The ChemSep Book

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Chapter 18

Design Models for Distillation Columns

This chapter serves as a guide to the correlations in ChemSep for estimating mass transfer coefficients and the pressure drop in distillation (and absorption) columns. The methods used in Design Mode to determine column design parameters also are discussed in detail. The chapter ends with the comparison of experimental distillation data and nonequilibrium model simulations.

18.1 Mass Transfer Coefficient Correlations

Table 18.1 provides a summary of the available correlations for trays and packings; the various correlations are discussed in more detail below. Recommended models are shown in boldface.

18.1.1 Trays

Binary mass transfer coefficients (MTC’s) can be computed from the Number of Transfer Units (NTU’s = N) by:

\[
\begin{align*}
  k^V &= \frac{N^V}{t_V a^V} \quad \text{(18.1)} \\
  k^L &= \frac{N^L}{t_L a^L} \quad \text{(18.2)}
\end{align*}
\]
Table 18.1: Available mass transfer coefficient correlations per internals type

<table>
<thead>
<tr>
<th>Bubble-Cap tray</th>
<th>Sieve tray</th>
<th>Valve tray</th>
<th>Dumped packing</th>
<th>Structured packing</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIChe</td>
<td>AIChe</td>
<td>AIChe</td>
<td>Onda 68</td>
<td>Bravo 85</td>
</tr>
<tr>
<td>Hughmark</td>
<td>Chan-Fair</td>
<td>Bravo 82</td>
<td>Bravo 92</td>
<td>Bravo 92</td>
</tr>
<tr>
<td>Zuiderweg</td>
<td>Chen-Chuang</td>
<td>Billet 92</td>
<td>Billet 92</td>
<td>...</td>
</tr>
<tr>
<td>Harris</td>
<td>Bubble-Jet</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
</tbody>
</table>

where the vapor and liquid areas are calculated with

\[ a^V = a_d/\epsilon h_f \]  \hspace{1cm} (18.3)
\[ a^L = a_d/\alpha h_f \]  \hspace{1cm} (18.4)

the interfacial area density may be estimated from Zuiderweg’s (1982) method (see below).

AIChe One of the oldest methods for estimating numbers of transfer units came from the AIChe tray efficiency research program of the 1950s. The correlations can be used for sieve trays, valve trays, and bubble-cap trays.

\[ N^V = (0.776 + 4.57h_w - 0.238F_s + 104.8Q_L/W_l)/\sqrt{Sc^V} \]  \hspace{1cm} (18.5)
\[ N^L = 19700\sqrt{D^L}(0.4F_s + 0.17)t_L \]  \hspace{1cm} (18.6)

where

\[ F_s = u_s\sqrt{\rho^V} \]  \hspace{1cm} (18.7)
\[ Sc^V = \eta^V/\rho_i^V D^V \]  \hspace{1cm} (18.8)
\[ t_L = h_LZW_l/Q_L \]  \hspace{1cm} (18.9)

The clear liquid height \( h_L \) is computed from a correlation due to Bennett et al. (1983):

\[ h_L = \alpha_e (h_w + C(Q_L/\alpha_e W_l)^{0.67}) \]  \hspace{1cm} (18.10)
\[ \alpha_e = \exp(-12.55(u_s(\rho^V/(\rho^L - \rho^V))^{0.5})^{0.91}) \]  \hspace{1cm} (18.11)
\[ C = 0.50 + 0.438\exp(-137.8h_w) \]  \hspace{1cm} (18.12)
The number of transfer units for the vapor phase is:

\[
N^V = \frac{(10300 - 8670FF)FF\sqrt{DVt_V}}{\sqrt{h_L}}
\]  
(18.13)

\[
t_V = (1 - \alpha_e)\frac{h_L}{(\alpha_e u_s)}
\]  
(18.14)

The AIChE correlation is used for the number of transfer units for the liquid phase. \((h_L\) and \(\alpha_e\) also are computed with the correlation of Bennett et al.).

The vapor phase mass transfer coefficient is

\[
k^V = 0.13/p_V^V - 0.065/(p_V^V)^2
\]  
(18.15)

Note that \(k^V\) is independent of the diffusion coefficient. The liquid mass transfer coefficient is computed from either:

\[
k^L = 2.6 \times 10^{-5} (\eta^L)^{-0.25}
\]  
(18.16)

or

\[
k^L = 0.024(D^L)^{0.25}
\]  
(18.17)

The interfacial area in the spray regime is computed from:

\[
a_dh_f = 40 \frac{U_s^2 \rho_V^V h_L FP}{\sigma}^{0.37}
\]  
(18.18)

and in the froth-emulsion regime from:

\[
a_dh_f = 43 \frac{U_s^2 \rho_V^V h_L FP}{\sigma}^{0.37}
\]  
(18.19)

The transition from the spray to mixed froth-emulsion flow is described by:

\[
FP > 3bh_L
\]  
(18.20)

where \(b\) is the weir length per unit bubbling area:

\[
b = W_l/A_b
\]  
(18.21)

The clear liquid height is given by:

\[
h_L = 0.6h_w^{0.5}(pFP/b)^{0.25}
\]  
(18.22)

The numbers of transfer units are given by:

\[
N^V = (0.051 + 0.0105F_s)\sqrt{\frac{\rho_L}{F_s}}
\]  
(18.23)

\[
N^L = (-44 + 10.7747 \times 10^4 Q_L/W_l + 127.1457 F_s)\sqrt{D_L A_{bub}/Q_L}
\]  
(18.24)
Harris The numbers of transfer units are given by:

\[
N^V = \frac{0.3 + 15G}{\sqrt{Sc_G}} \quad (18.25)
\]

\[
N^L = \frac{5 + 10t_L(1 + 0.17(0.82F_s - 1)(39.3h_w + 2))}{\sqrt{Sc_L}} \quad (18.26)
\]

Chen-Chuang The numbers of transfer units for the vapor is:

\[
t^V = \frac{h_1}{u_s} \quad (18.27)
\]

\[
F_s = U_s\sqrt{\rho V} \quad (18.28)
\]

\[
N^V = 11 \frac{1}{\eta_{L}^{0.1}\beta_{L}^{0.14}} \left( \frac{\rho_L F_s^2}{\sigma^2} \right)^{1/3} \sqrt{D_V t_V} \quad (18.29)
\]

and for the liquid

\[
t_L = \frac{\rho_L t_V}{\rho V} \quad (18.30)
\]

\[
N^L = 14 \frac{1}{\eta_{L}^{0.1}\beta_{L}^{0.14}} \left( \frac{\rho_L F_s^2}{\sigma^2} \right)^{1/3} \left( \frac{V}{L} \right) \sqrt{D_L t_L} \quad (18.31)
\]

Bubble-Jet This is a combination of a theoretical model described by Taylor and Krishna (1993) and empirical models (Prado, 1986, Prado and Fair, 1990) to determine bubble sizes and velocities.

18.1.2 Random Packings

OTO-68 Onda et al. (1968) \{parameters \(a_p, d_p, \sigma_c\}\} developed correlations of mass transfer coefficients for gas absorption, desorption, and vaporization in random packings. The vapor phase mass transfer coefficient is obtained from

\[
k^V = A\Re_{V}^{0.7}Sc_{V}^{0.333}(a_pD_V)(a_p d_p)^{-2} \quad (18.32)
\]

where \(A = 2\) if \(d_p < 0.012\) and \(A = 5.23\) otherwise. Vapor and liquid velocities are calculated from

\[
u_V = VM^V / \rho^V A_t \quad (18.33)
\]

\[
u_L = LM^L / \rho^L A_t \quad (18.34)
\]

and Reynolds and Schmidt numbers defined by:

\[
\text{Re}_V = \frac{\rho^V u_V}{(\eta^V a_p)} \quad (18.35)
\]
\[ \text{Re}_L = \frac{\rho_L u_L}{(\eta^L a_p)} \quad (18.36) \]
\[ \text{Sc}_V = \frac{\eta^V}{(\rho_i^V D^V)} \quad (18.37) \]
\[ \text{Sc}_L = \frac{\eta^L}{(\rho_i^L D^L)} \quad (18.38) \]

