Distillation Absorption 2010
A.B. de Haan, H. Kooijman and A. Górak (Editors)

SHORT-CUT METHODS FOR THE OPTIMAL DESIGN OF SIMPLE AND COMPLEX DISTILLATION COLUMNS

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Abstract

New short-cut methods providing optimal design parameters for distillation columns with simple and complex configurations including two-feed and one-feed-one-side-stream columns are presented. The methods assume constant relative volatilities and constant molar flow rates within each distillation section. The constituting design equations are based on the Underwood equations for the calculation of minimum reflux ratio, the analytical formulations of the distillation line, the Eigenfunction and the number of theoretical stages for each mass transfer section[1]. Additional design equations have been established based on the analysis of the geometrical properties for a given separation with respect to the type of split, the configuration of the column (simple or complex) and the mass balance around each feed section for an arbitrary feed quality. Optimization algorithms based on the minimization of the total number of theoretical stages of the column under the constraint of the mass balance at each feed section were elaborated providing the reflux ratio, the minimum number of theoretical stages of the column, the optimal feed location and the product compositions for a given separation. In comparison to the boundary value method[2] the new short-cut methods require a minimum number of specifications, they are completely numerical and provide a lower total number of theoretical stages particularly for complex configurations. The new short-cut methods have been extended to the design of columns separating azeotropic mixtures by approximating the latter by appropriate pseudo-ideal mixtures[3,4]. Several separation examples including ideal and azeotropic mixtures, different types of splits as well as columns with simple and complex configurations were tested and show a very good agreement with the simulation results obtained with Radfrac (Aspenplus).

Keywords: Distillation, short-cut methods, azeotropic mixtures, geometrical properties, complex configurations

1. Introduction

Despite extensive investigations on the conceptual design of multicomponent distillation columns, the calculation of the total number of transfer units of a column, the feed location and the side stream location are still based on approximate methods like the empirical correlations of Gilliland-Kirkbride[5] or the boundary value method (BVM)[2] based on a geometrical and graphical approach. Therefore, the incorporation of such methods into a systematic procedure for screening of distillation flowsheets is not reliable, particularly if complex configurations are involved. In this paper new short-cut methods are presented for three basic configurations as presented in Fig. 1, i.e. (a) a column of a simple configuration, (b) a two-feed column and (c) a column with one feed and one side stream.

2. Design equations

The new design methods assume constant relative volatilities α and constant molar flow rates within each distillation section. The calculation of the minimum reflux ratio is based on the Underwood equations. Each mass transfer section k is defined by the respective Eigenfunction [1]

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$$\sum_{i=1}^{c}\frac{\alpha_i \cdot a_i^k}{\alpha_i - r^k \cdot E^k} = 1, \tag{1}$$

where a_i^k and r^k are the constant and the ratio of the internal liquid and vapor flow rate of the operating line for the section k. The solutions of the Eigenfunction of the section k are the c Eigenvalues E^k of the pure components which define the distillation space and the parameters of the respective distillation line given by

$$\frac{\xi_j^k}{\xi_1^k} = \chi_j^k \cdot \left(\frac{\xi_c^k}{\xi_1^k}\right)^{e_j^k}, \chi_j^k = \frac{\dfrac{\xi_{j,0}^k}{\xi_{i,0}^k}}{\left(\dfrac{\xi_{c,0}^k}{\xi_{i,0}^k}\right)^{e_j^k}}, \text{ j=2,…,c-1, , with } \sum_{i=1}^{c}\xi_i^k = 1\ , \tag{2}$$

where χ^k is the initial composition of the distillation line and e^k are the exponents of the distillation line in the section k given by

$$e_j^k = \frac{\mathrm{Ln}E_i^k - \mathrm{Ln}E_j^k}{\mathrm{Ln}E_i^k - \mathrm{Ln}E_c^k}, \text{j=2,c-1.} \tag{3}$$

ξ^k are transformed mole fractions and the actual composition profiles are obtained by the following transformations for the liquid and vapour phase, respectively,

$$\left|x^k\right| = \left|\Xi_L^k\right| \cdot \left|\xi^k\right|, \text{and} \left|y^k\right| = \left|\Xi_V^k\right| \cdot \left|\eta^k\right|\ , \tag{4}$$

where $\left|\Xi_L^k\right|$ and $\left|\Xi_V^k\right|$ are the matrices representing the liquid and vapor distillation space for the mass transfer section k, respectively. For each mass transfer section the number of theoretical stages writes

$$N^k = \frac{\mathrm{Ln}\left[\left(\dfrac{\xi_i^k}{\xi_c^k}\right)\cdot\left(\dfrac{\xi_{c,0}^k}{\xi_{i,0}^k}\right)\right]}{\mathrm{Ln}\left(\dfrac{E_i^k}{E_c^k}\right)}. \tag{5}$$

