

$$Ar = \frac{(0.6 \cdot 10^{-3})^3 \cdot 9.81 \cdot 1.2(1000 - 1.2)}{(15 \cdot 10^{-6})^2} = 52.26$$

$$Re = \left(\frac{52.26}{13.9}\right)^{1/14} = 2.575$$

$$w_{\mathrm{Fall}} = \frac{2.575 \cdot 15 \cdot 10^{-6}}{0.1 \cdot 10^{-3} \cdot 1.2} = 0.32\,\mathrm{m/s}$$

Example 2: Data as in Example 1, but $\boldsymbol{\rho_G}$ = 0.1 kg/m^3

$$Ar = 4.359 \quad Re = 0.436$$

$$w_{\mathrm{Fall}} = \frac{0.436 \cdot 15 \cdot 10^{-6}}{0.1 \cdot 10^{-3} \cdot 0.1} = 0.65\,\mathrm{m/s}$$

Example 3: Data as in Example 1, but $\boldsymbol{\rho_G}$ = 10 kg/m^3

$$Ar = 431.6 \quad Re = 11.64$$

$$w_{\mathrm{Fall}} = \frac{11.64 \cdot 15 \cdot 10^{-6}}{0.1 \cdot 10^{-3} \cdot 10} = 0.17\,\mathrm{m/s}$$

Conclusion Falling velocity increases with decreasing gas density (in a vacuum)!

Example 4: Check of Example 1 using Eq. (11.13d)

$$w_{\mathrm{Fall}} = \frac{0.153 * 9.81^{0.71} * 0.0001^{1.143} * (1000 - 1.2)^{0.714}}{1.2^{0.286} * (15 * 10^{-6})^{0.429}}$$

$$w_{\mathrm{Fall}} = 0.32\,\mathrm{m/s}$$

Example 5: Check of Example 2 using Eq. (11.13c)

$$w_{\mathrm{Fall}} = \sqrt{\frac{4}{3} \cdot \frac{0.1 \cdot 10^{-3}}{30.44} \cdot \frac{9.81 \cdot (1000 - 0.1)}{0.1}} = 0.65\,\mathrm{m/s}$$

$$c = 18.5/0.436^{0.6} = 30.44$$

Example 6: Data as in Example 1, but d = 2 mm

$$Ar = \frac{(2 \cdot 10^{-3})^3 \cdot 9.81 \cdot 1.2(1000 - 1.2)}{(15 \cdot 10^{-6})^2} = 418{,}058$$

$$Re = 1.73 \cdot \sqrt{418058} = 1118.6$$

$$w_{\mathrm{Fall}} = 1118.6 \cdot \frac{15 \cdot 10^{-6}}{2 \cdot 10^{-3} \cdot 1.2} = 7\,\mathrm{m/s}$$

Check of the falling velocity using Eq. (11.13b):

$$w_{\mathrm{Fall}} = 5.48 \cdot \sqrt{\frac{0.002 \cdot (1000 - 1.2)}{1.2}} = 7\,\mathrm{m/s}$$

Check of the Archimedes number using Eq. (11.11a):
Fr = Froude number

Table 11.2 ρ_G = 1.2 kg/m^3 ρ_{Fl} = 995 kg/m^3η_G = 0.018 mPa

d (μm)	Ar –	Re –	w_{Fall} (m/s)
100	36.1	1.977	0.297
200	288.9	8.73	0.65
300	974.9	20.82	1.04
400	2310.9	38.57	1.44
500	4513.5	62.22	1.87
600	7799.3	91.96	2.29
800	18,487.3	170.34	3.19
1000	36,108	274.8	4.12

Table 11.3 $\rho_G = 0.1\ \mathrm{kg/m^3}$ $\rho_{Fl} = 995\ \mathrm{kg/m^3}$ $\eta_G = 0.018$ mPa

d (μm)	Ar –	Re –	w_{Fall} (m/s)
100	3.01	0.167	0.6
200	24.1	1.48	1.33
300	81.3	3.53	2.1
400	192.7	6.54	2.9
500	376.5	10.55	3.79
600	650.7	15.55	4.67
800	1542	28.89	6.5

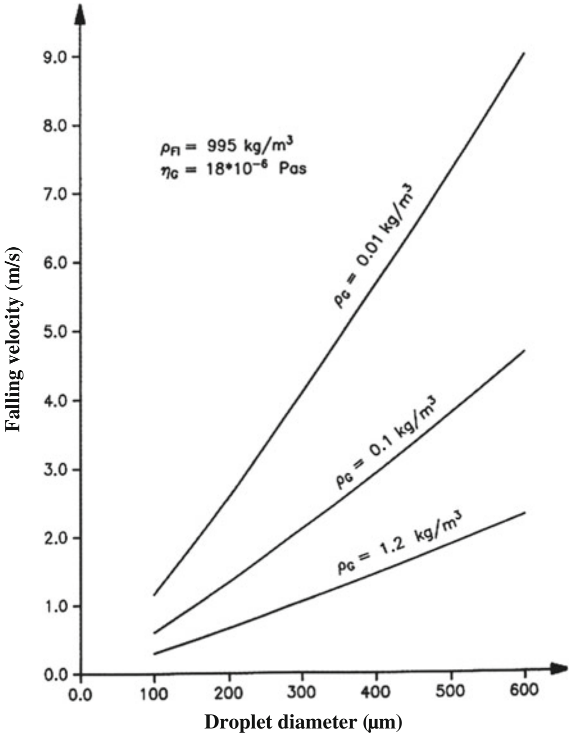


Fig. 11.11 Falling velocities of water droplets in air rat different gas densities

$$Fr = \frac{w^2}{d \cdot g} = \frac{7^2}{0.002 \cdot 9.81} = 2497.4$$

$$Ar = \frac{1118.6^2 \cdot (1000 - 1.2)}{2497.4 \cdot 1.2} = 417013$$

Results tables

See Tables 11.2 and 11.3; Fig. 11.11.

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