The liquid phase mass transfer coefficient is
\[ k^L = 0.0051 \left( \text{Re}_L^f \right)^{2/3} \text{Sc}_L^{-0.5} (a_p d_p)^{0.4} \left( \frac{\eta^L g}{\rho^L} \right)^{1/3} \quad (18.39) \]
where \( \text{Re}_L^f \) is the liquid Reynolds number based on the interfacial area density
\[ \text{Re}_L^f = \frac{\rho_L u_L}{(\eta^L a_d)} \quad (18.40) \]

The interfacial area density, \( a_d \left( m^2/m^3 \right) \), is computed from
\[ a_d = a_p \left( 1 - \exp \left( -1.45 (\sigma_c/\sigma)^{0.75} \text{Re}_L^{0.1} \text{Fr}_L^{-0.05} \text{We}_L^{0.2} \right) \right) \quad (18.41) \]

where
\[ \text{Fr}_L = \frac{a_p u_L^2}{g} \quad (18.42) \]
\[ \text{We}_L = \frac{\rho_L u_L^2}{a_p \sigma} \quad (18.43) \]

**BF-82** Bravo and Fair (1982) [parameters \( a_p, d_p, \sigma_c \)] used the correlations of Onda et al. for the estimation of mass transfer coefficients for distillation in random packings but proposed an alternative relation for the interfacial area density:
\[ a_d = 19.78 (\text{Ca}_L \text{Re}_V)^{0.392} \sqrt{\sigma} H^{-0.4} a_p \quad (18.44) \]

where \( H \) is the height of the packed section and \( \text{Ca}_L \) is the capillary number
\[ \text{Ca}_L = \frac{u_L \eta^L}{\rho^L \sigma} \quad (18.45) \]

Since the interfacial area density is used in the calculation for the liquid phase Reynolds number the Bravo and Fair method will predict different mass transfer coefficients for the liquid phase.

**BS-92** Billet and Schultes (1992) [parameters \( a_p, \epsilon, C_{fL}, C_h, C_p, C_v, C_l \)] describe an advanced empirical/theoretical model which is dependent on the pressure drop/holdup calculation \( (C_h, C_p, C_{fL}) \). The correlation can be used for both
random and structured packings. Vapor and liquid phase coefficients are adjusted by parameters $C_v$ and $C_l$, bringing the total number of parameters to five. There are trends in the parameters that can be observed from the tabulated data. Unfortunately, no such generalization was done by Billet, making use of the model dependent on the availability of the parameters or experimental data. The mass transfer coefficients are computed from

$$
k^L = C_l \left( \frac{g ho_l}{\eta_l} \right)^{1/6} \sqrt{\frac{D_L}{d_h} \left( \frac{u_L}{a_p} \right)^{1/3}} \tag{18.46}
$$

$$
k^V = C_v \left( \frac{1}{\sqrt{\epsilon - h_t}} \right) \sqrt{\frac{a}{d_h} D^V (Re_V)^{3/4} (Sc_V)^{1/3}} \tag{18.47}
$$

with Reynolds and Schmidt numbers calculated as in the method of Onda et al.

The hydraulic diameter $d_h$ is

$$
d_h = 4 \epsilon / a_p \tag{18.48}
$$

and the liquid holdup fraction, $h_t$, is calculated as described below under the pressure drop section. The interfacial area density is given by:

$$
a_d = a_p (1.5 / \sqrt{a_p d_h})(u_L d_h \rho^L / \eta^L)^{-0.2} (u_L^2 \rho^L d_h / \sigma)^{0.75} (u_L^2 / gd_h)^{-0.45} \tag{18.49}
$$

### 18.1.3 Structured Packings

**BRF-85** Bravo et al. (1985) [parameters $a_p$, $\epsilon$, $B$, $h_c$, $S$, $D_{eq}$, $\theta$] published correlations for structured packings. This method is based on the assumption that the surface is completely wetted and that the interfacial area density is equal to the specific packing surface: $a_d = a_p$. The Sherwood number for the vapor phase is

$$
Sh_V = 0.0338 Re_V^{0.8} Sc_V^{0.333} \tag{18.50}
$$

and is defined by

$$
Sh_V = \frac{k^V d_{eq}}{D^V} \tag{18.51}
$$

The equivalent diameter of a channel is given by

$$
d_{eq} = B h_c \left[ 1/(B + 2S) + 1/2S \right] \tag{18.52}
$$

where $B$ is the base of the triangle (channel base), $S$ is the corrugation spacing (channel side), and $h_c$ is the height of the triangle (crimp height). The vapor phase Reynolds number is defined by

$$
Re_V = \frac{d_{eq} \rho^V (u_{V,eff} + u_{L,eff})}{\eta^V} \tag{18.53}
$$
The effective velocity of vapor through the channel, $u_{V,\text{eff}}$, is

$$u_{V,\text{eff}} = \frac{u_V}{(\epsilon \sin \theta)} \quad (18.54)$$

($u_V$ is the superficial vapor velocity, $\epsilon$ the void fraction, and $\theta$ the angle of the channel with respect to the horizontal). The effective velocity of the liquid is

$$u_{L,\text{eff}} = \frac{\Gamma}{2 \rho L} \left( \frac{(\rho L)^2 g}{3 \eta L \Gamma} \right)^{1/3} \quad (18.55)$$

where $\Gamma$ is the liquid flow rate per unit of perimeter

$$\Gamma = \rho L u_L / P \quad (18.56)$$

where $P$ is the perimeter per unit cross-sectional area, computed from

$$P = (4S + B)/Bh_c \quad (18.57)$$

The penetration model is used to predict the liquid phase mass transfer coefficients with the exposure time assumed to be the time required for the liquid to flow between corrugations (a distance equal to the channel side):

$$t_L = S/u_{L,\text{eff}} \quad (18.58)$$

$$k_L = 2 \sqrt{\frac{D_L}{\pi t_L}} \quad (18.59)$$

**BRF-92** Bravo et al. (1992) [parameters $a_p$, $\epsilon$, $S$, $\theta$, $F_{se}$, $K_2$, $C_e$, $dPdz_{\text{flood}}$] developed a theoretical model for modern structured packings. Four parameters can be supplied. However, the authors advise using a fixed value for the surface renewal correction ($C_e$), normally 0.9. They provide a relation for parameter $K_2$ as well:

$$K_2 = 0.614 + 71.35S \quad (18.60)$$

The mass transfer calculations depend on the pressure drop and holdup calculation. The effective area can be adjusted with the surface enhancement factor $F_{se}$, and the liquid resistance with a correction on the surface renewal following the penetration model (parameter $C_e$). Effective velocities are computed with

$$u_{L,\text{eff}} = \frac{u_L}{eh_1 \sin \theta} \quad (18.61)$$

$$u_{G,\text{eff}} = \frac{u_V}{\epsilon (1 - h_1) \sin \theta} \quad (18.62)$$

where $h_1$ is the fractional liquid holdup (see below at the section on pressure drop calculation). Reynolds numbers and liquid mass transfer coefficient is now calculated as in Bravo et al. (1985) but with

$$t_L = C_e S / u_{L,\text{eff}} \quad (18.63)$$
The vapor phase mass transfer coefficient is obtained from

\[ k_V = 0.054 \left( \frac{D^V}{S} \right) Re_V^{0.8} Sc_V^{1/3} \]  

(18.64)

where the equivalent diameter is replaced with the channel side \( S \) and a different coefficient is used. The assumption of a completely wetted packing is dropped. Instead, the interfacial area density is given by

\[
\alpha_d = F_t F_{sc} a_p
\]

(18.65)

\[
F_t = \frac{29.12 (We_L Fr_L)^{0.15} S^{0.359}}{Re_L^{0.2} \epsilon^{0.6} (\sin \theta)^{0.3} (1 - 0.93 \cos \gamma)}
\]

(18.66)

where \( \cos \gamma \) is equal to 0.9 for \( \sigma < 0.0453 \), otherwise it is computed from

\[
\cos \gamma = 5.211 \times 10^{-16.835 \sigma}
\]

(18.67)

Note that a switch point different from that used by Bravo et al. (1992) is employed to guarantee continuity in \( \cos \gamma \).