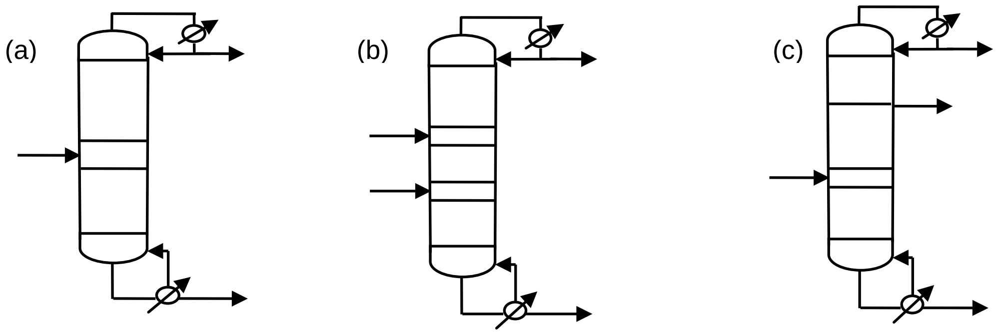

Figure 1. Basic configurations of a distillation column

The analytical formulation of the parameters of the Eigenfunction of the middle section for two-feed columns as well as for one-feed-one-side-stream columns shows[4] that the respective distillation space is independent of the initial conditions, i.e. the composition of the side stream and the location of the upper (lower) feed, respectively.

3. Design algorithms

For each column configuration three main calculation steps are carried out: 1) initialization procedure, 2) optimization procedure, and 3) calculation of the composition profiles in the column. For given design specifications the initialization procedure provides analytically the geometrical structure of the problem as well as initial values for the optimization parameters as illustrated in Fig. (2) for a column with a simple configuration separating a mixture of methanol, ethanol and 1-propanol (Table 1). For a given separation the optimization procedure deals with the minimization of the total number of theoretical stages in the column by adjusting the appropriate design parameters and satisfying the mass balance equations at the feed section[4] such that the point above the feed section ($x_{F,ab}$, $y_{F,ab}$) belongs to the distillation line of the rectifying section and the one below the feed section ($x_{F,bel}$, $y_{F,bel}$) belongs to the distillation line of the stripping section. The number of theoretical stages in the stripping (rectifying) section (minimum value provided by the initialization procedure) is used as an optimization parameter in the case of a direct (indirect) split since the invariant distillation line corresponds to the stripping (rectifying) section. Once the optimization has been performed then the composition profiles are determined analytically (Eq. (2)) by using the equation of distillation line within an initial condition problem. Such calculations are executed from the bottom upwards for a direct split, and from the top downwards for an indirect split.

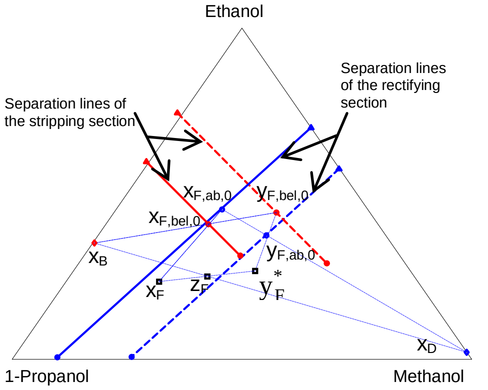

Figure 2. Geometry of the direct separation in a simple column (q_F =0.5)

Table 1. Separation examples for ideal systems

Simple configuration	Two-feed column	One feed-one side stream column
Methanol (1)	Methanol (1)	Benzene (1)
Ethanol (2)	Ethanol (2)	Toluene (2)
1-Propanol (3)	1-Propanol (3)	O-xylene (3)
$\alpha = [3.6\ \ 2.1\ \ 1]$	$\alpha = [3.6\ \ 2.1\ \ 1]$	$\alpha = [6.4\ \ 2.7\ \ 1]$
x_F =[0.3 0.25 0.45]	x_{FL} =[0.1 0.2 0.7], x_{FU} =[0.4 0.5 0.1] Fr = 1	x_F =[0.1 0.45 0.45] B/F= 0.443 (side stream above the feed)
$x_{D,1} \geq 0.99$, $x_{B,1} \leq 0.01$	$x_{B,3} \geq 0.99$, $x_{D,1} \leq 0.01$	$x_{D,1} \geq 0.99$, $x_{B,3} \geq 0.99$, q_W =1

3.1 Two-feed column

For given feed compositions, feed qualities, feed ratio and product purities, the design specifications for a two-feed column are augmented by one[6] in comparison to a column with a simple configuration. The additional design parameter provides the location of the additional feed. As for single-feed columns, the invariant distillation line corresponds to the rectifying section for an indirect split and to the stripping section for a direct split. Thus, it is more convenient to specify the upper feed location for an indirect split and the lower feed location for a direct split independently of which feed is controlling. Levy et al. (1986)[7] proposed an approximate graphical procedure to assess the location of the upper (lower) feed for an indirect (direct) split. In this work an analytical procedure is proposed to determine systematically the optimal location of the first feed. For this purpose let us consider the indirect separation in a two-feed column of a mixture of methanol, ethanol and 1-propanol (Table 1) where the upper feed was found to be the

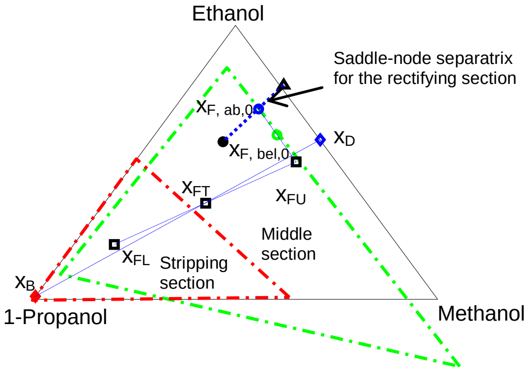

Figure 3. Determination of the upper feed location

controlling feed[6]. In this case, the upper feed is the first to be determined. For this purpose, the intersection of the saddle-stable node separatrix of the rectifying section and the unstable node-saddle separatrix of the middle section provides the point $x_{F,ab,0}$ which represents the initial value for the composition above the upper feed location. Since the distillation space of the middle section is invariant it is straightforward to check analytically whether the point $x_{F,bel,0}$, representing the location below the upper feed section and obtained by mass balance around the upper feed location, belongs to the above mentioned distillation space (see Fig. (3)).

3.2 Column with one feed and one side stream

The side stream may be a saturated liquid above the feed location with the primary separation 1-2/3 and the secondary separation 1/2-3 or a saturated vapor below the feed location with the primary separation 1/2-3 and the secondary separation 1-2/3. In addition to the specification of the distillate and the bottom product purities, the flow rate of the bottom product B (the distillate) is specified if the side stream is above (below) the feed location. Thus, the flow rate of the bottom product (the distillate) allows to determine the distillation spaces of both the middle and the stripping sections (middle and rectifying sections) as well as the flow rate of the distillate D (bottom product) at the pinch conditions. In the case where the side stream is above the feed location, the feasibility of the primary separation depends on a sufficient vapor flow rate supplied by the reboiler[6], whereas that of the secondary separation is satisfied if the side-stream location belongs to the distillation lines of both the rectifying and middle sections, i.e. the composition of the side stream must be located within the distillation spaces of both the middle and rectifying sections. In this work it is shown that this condition is fulfilled if the distillate flow rate is lower than the value corresponding to the pinch condition so that the composition x_s and the flow rate S of the side stream are then obtained straightforwardly by a mass balance as illustrated in Fig. (4) for a mixture of benzene, toluene and o-xylene with the side stream above the feed location (Table 1). Once the side stream location is calculated then the optimal feed location for the primary separation is determined analytically similarly to the simple configuration procedure for an indirect split involving the middle section (invariant) and the stripping section. Likewise, if the side stream is below the feed location the calculation of the optimal feed location is carried out similar to the simple configuration procedure for a direct split involving the rectifying section and the middle section (invariant). The design parameters for the separation examples (Table 1) are obtained for an operating reflux (reboil) ratio R taken as 1.2 times their minimum value (Underwood equations). The results are presented numerically and graphically in Fig. (5) for the three configurations. The values of the reflux (reboil) ratio and the product compositions obtained by the new short-cut methods are introduced into the BVM procedure. The comparison of the total number of theoretical stages N_T determined by both methods shows (see Fig. 5) that a lower total number of theoretical stages for the complex configurations has been found in this work.