BS-92 Billet and Schultes (1992) [parameters \( a_p, \epsilon, C_{fl}, C_h, C_p, C_v, C_l \)] developed a model for both random and structured packings, see the section on random packings above.

### 18.2 Pressure Drop Models

There are as many ways to compute tray pressure drops as there to estimate mass transfer coefficients. For packings there is a move away from the use of generalized pressure drop charts (GPDC) to more theoretically based correlations. We have chosen to employ the most recently published models. For packings there are at least 7 methods available (see Table 18.2). For packings operating above the loading point \((FF > 0.7)\) we advise the use of models that take the correction for the liquid holdup into account, such as the SBF-89. However, disadvantage is that these models can have complex (imaginary) solutions, especially at high fractions of flood. This can cause non-convergence! The Lev-92 model can be an alternative for it includes a dependence on the liquid flow rate to simulate the increased pressure drop at loading conditions. When the pressure drop is specified as fixed, it is assumed zero.
Table 18.2: Pressure drop correlations per internals type

<table>
<thead>
<tr>
<th>Bubble-Cap</th>
<th>Sieve</th>
<th>Valve</th>
<th>Dumped packing</th>
<th>Structured packing</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
<td>Fixed</td>
</tr>
<tr>
<td>Estimated</td>
<td>Estimated</td>
<td>Estimated</td>
<td>Ludwig 79</td>
<td>Billet 92</td>
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<td></td>
<td></td>
<td></td>
<td>Leva 92</td>
<td>Bravo 86</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>Billet 92</td>
<td>Stichlmair 89</td>
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<td>Bravo 92</td>
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</tr>
</tbody>
</table>

18.2.1 Tray pressure drop Estimation

The liquid heights on the trays are evaluated from the tray pressure drop calculations. The wet tray pressure drop liquid height is calculated from:

$$h_{wt} = h_d + h_l$$

(18.68)

where $h_d$ is the dry tray pressure drop liquid height and $h_l$ the liquid height:

$$h_l = h_{cl} + h_r + \frac{h_{tg}}{2}$$

(18.69)

The clear liquid height, $h_{cl}$, is calculated with

$$h_{cl} = \alpha h_w + h_{ow}$$

(18.70)

where the liquid fraction of the froth, $\alpha$, is computed with the Barker and Self (1962) correlation:

$$\alpha = \frac{0.37h_w + 0.012F_s + 1.78Q_L/W_l + 0.024}{1.06h_w + 0.035F_s + 4.82Q_L/W_l + 0.035}$$

(18.71)

The choice of correlation for the liquid fraction turns out to be important as certain correlations are dynamically unstable. The height of liquid over the weir, $h_{ow}$, is computed by various correlations for different types of tray weirs (see Perry’s Handbook, 1984) and a weir factor ($F_w$) correction (see Smith, pp. 487) is employed. For example for a segmental weir:

$$h_{ow} = 0.664F_w \left( \frac{Q_L}{W_l} \right)^{2/3}$$

(18.72)

$$w = \frac{W_l}{D_c}$$

(18.73)

$$F_w^3 = \frac{w^2}{1 - (F_ww(\left( \frac{1.668Q_L}{W_l^2} \right)^{2/3} + \sqrt{1 - w^2})^2)}$$

(18.74)
where $Q_L$ is the volumetric flow over the weir per weir length. The residual height, $h_r$, is only taken into account for sieve trays. Bennett’s method (see Lockett, 1986, pp. 81) is:

$$h_r = \left( \frac{6}{1.27\rho_L} \right) \left( \frac{\sigma V}{g} \right)^{2/3} \left( \frac{\rho_L - \rho_v}{d_h} \right)^{1/3}$$  \hspace{1cm} (18.75)

Dry tray pressure, $h_d$, is calculated with:

$$h_d = K \frac{\rho G}{\rho_L} u_h^2$$  \hspace{1cm} (18.76)

$$K = \frac{\xi}{2g}$$  \hspace{1cm} (18.77)

where the orifice coefficient $\xi$ for sieve trays is computed as described by Stichlmair and Mersmann (1978). For valve trays we use the method of Klein (1982) as described in Kister (1992, pp. 309–312) where $K$ is given for the cases with the valves closed or open. It is extended for double weight valve trays as discussed by Lockett (1986, pp. 82–86). The dry tray pressure drop is corrected for liquid fractional entrainment.

The froth density is computed from

$$h_f = \frac{h_{cl}}{\alpha}$$  \hspace{1cm} (18.78)

The liquid gradient, $h_{lg}$, is estimated from a method due to Fair (Lockett, 1986, pp. 72):

$$R_h = \frac{W h_f}{W + 2h_f}$$  \hspace{1cm} (18.79)

$$U_f = \frac{Q_L}{Wh_{cl}}$$  \hspace{1cm} (18.80)

$$Re_f = \frac{R_h U_f \rho_L}{\eta_L}$$  \hspace{1cm} (18.81)

$$f = 7 \times 10^4 h_w Re_f^{-1.06}$$  \hspace{1cm} (18.82)

$$h_{lg} = \frac{Z f U_f^2}{g R_h}$$  \hspace{1cm} (18.83)

where $W$ is the average flow-path width for liquid flow, and $Z$ the flow path length. The height of liquid at the tray inlet is:

$$h_i = \sqrt{\left(\frac{2}{g} \left(\frac{Q_L}{W_f}\right)^2 \left(\frac{1}{h_{cl}} - \frac{1}{h_c}\right) + \frac{2\alpha h_f^2}{3}\right)}$$  \hspace{1cm} (18.84)

where $h_c$ is the height of the clearance under the downcomer. The pressure loss under downcomer (expressed as a liquid height) is

$$h_{ude} = \left(\frac{1}{2g}\right) \left(\frac{Q_L}{C_d W_f h_c}\right)^2$$  \hspace{1cm} (18.85)
where \( C_d = 0.56 \) according to Koch design rules. The height of liquid in the downcomer can now be calculated with the summation:

\[
h_{db} = h_w + h_i + h_{udc} \tag{18.86}
\]


### 18.2.2 Random packing Pressure Drop Correlations

For packings the vapor and liquid mass flow per cross sectional area (\( kg/m^2s \)) and velocities (\( m/s \)) are:

\[
L_a = LM^L/A_t \tag{18.87}
\]
\[
V_a = VM^V/A_t \tag{18.88}
\]
\[
u_L = L_a/\rho^L \tag{18.89}
\]
\[
u_V = V_a/\rho^V \tag{18.90}
\]

**Lud-79** Ludwig (1979) [parameters \( A, B \)] supplied a simple empirical equation for the pressure drop requiring two fitted parameters (see Wankat, 1988, 420–428):

\[
\frac{\Delta p}{\Delta z} = 3.281242A \left( \frac{0.2048V_a}{0.06243L_a} \right)^2 10^{B(0.06243L_a)} \tag{18.91}
\]

where 3.281242, 0.2048, and 0.06243 are conversion factors so that we can use \( A \) and \( B \) parameters from Wankat. Its accuracy is limited since the influence of physical properties such as viscosity or surface tension on \( A \) and \( B \) are not included. Even more, the fitted parameters can be flow regime dependent. The loading regime is not well described with the simple exponential term.

**Lev-92** Leva (1992) [parameter \( F_p \)] devised a modified version of the Generalized Pressure Drop Correlation (GPDC) presented long ago by Leva (1951). The GPDC has been the standard design method for decades. Some modifications that were actually simplifications made the GPDC lose its popularity. The function worked back from the GPDC and limiting \((L_a = 0)\) behavior is (in SI units):

\[
\frac{\Delta p}{\Delta z} = 22.3F_p(\eta^L)^{0.2} \phi V_a^2 \frac{10^{0.035L_a\phi}}{g\rho^V} \tag{18.92}
\]

with \( \phi = \rho_{water}/\rho_l = 1000/\rho_l \). This expression is similar to the Ludwig (1979) equation with corrections for the influence of the liquid density and viscosity. The only parameter is the packing factor \( F_p \) that can be obtained from
dry pressure drop experiments (see Leva, 1992) or estimated from the specific packing area over the void fraction cubed. Again, the loading regime is not well described with the simple exponential term. This model is the default method for random packings if no model is specified, since it requires only the packing factor.

SBF-89 Stichlmair et al. (1989) [parameters \( a_p, \epsilon, C_1, C_2, C_3 \)] published a semi-empirical method from an analogy of the friction of a bed of particles and the pressure drop. It contains a correction for the actual void fraction corrected for the holdup, that is dependent on the pressure drop. It is, therefore, an iterative method. It is suitable for both random and structured packings, but there are few published parameters for structured packings. The pressure drop is

\[
\frac{\Delta p}{\Delta z} = 0.75 f_0 (1 - \epsilon_p) \rho V U^2 / (d_p \epsilon_p^{4.65})
\]  

(18.93)

where the void fraction of the irrigated bed, equivalent packing diameter, Reynolds number, and friction factor for a single particle are:

\[ \epsilon_p = \epsilon - h_t \]  

(18.94)

\[ d_p = 6(1 - \epsilon_p) a_p \]  

(18.95)

\[ \text{Re}_V = \frac{u_V d_p \rho V}{\eta V} \]  

(18.96)

\[ f_0 = \frac{C_1}{\text{Re}_V} + \frac{C_2}{\sqrt{\text{Re}_V}} + C_3 \]  

(18.97)

The iterations are started by assuming a dry bed for which \( \epsilon_p = \epsilon \) and the holdup fraction is computed with the liquid Froude number:

\[ \text{Fr}_L = \frac{u_L^2 a_p}{g \epsilon^{4.65}} \]  

(18.98)

\[ h_t = 0.555 \text{Fr}_L^{1/3} \]  

(18.99)

The liquid holdup is limited to 0.5 in order to handle flooding.

BS-92 Billet and Schultes (1992) and Billet’s monograph (1979) [parameters \( a, \epsilon, C_{fl}, C_h, C_p \)] include a model with a comprehensive list of packing data and fitted parameters. The method corrects for the holdup change in the loading regime but employs an empirical exponential term, and is not iterative.

Packing dimension, hydraulic diameter and F-factor are

\[ d_p = \frac{6(1 - \epsilon)}{a_p} \]  

(18.100)

\[ d_h = \frac{4 \epsilon}{a_p} \]  

(18.101)

\[ F_s = \frac{u_V \sqrt{\rho V}}{g} \]  

(18.102)

Liquid Reynolds and Froude number are

\[ \text{Re}_{L} = \frac{u_L \rho_L}{\eta^L a_p} \]  

(18.103)

\[ \text{Fr}_{L} = \frac{u_L^2 a_p}{g} \]  

(18.104)
If $Re_L < 5$ then
\[ q = C_h Re_L^{0.15} Fr_L^{0.1} \] (18.105)
else
\[ q = 0.85 C_h Re_L^{0.25} Fr_L^{0.1} \] (18.106)

\[ h_{t,1} = \left( \frac{12\eta L a_p^2 u_L}{\rho g} \right)^{1/3} \] (18.107)
\[ h_{t,2} = h_{t,1} q^{2/3} \] (18.108)
\[ h_{t,fl} = 0.3741 \left( \frac{\eta L \rho}{\eta w \rho L} \right)^{0.05} \] (18.109)

\[ \epsilon_{fl} = \left( \frac{u_L}{u_V} \right) \left( \frac{\rho L}{\rho V} \right) \left( \frac{\eta L}{\eta V} \right)^{0.2} \] (18.110)
\[ \epsilon_{fl} = \frac{g}{(C_{fl}^2 \epsilon_{fl})^{0.39}} \] (18.111)
\[ u_{v,fl} = \sqrt{2g/\epsilon_{fl}(\epsilon - h_{t,fl})^{1.5}} \sqrt{h_{t,fl}/a_p} \sqrt{\rho L / \rho V} / \sqrt{\epsilon} \] (18.112)

if $u_V > u_{V,fl}$ then $h_t = h_{t,fl}$ else
\[ h_t = h_{t,2} + (h_{t,fl} - h_{t,2})(u_V / u_{V,fl})^{1.3} \] (18.113)

The pressure drop is then
\[ K_1 = 1 + (2/3)(1/1 - \epsilon)(d_p / D_c) \] (18.114)
\[ Re_V = u_V d_p \rho V / (1 - \epsilon) \eta V K_1 \] (18.115)
\[ \phi_{t1} = C_p (64 / Re_V + 1.8 / Re_V^{0.08}) \exp(Re_L / 200)(h_t / h_{t,1})^{0.3} \] (18.116)
\[ \frac{\Delta p}{\Delta z} = \phi_{t1}(a_p / (\epsilon - h_t)^3)(F_{eff}^2 / 2)K_1 \] (18.117)

### 18.2.3 Structured packing Pressure Drop Correlations

**BRF-86** Bravo et al. [parameters $\epsilon$, $S$, $\sin(\theta)$, $C_3$] compute the pressure drop from an empirical correlation with one fitted parameter, called $C_3$. This model is unsuitable for pressure drop correlations in the loading regime ($FF > 0.7$). The pressure drop per height of packing is:

\[ \frac{\Delta p}{\Delta z} = (0.171 + 92.7 / Re_V)(\rho V u_{V,eff}^2 / d_{eq}) \left( \frac{1}{1 - C_3 \sqrt{Fr}} \right)^5 \] (18.118)
where

\[
\begin{align*}
  u_{V,\text{eff}} &= u_V/(\varepsilon \sin \theta) \quad (18.119) \\
  \text{Re}_V &= \frac{d_{eq} \rho^V u_{V,\text{eff}}}{\eta^V} \quad (18.120) \\
  \text{Fr}_L &= \frac{u_L^2}{d_{eq} g} \quad (18.121)
\end{align*}
\]

SBF-92 Stichlmair et al. (1989) [parameters \(a, \varepsilon, C_1, C_2, C_3\)] published a semi-empirical method, see the section on pressure drop of random packed columns above.

BRF-92 Bravo et al. (1992) [parameters \(a_p, \varepsilon, S, \theta, K_2, dPdz_{\text{flood}}\)] developed a theoretical model developed for modern structured packings. Two parameters need to be supplied for pressure drop calculations, however, the \(K_2\) parameter was fitted by the authors. The pressure of flooding (\(dPdz_{\text{flood}}\)) can be easily obtained from data or via Kister’s correlation and the packing factor. The model includes an iterative method with a dependence of the liquid holdup on the pressure drop (and vice versa). The Weber, Froude, and Reynolds numbers are

\[
\begin{align*}
  \text{We}_L &= \frac{u_L^3 \rho^L S}{\sigma} \quad (18.122) \\
  \text{Fr}_L &= \frac{u_L^2}{(Sg)} \quad (18.123) \\
  \text{Re}_L &= \frac{u_L S \rho^L}{\eta^L} \quad (18.124)
\end{align*}
\]

The effective \(g\) (as a function of \(h_t\)) is obtained from:

\[
geff = \left(1 - \frac{dPdz}{dPdz_{\text{flood}}}\right) \frac{(\rho^L - \rho^V)}{\rho^L} g \quad (18.125)
\]

Then \(F_t\) (see above), \(h_t\), and \(dPdz\) are computed

\[
\begin{align*}
  h_t &= \left(\frac{AF_t}{S}\right)^{2/3} \left(\frac{3\eta^L u_L}{\rho^V \sin \theta \varepsilon g_{\text{eff}}}\right)^{1/3} \quad (18.126) \\
  A &= \frac{0.177 \rho^V}{S \epsilon^2 (\sin \theta)^2} \quad (18.127) \\
  B &= \frac{88.774 \eta^V}{S^2 \epsilon \sin \theta} \quad (18.128) \\
  \frac{\Delta \rho}{\Delta z} &= (Au_V^2 + B u_V) \left(\frac{1}{1 - K_2 h_t}\right)^5 \quad (18.129)
\end{align*}
\]

The calculation is repeated until pressure drop converges or when it becomes larger than the pressure drop at flood. There can be problems converging this method.

BS-92 Billet and Schultes (1992) and Billet’s monograph (1979?) [\(a_p, \varepsilon, C_{fl}, C_h, C_p\)] See the section on pressure drop of random packed columns above.
18.3 Entrainment and Weeping

Entrainment and weeping flows (for trays only) change the internal liquid flows and influence the performance of the column internals. **ChemSep currently does not support the handling of these flows.** This is due to the fact that few entrainment models behave properly. Neither is the effect of the entrainment and weeping flows on the mass transfer properly taken into account.

Entrainment can be estimated from the fractional liquid entrainment from Hunt’s correlation and from Figure 5.11 of Lockett (1986) for sieve trays:

$$\phi_L = 7.75 \times 10^{-5} \left( \frac{0.073}{\sigma} \right) M_v \left( \frac{U_v}{T_s - 2.5 h_{cl}} \right)^{3.2}$$  \hspace{1cm} (18.130)

The weep factor is estimated from a figure from Smith (1963, p. 548), that was fitted to the following correlation

$$WF = 0.135 \phi \ln\left(34(H_w + H_{ow}) + 1\right) \left(\frac{H_d + H_r}{H_d + H_r} \right)$$  \hspace{1cm} (18.131)

where $\phi$ is the open area ratio.

18.4 Packing Flooding and Minimum Wetting

The fraction of flooding for packings is computed by dividing the superficial gas velocity by the gas velocity at flood. The latter is found in an iterative process from the pressure drop correlation (keeping the liquid to vapor ratio constant!) and the specified pressure drop of flood. If no flood pressure drop is specified it is computed from the packing factor with the Kister and Gill correlation. If no pressure drop model is selected, the Leva’s method is used, which also has the packing factor as only parameter.

The minimum operating conditions, similar to the weep point for tray operation, is set to the minimum wetting rate predicted by Schmidt (1979). Schmidt calculates a liquid falling number

$$C_L = 1633.6(0.062428 \rho_L)(1000\sigma)^3/(1000\eta_L)^4$$  \hspace{1cm} (18.132)

and the minimum wetting rate is (in USgal/min/ft²):

$$Q_{MW} = \frac{0.3182C_L^{2/3}(1 - \cos \phi)^{2/3}}{\sqrt{(1 - T_L)\alpha_p/0.3048}}$$  \hspace{1cm} (18.133)
where $\phi$ is the liquid contact angle and $T_L$ is the shear stress number:

$$T_L = 0.9FF^{-2.8}$$

(18.134)

with $FF$ as the fraction of flood. The contact angle for metals is $10^\circ$ (0.1745 rad).

To obtain contact angles for other packings the contact angle is assumed inverse proportional to the critical surface tension, $\sigma_c$. For metals we have $\sigma_c = 0.075$, so the contact angle is computed with

$$\phi = 0.1745 \left( \frac{0.075}{\sigma_c} \right)$$

(18.135)

With this approach we obtain higher minimum wetting rates for plastic packings than for metal packings. The minimum operating or ‘weep’ fraction $WF$ is then taken as

$$WF = \frac{Q_{MW}}{u_L}$$

(18.136)

where $u_L$ is the superficial liquid flow.

### 18.5 Column Design

Tray layout parameters that specify a complete design (for the calculation of mass transfer coefficients and pressure drops) are shown in Table 18.3. For packings only the column diameter and bed height are design parameters, other parameters (such as void fraction, nominal packing diameter, etc.) are fixed once the type of packing has been selected. The packed bed height must be specified since it determines the desired separation and the capacity.

A very important parameter in tray column design is the system factor (SF). It represents the uncertainty in design correlations with regard to phenomena that are currently still not properly modeled, such as foaming.

Different design methods can be employed:

- **Fraction of flooding**: this is the standard design method for trays, we have employed a modified version of the method published by Barnicki and Davis (1989).
- **Pressure drop**: this is the usual design method for packed columns, but is very useful as well for tray design with pressure drop constraints.

other design methods can be thought of: ones that minimize pressure drop and cost, or maximize flexibility and efficiency. ChemSep has a modular structure to allow different design methods to be implemented.
### Table 18.3: Tray layout data

<table>
<thead>
<tr>
<th>General (sieve) tray layout data:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Column diameter</td>
<td>Active area</td>
</tr>
<tr>
<td>Number of flow passes</td>
<td>Total hole area</td>
</tr>
<tr>
<td>Tray spacing</td>
<td>Downcomer area</td>
</tr>
<tr>
<td>Liquid flow path length</td>
<td>Weir length</td>
</tr>
<tr>
<td>Hole diameter</td>
<td>Weir height</td>
</tr>
<tr>
<td>Hole pitch</td>
<td>Deck thickness</td>
</tr>
<tr>
<td>Downcomer clearance</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Additional data for bubble caps:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Cap diameter</td>
<td>Slot area</td>
</tr>
<tr>
<td>Slot height</td>
<td>Riser area</td>
</tr>
<tr>
<td>Skirt clearance</td>
<td>Annual area</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Additional data for valves:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Closed Loss K</td>
<td>Open Loss K</td>
</tr>
<tr>
<td>Eddy Loss C</td>
<td>Ratio Valve Legs</td>
</tr>
<tr>
<td>Valve Density</td>
<td>Valve Thickness</td>
</tr>
<tr>
<td>Fraction Heavy Valves</td>
<td>Heavy Valve Thickness</td>
</tr>
</tbody>
</table>

#### 18.5.1 Tray Column Design: Fraction of flooding

The first task in this approach to tray design is to assign all layout parameters to consistent values corresponding to the required capacity defined by the fraction of flooding and current flowrates. These defaults function as starting points for subsequent designs.

The initial free area ratio is taken to be 15% of the active area. The active area is determined from a capacity factor calculation with internals specific methods (for sieve and bubble-cap trays the default is Fair’s correlation by Ogboja and Kuye (19), and the Glitsch method is used for valve trays). The tray spacing is initially set to the default value (of 0.5m) and the downcomer area is calculated according to a method in the Glitsch manual (limited by a minimum time residence check). From the combined areas the column diameter is computed. The number of liquid passes on a tray is initially set by the column diameter; under 5ft one pass, under 8ft two, 10ft three, under 13ft four, else five passes. With the number of passes and the column diameter the total weir length is computed. Once the weir length is determined the liquid weir load is checked, if too high the number of passes is incremented and a new weir length is evaluated until the weir load is below a specified maximum.
Initial weir height is taken as 2”, but limited to a maximum of 15% of the tray spacing. For notched or serrated weirs the notch depth is a third of the weir height. For serrated weirs the angle of serration is 45°. Circular weirs have diameters 0.9 times the weir length. The hole diameter is set to 3/16” for sieve trays and tray thickness 0.43 times the hole diameter (or 1/10”). The hole pitch is computed from the free area ratio and hole diameter according to a triangular pitch. The default downcomer clearance is 1.5” but is limited by the maximum allowed downcomer velocity according to the Glitch method, de-rated with the system factor. The clearance is set to be at least 0.5” lower than the weir height to maintain a positive liquid seal but is limited to a minimum of 0.5”.

For bubble-cap trays the cap diameter is 3” for column diameters below 4.5 ft and 4” for above. The hole diameter can vary between 60% to 71% of the cap diameter, and default taken as 70%. Default skirt clearance is 1” with minimum of 0.5” and maximum of 1.5”. The slot height can vary in between 0.5” and 1.5”, where the default is 1” for cap diameters below 3.5” and 1.25” for larger cap diameters. The pitch can vary from 1.25” to half the flow path length (minimum number of rows is two), with the default value set to 1.25”.

Valve trays are initialized to be Venturi orifice uncaged, carbon steel valves of 3mm thick with 3 legs (see Kister, 1992, p312). The hole diameter is 1” for column smaller than 4.5 ft, otherwise 2”. No double weight valves are present.

The second task in the fraction of flooding method consists of finding the proper free area ratio ($\beta = A_h / A_b = \text{hole area} / \text{active area}$) so that no weeping occurs. This ratio can vary between a minimum of 5% (for stable operation) and a maximum of 20%. To test whether weeping occurs, we use the correlation of Lockett and Banik (1984): $Fr_{hole} > 2/3$. The method requires all liquid heights to be evaluated at weep rate conditions. This task is ignored for bubble-cap trays. The weep test is done at weeping conditions, with a weep factor at 60% (this can be changed). Calculation of the liquid heights was described in Section 18.2. If weeping occurs at the lower bound for the free area ratio, a flag is set for the final task to adapt the design.

The final task consists of evaluating all liquid heights at normal conditions and to do a number of checks:

- vapor distribution (for bubble-cap trays),
- weeping (for sieve trays/valve trays),
- hydraulic flooding,
- excessive liquid entrainment,
• froth height limit, and
• excessive pressure drop

If a check fails, the design is modified to correct the problem, according to the adjustments shown in Table 18.4 after which new areas are calculated from the capacity correlations. Part of this task is also to keep the layout parameters within certain bounds to maintain a proper tray design. Finally, the number of iterations for the design method is checked against a maximum (default 30) to prevent a continuous loop.

The adjustment factors $f_1$, $f_2$, and $f_3$ are percentile in/decrements, normally set at 5, 2, and 1%. These factors – together with all the default, lower, and upper settings that are used in the design routine – are stored in a “design file” (TDESIGN.DEF, described in Section ??) that can be tailored to handle specific kinds of designs and columns. This allows the selection of different methods for capacity and hydrodynamic calculations as well. Also the fraction that the flows need to change before a re-design is issued can be changed in this manner together with other design criteria. The design file must be in the current directory for the nonequilibrium program to use it, otherwise the normal defaults will be used. To obtain the best results, it would be best to have different TDESIGN.DEF files for distillation and absorption. However, a compromise between these operations was struck and ChemSep currently has one file to handle both.

### 18.5.2 Tray Column Design: Pressure drop

The same design routine for a tray design at a specific fraction of flood may also be used to design a tray with a certain maximum pressure drop, using a default fraction of flood of 75%. Note that this method of designing trays does not fix the pressure drop: it only applies a maximum allowed pressure drop over the tray. If the tray design results in a pressure drop larger than that specified the layout is adjusted according to the steps for excessive pressure drop per Table 18.4. To obtain a layout which has a lower pressure drop is to raise the bubbling area, in effect lowering the fraction of flood. However, the weir height is also lowered and the hole diameter is increased (albeit with a smaller factor).

### 18.5.3 Packed Column Design: Fraction of flooding

For packed columns only the column diameter is to be estimated. Default packing data are used for all parameters that are not specified; values of 1” metal Pall rings
Table 18.4: Tray design checks and adjustments

<table>
<thead>
<tr>
<th>Problem</th>
<th>Test</th>
<th>Adjustments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble cap vapor distribution</td>
<td>$h_{tg}/h_d &gt; 0.5$</td>
<td>$p + f_1,$ $h_{skirt} + f_2,$ $h_{slot} + f_3,$ $d_h - f_3$</td>
</tr>
<tr>
<td>Weeping</td>
<td>$Fr_{h}/(2/3) &lt; 1 - f_a$</td>
<td>$h_{w} &lt; f_1$: $A_b = A_{bf}$ $W_f + f_1$ $A_b - f_1$ $d_h - f_3$ $h_{w} - f_3$ $t_v + f_2 (vt)$</td>
</tr>
<tr>
<td>Hydrodynamic (downcomer) flooding</td>
<td>$T_s &lt; h_{db}/FF$</td>
<td>$T_s + f_1$ $A_d + f_1$ $h_w + f_2$ $h_c + f_3$</td>
</tr>
<tr>
<td>Excessive liquid entrainment</td>
<td></td>
<td>$A_b + f_1$ $T_s + f_2$ $d_h - f_2$ $h_w - f_3$</td>
</tr>
<tr>
<td>Froth height limit</td>
<td>$h_f &gt; 0.75T_s$</td>
<td>$A_b + f_1$ $T_s + f_2$ $h_w - f_3$</td>
</tr>
<tr>
<td>Excessive pressure drop</td>
<td>$gph_{w} &gt; \Delta p_{max}$</td>
<td>$A_b + f_1$ $h_w - f_1$ $d_h + f_2$ $p + f_1 (bc)$ $h_{skirt} + f_2 (bc)$ $h_{slot} + f_3 (bc)$</td>
</tr>
<tr>
<td>Excessive vapor entrainment</td>
<td></td>
<td>$A_d + f_1$</td>
</tr>
</tbody>
</table>
for random packed sections and of Koch Flexipack 2 (316SS) for structured sections. To determine the packed column diameter, the diameter that gives rise to the flooding pressure drop (as specified) is computed using the selected pressure drop model. The resulting diameter is corrected for the fraction of flooding and the system factor:
\[
D_c = \frac{D_{c,flood}}{\sqrt{FF SF}}
\]  
(18.137)

This makes the resulting column diameter depend on the selected pressure drop model. If no pressure drop model is selected the Leva (1992) model is selected (which is a function only of the packing factor). If no pressure drop at flood is specified, it is estimated with Kister and Gill correlation (1992):
\[
\Delta P_{flood} = 0.115 F_p^{0.7}
\]  
(18.138)
(with pressure drop as liquid height and English units!). This correlation is a function only of the packing factor but has been tested on a wide range of packings and an accuracy of 15 %. As long as the packing factor is known, this design method will not fail.

### 18.5.4 Packed Column Design: Pressure drop

Tray design based on a specified pressure drop is done as discussed above but with a default fraction of flooding of 75 %. However, the specified pressure drop functions as a maximum allowed pressure drop per tray. No adjustment is done if the pressure drop is below this specified pressure drop.

Packed column design automatically finds the diameter leading to the specified pressure drop (with the selected pressure drop model). This is done by using a linear search technique as the different packing pressure drop correlations can behave quite erratically. The maximum allowed pressure drop is the flooding pressure drop as specified or computed from Kister’s correlation and the packing factor. If the pressure drop is specified to be very low the column diameter might converge to unrealistic diameters. A zero or larger than flooding pressure drop specification results in a 70 % fraction of flooding design.

### 18.6 Comparison with Experimental Distillation Data

Here, we illustrate the performance of the nonequilibrium model by simulating several systems for which experimental data is available in the literature. We focus our
attention on ternary systems; only in mixtures with more than two species can the molecular interaction between them influence the mass transfer resulting in different individual component Murphree efficiencies.

The complete process of comparing experimental data with the current version of ChemSep has been automated and provides a test for the correct behavior of the simulator. We hope to build up an extensive database of distillation experiments and welcome additional data. The experimental literature data is entered in a database file that consists of keywords and the data. Then we carry out simulations and store each simulation in a sep-file. With the use of some utility programs we convert the simulation information and compare it to the experimental measured values. We can create parity plots and calculate average and maximum errors.

18.6.1 Ternary Distillation Experiments

The experiments discussed below were carried out at total reflux in columns with bubble-cap trays.

Vogelpohl (1979) has reported some results for the distillation of two non-ideal systems: acetone, methanol, and water as well as methanol, isopropanol, and water. The experiments were done in a column with 38 bubble-cap trays of 0.3 m in diameter. Due to the ease of separation, only up to 13 trays were active for the experimental runs. The experimental data clearly shows that the component Murphree efficiencies are unequal; indeed, in the acetone-methanol-water system the composition of methanol passes through a maximum in the column and the efficiency for this component becomes unbounded. Vogelpohl shows that the assumption of equal component efficiencies gives rise to large differences between the predicted and measured composition profiles.

The simulations were done using the total reflux mode of the nonequilibrium model. For total reflux specifications one must use a column configuration with a condenser and reboiler plus one feed. Either the distillate flow is set to zero and a reboiled vapor flow is specified, or, the bottoms flow is set to zero and a reflux flowrate is specified. Only these specifications of the column operation will trigger the total reflux mode of the column simulator. In this mode the feed specifications are employed as the specification of the vapor or liquid compositions on a specific stage. The compositions (and stage) that are to be fixed are set by the feed compositions and stage. Thus, if we know the compositions of the vapor leaving the reboiler we specify a feed to the reboiler and set the feed component flows equal to the known mole fractions. To indicate that these are vapor mole fractions I set the vapor fraction of the feed as 1. On the other hand, if the liquid reboiler compositions are known we would specify the
feed vapor fraction as 0.

For Vogelpohl’s data the compositions of the vapor leaving the (total) reboiler were specified to match the measured values. The reboiler vapor flowrate was specified at 0.65 \( \text{kmol/h} \) resulting in an effective F-factor around 0.1. The calculated fraction of flood was around 20 %. Table 18.5 shows the UNIQUAC interaction parameters used for the acetone, methanol, and water column. These interaction parameters were fitted to binary VLE data. The bubble-cap trays were specified with 0.3 \( m \) tray diameter, tray spacing as 0.2 \( m \), bubbling area of 0.06008 \( m^2 \), a weir height of 0.03 \( m \), and a flow path width of 0.24 \( m \). The other layout parameters are assigned/computed by the simulator. The AIChE MTC model was used together with the vapor plug flow and liquid mixed flow models.

Table 18.5: UNIQUAC interaction parameters (cal/mol) for the Acetone (1) - Methanol (2) - Water (3) system

<table>
<thead>
<tr>
<th>Components i-j</th>
<th>( A_{ij} )</th>
<th>( A_{ji} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>acetone - methanol</td>
<td>403.8524</td>
<td>-84.2364</td>
</tr>
<tr>
<td>acetone - water</td>
<td>698.7989</td>
<td>-110.382</td>
</tr>
<tr>
<td>methanol - water</td>
<td>-337.129</td>
<td>549.2958</td>
</tr>
</tbody>
</table>

Figure 18.1: Experimental compositions (points) and the predicted composition profiles (lines) for the acetone-methanol-water system.
Figure 18.2: Parity plot for the acetone-methanol-water system.

Figure 18.3: Experimental compositions (points) and the predicted composition profiles (lines) for the methanol-isopropanol-water system.
For the methanol, isopropanol, and water column UNIQUAC interaction parameters were taken from DEHEMA (p. 575) that were fitted to ternary VLE data, see Table 18.6. The same bubble-cap tray layout, column specifications, and model selections were used as for the acetone-methanol-water column.

Figure 18.1 shows the measured compositions and the simulated mole fraction profiles for the acetone-methanol-water system. Figure 18.2 shows that the nonequilibrium model does an excellent job in predicting the mole fractions for this very nonideal system. Figure 18.3 and Figure 18.4 show that the methanol-isopropanol-water system is predicted less well. We suspect this may be due to the interaction parameters of the activity coefficients. These simulations are extremely sensitive to these parameters, especially as isopropanol is going through a maximum in concentration. The average and maximum discrepancies in the predicted and experimentally measured compositions are shown in Table 18.8.

Ternary distillation experiments using acetone, methanol, and ethanol were performed by Free and Hutchison (1960) in a column with 7 bubble-cap trays of 0.1016 m in diameter. They also find that equal Murphree efficiencies cannot explain the behavior of this system. Twelve runs were conducted covering different regions of the ternary composition triangle. The column they used had a tray diameter of 0.1016 m, bubbling area of 0.00689 m², 0.015 m weir height and a flow path length of 0.0813 m.
Table 18.6: UNIQUAC interaction parameters (cal/mol) for the Methanol (1) - Isopropanol (2) - Water (3) system

<table>
<thead>
<tr>
<th>Components i-j</th>
<th>( A_{ij} )</th>
<th>( A_{ji} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>methanol - isopropanol</td>
<td>754.216</td>
<td>-457.107</td>
</tr>
<tr>
<td>methanol - water</td>
<td>670.563</td>
<td>-442.713</td>
</tr>
<tr>
<td>isopropanol - water</td>
<td>355.536</td>
<td>28.874</td>
</tr>
</tbody>
</table>

The F-factor was assumed to be around 0.9 \( \sqrt{kg/m/s} \) and a vapor boilup of 0.65 \( kmol/h \) was specified, resulting in fraction of flood around 35%. Table 18.7 shows the UNIQUAC Q prime interaction parameters were used (Prausnitz et al., 1980). The UNIQUAC Q prime activity coefficient model gives excellent results for these experiments. Figure 18.5 shows the data and the predicted column profiles for some of the experimental runs. The agreement is excellent, as can also be seen from the parity plot, Figure 18.6.

Figure 18.5: Comparison of experimental compositions (points) and the predicted composition profiles (lines) for the acetone-methanol-ethanol system.

All these simulations were done by specifying the bottom compositions in the column, just as was done by Krishnamurthy and Taylor (1985). The errors in Table 18.8 would be reduced if we would specify the compositions in the middle of the column, as the errors in the predicted mole fractions often accumulate from stage to stage.
Figure 18.6: Comparison of experimental and predicted mole fractions for the acetone-methanol-ethanol system.

Table 18.7: UNIQUAC interaction parameters (cal/mol) for the Acetone (1) - Methanol (2) - Ethanol (3) system

<table>
<thead>
<tr>
<th>Components i-j</th>
<th>$A_{ij}$</th>
<th>$A_{ji}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>acetone - methanol</td>
<td>359.10</td>
<td>-96.90</td>
</tr>
<tr>
<td>acetone - ethanol</td>
<td>404.49</td>
<td>-131.25</td>
</tr>
<tr>
<td>methanol - ethanol</td>
<td>660.19</td>
<td>-292.39</td>
</tr>
</tbody>
</table>

Table 18.8: Summary of the average and maximum discrepancies between model prediction and experimental measurement

<table>
<thead>
<tr>
<th>System</th>
<th>No. of Runs</th>
<th>No. of Samples</th>
<th>Average Error</th>
<th>Maximum Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>acetone - methanol - water</td>
<td>3</td>
<td>22</td>
<td>0.015</td>
<td>0.070</td>
</tr>
<tr>
<td>methanol - isopropanol - water</td>
<td>3</td>
<td>27</td>
<td>0.024</td>
<td>0.087</td>
</tr>
<tr>
<td>acetone - methanol - ethanol</td>
<td>12</td>
<td>67</td>
<td>0.010</td>
<td>0.051</td>
</tr>
</tbody>
</table>
18.6.2 Significance of Multicomponent Interaction Effects

Figure 18.7 is a comparison for the acetone-methanol-water experiments of the nonequilibrium model with an ‘equal diffusivity’ model. This model uses a single average value of the diffusion coefficients for each component. It yields equal component stage efficiencies and, therefore, corresponds to the conventional equilibrium stage model with efficiencies. The comparison clearly shows that the predicted top compositions of the ‘equal diffusivity’ model are qualitatively different from the experimental values.

This can be explained by inspecting the back-calculated Murphree component efficiencies of the nonequilibrium model, see Figure 18.8. We see that the efficiencies of water and acetone differ by about 10%! This explains the observed 10% difference in top compositions. The methanol efficiencies show an even more weird behavior: they become unbounded between plate 6 and 7. When we look at the compositions, we see that the reason for this is that methanol goes through a maximum around stage 6. Whenever a component goes through an extreme in composition (the driving force becomes zero) and there is still mass transfer occurring (however little) than the efficiencies are unbounded. If we had more stages in the column, we would observe that the methanol efficiency below this maximum stays at the higher value of the Murphree efficiency of water. Apparently, the direction of the mass transfer is important!

18.6.3 Binary Distillation Experiments: Mass Transfer Coefficients and Flow Models

To illustrate the behavior of the various tray MTC models as well as the different flow models we include here some comparisons with experimental data of the FRI by Yanagi and Sakata (1979, 1981). Two systems were used in these tests: the cyclohexane - n-heptane system at pressures of 28, 34, and 165 kPa, and the i-butane - n-butane system at pressures of 1138, 2056, and 2756 kPa. The experiments were carried out in sieve tray columns operated at total reflux. Nonequilibrium simulations were done for a column with the same tray design (the design parameters are summarized in Table 18.9) at total reflux (Kooijman, 1995). The Murphree efficiencies were calculated for each component on each tray from the results of a simulation and averaged (over those trays not adjacent to condenser/reboiler). Simulations were done using different combinations of flow models:

- Mixed vapor - Mixed liquid
- Plug flow vapor - Mixed liquid
- Plug flow vapor - Plug flow liquid
Figure 18.7: Experimental compositions (points) and the predicted composition profiles for the acetone-methanol-water system using the nonequilibrium model (solid lines) and the ‘equal diffusivity’ model (broken lines).

Table 18.9: Sieve Plate Dimensions of FRI Column

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Column diameter ((m))</td>
<td>1.2</td>
</tr>
<tr>
<td>Tray spacing ((m))</td>
<td>0.61</td>
</tr>
<tr>
<td>Sieve plate material</td>
<td>316SS</td>
</tr>
<tr>
<td>Plate thickness ((mm))</td>
<td>1.5</td>
</tr>
<tr>
<td>Hole diameter ((mm))</td>
<td>12.7</td>
</tr>
<tr>
<td>Hole pitch ((mm))</td>
<td>30.2</td>
</tr>
<tr>
<td>Weir length ((m))</td>
<td>0.94</td>
</tr>
<tr>
<td>Weir height ((mm))</td>
<td>25.4, 50.8</td>
</tr>
<tr>
<td>Downcomer clearance ((mm))</td>
<td>22, 23.8</td>
</tr>
<tr>
<td>Effective bubbling area ((m^2))</td>
<td>0.859</td>
</tr>
<tr>
<td>Hole area ((m^2))</td>
<td>0.118</td>
</tr>
</tbody>
</table>

Simulations were carried out with flows that go from 20% to 100% of flooding. Figure 18.9 shows some of these results with the Chan and Fair (1984) mass transfer coefficients correlations. The experimental efficiencies show a decline at low and high fractions of flooding, probably due to weeping and liquid entrainment. The Chan
and Fair model includes a quadratic dependence of $N^V$ on the fraction of flooding in order to account for the decrease in mass transfer at both low and high fractions of flooding. For this reason the Chan and Fair method usually describes the mass transfer (and hence, the efficiencies) better than the other mass transfer coefficient models.

Note that the Mixed-Mixed flow model underpredicts the efficiencies, as is true for the Plug flow vapor - Mixed flow liquid model. The Plug-Plug flow model fits the experimental efficiencies quite well. This should not be too surprising as this data was actually used in the development of the Chan and Fair correlations. We are, however, using the correlations in a nonequilibrium model rather than in an efficiency calculation.

Four different methods for estimating the binary mass transfer coefficients for sieve trays were tested: AIChE (1958), Chan and Fair (1984), Zuiderweg (1982), and Chen and Chuang (1994). Figure 18.10 shows the results for the i-butane/n-butane tests using the plug-plug flow model. In general, the AIChE and the Chan-Fair correlations behave in similarly, except for the strong dependence on the fraction of flooding of the Chan-Fair model. This is not surprising since both use the same expression for the liquid mass transfer coefficients. The Zuiderweg and Chen-Chuang models predict higher efficiencies as they have higher values for the liquid number of transfer units.
than the first two correlations. For this test they perform well; in many other tests these two models tend to overpredict the Murphree efficiencies.

The Chan-Fair correlation tends to describes the overall behavior of the Murphree efficiencies better than the other methods considered. However, it's formulation causes it always to have a maximum efficiency at 60% fraction of flood. This limits the model to sieve trays only and to the range of fractions of flooding where the quadratic term is positive (0-1.2). Presumably, the fall-off in tray performance at low and high fractions of flooding is due to increases in weeping or entrainment at these extreme flows. It is not clear to us that mass transfer coefficient correlations should account for these effects. Rather, we suggest that these effects should be separated. We have also encountered situations where the Chan and Fair correlations provide negative mass transfer coefficients because the flows are outside its range. Not only are negative mass transfer coefficients physically meaningless, they may prevent the program that implements our nonequilibrium model from converging to a solution! Despite these
Figure 18.10: Murphree efficiencies for different Mass Transfer Coefficient models for a (14% hole area) sieve tray column with $i$-butane - $n$-butane system operating at 1138 kPa. Chan and Fair (thick dotted line), AIChE (thick dashed line), Zuiderweg (dashed line), and Chen and Chuang (solid line).

problems with the Chan and Fair method we think its limitations are less serious (from our perspective) than are the limitations of other methods and, for now, it is our method of choice.

Symbol List

Latin Symbols

- $a_d$  
  interfacial area density ($m^2/m^3$)
- $a$  
  area ($m^2$)
- $A_h$  
  hole area ($m^2$)
- $A_b$, $A_{bub}$  
  bubbling area ($m^2$)
- $A_d$  
  downcomer area ($m^2$)
$B$ packing base ($m$)
c number of components, molar concentration ($kmol/m^3$)
$Ca$ Capillary number
d$_h$ hole diameter ($m$)
d$_{eq}$ equivalent diameter
$D$ binary diffusivity coefficient ($m^2/s$)
$D_c$ column diameter ($m$)
$D_e$ eddy dispersion coefficient ($m^2/s$)
$f_1$, $f_2$, $f_3$ design adjustment factors
$F_p$ packing factor ($1/m$)
$F_s$ F factor $F_s = U_w \sqrt{\rho V}$ ($kg^{0.5}/m^{0.5}/s$)
$FF$ fraction of flooding
$FP$ flow parameter $FP = M_L/M_V \sqrt{\rho_L/\rho_V}$
$Fr$ Froude number
g gravitational constant, 9.81 ($m/s^2$)
h$_c$ clearance height under downcomer ($m$)
h$_{cl}$ clear liquid height ($m$)
h$_d$ dry tray pressure drop height ($m$)
h$_{db}$ downcomer backup liquid height ($m$)
h$_f$ froth height ($m$)
h$_i$ liquid height at tray inlet ($m$)
h$_tg$ liquid gradient pressure drop height ($m$)
h$_l$, $h_L$ liquid pressure drop height ($m$)
h$_{ow}$ height of liquid over weir ($m$)
h$_r$ residual pressure drop liquid height ($m$)
h$_{wt}$ wet tray pressure drop liquid height ($m$)
h$_w$ weir height ($m$)
h$_{udc}$ liquid height pressure loss under downcomer ($m$)
k binary mass transfer coefficient ($m/s$)
$Le$ Lewis number ($Le = Sc/Pr$)
$M_w$ molecular weight ($kg/kmol$)
$N$ number of transfer units, NTU
$P$ perimeter ($m$)
p hole pitch ($m$), pressure ($Pa$)
$\Delta p$ pressure drop ($Pa$)
$\Delta P_{max}$ maximum design pressure drop ($Pa/tray$ or $Pa/m$)
$Pr$ Prandtl number
$Q$ volumetric flow ($m^3/s$)
$Re$ Reynolds number
\( S \)  
packing side (\( m \))

\( Sc \)  
Schmidt number

\( SF \)  
system derating factor

\( t \)  
residence time (\( s \))

\( t_v \)  
valve thickness (\( m \))

\( T \)  
temperature (\( K \))

\( T_s \)  
tray spacing (\( m \))

\( u, U \)  
velocity (\( m/s \))

\( V \)  
vapor flow rate (\( kmol/s \))

\( We \)  
Weber number

\( W_l \)  
weir length (\( m \))

\( x \)  
liquid mole fraction

\( y \)  
vapor mole fraction

\( z \)  
mole fraction

\( Z \)  
tray flow path length (\( m \))

**Greek Symbols**

\( \alpha \)  
fraction liquid in froth

\( \beta \)  
fractional free area \( \beta = A_h/A_b \)

\( \epsilon \)  
void fraction

\( \Gamma \)  
liquid flow per perimeter

\( \phi \)  
fractional entrainment

\( \rho \)  
density (\( kg/m^3 \))

\( \sigma \)  
surface tension (\( N/m \))

\( \eta \)  
viscosity (\( Pa s \))

\( \lambda \)  
thermal conductivity (\( W/m/K \))

**Superscripts**

\( I \)  
interface

\( L \)  
liquid

\( P \)  
phase \( P \)

\( V \)  
vapor
Subscripts

\( b, \text{ bub} \) bubbling
\( c \) critical, contact
\( \text{eff} \) effective
\( \text{fl, flood} \) at flooding conditions
\( i \) component \( i \)
\( j \) stage \( j \),
    component \( j \)
\( h \) hole
\( MW \) minimum wetting
\( p \) packing
\( \text{spec} \) specified
\( t \) total

Abbreviations

bc bubble-caps

References


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M. Nord, “Plate Efficiencies of Benzene-Toluene-Xylene Systems in Distillation”,