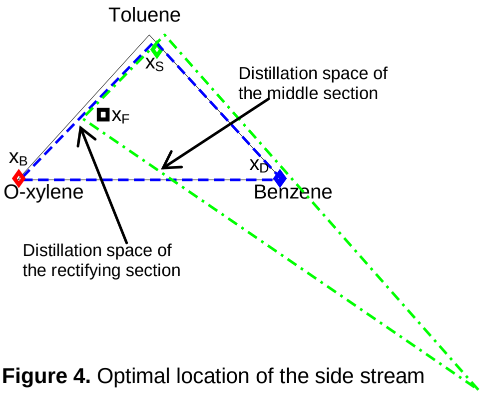

Figure 4. Optimal location of the side stream

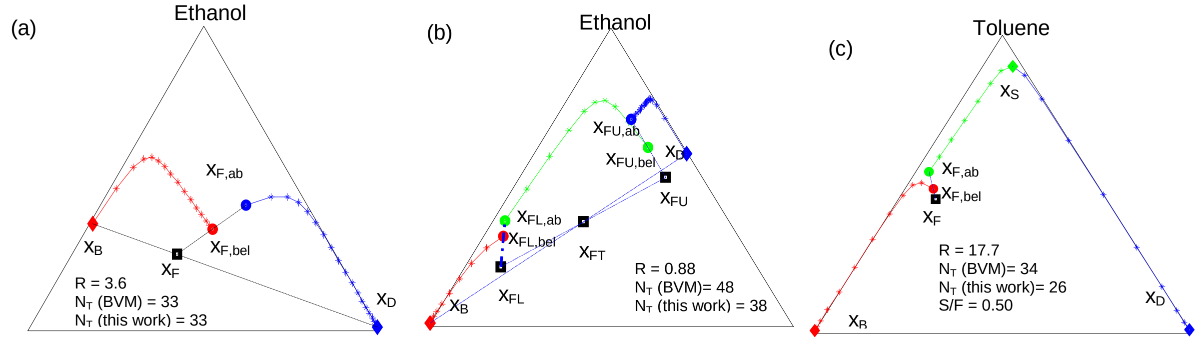

Figure 5. Design results for ideal mixtures, a) simple configuration, b) 2-feed column, c) column with one side tream above the feed

4. Extension to azeotropic systems

The new short-cut methods have been extended to the design of columns separating azeotropic mixtures by approximating the latter by pseudo-ideal mixtures based on the thermodynamic structure of the azeotropic mixture[8] and the identification of the relevant distillation region. Accordingly, an appropriate set of relative volatilities of the singular points forming the subsystem was determined in the transformed system of compositions by a rigorous thermodynamic model. All calculations in this work are carried out at atmospheric pressure. The activity coefficients and the vapor pressures are calculated using the Wilson and the Antoine equation, respectively. The data relating to the Wilson and the Antoine equation are taken from the DECHEMA liquid-vapor equilibrium data collection[9]. Separation examples including highly non-ideal mixtures are given in Table 2. For each case the azeotropic mixture is approximated by a pseudo-ideal mixture and average relative volatilities for the latter are calculated at the feed composition[4]. The design results are given numerically and graphically in Figs. (6) and (7). For each separation the calculated parameters are introduced into the model RadFrac (Aspen plus) and the obtained product compositions show a very good agreement with those obtained by the new short-cut method as illustrated in Table 3.

Table 2. Separation examples for azeotropic systems

Simple configuration	Two-feed column	One feed-one side stream column	
Methanol (1)	Methanol (1)	Methanol (1)	Acetone (1)
Isopropanol (2)	Isopropanol (2)	Isopropanol (2)	Chloroform (2)
Water (3)	Water (3)	Water (3)	Benzene (3)
x_F =[0.2 0.25 0.55]	x_{FL} = [0.1 0.2 0.7], $x_{F\,U}$ = [0.3 0.3 0.4] Fr = 1	q_S=0, D/F=0.3	q_S=1, B/F=0.3
$x_{D,3} \le 0.21$,	$x_{B,3} \ge 0.99$ $x_{D,3} \le 0.21$	x_F =[0.33 0.33 0.34]	
$x_{B,3} \ge 0.99$		$x_{D,1} \ge 0.99$ $x_{B,3} \ge 0.99$	

Table 3. Comparison of design and simulation results

	Distillate		Bottom product	
	This work	RadFrac	This work	RadFrac
Simple configuration				
Methanol	0.3547	0.355	0.001	769 PPB
Isopropanol	0.4400	0.404	0.0055	0.052
Water	0.2053	0.241	0.9935	0.947
2-feed column				
Methanol	0.3553	0.355	0.001	73 PPM
Isopropanol	0.4425	0.420	0.0023	0.031
Water	0.2022	0.224	0.9976	0.969

Side-stream below the feed

	Distillate		Bottom product		Side stream product	
	This work	RadFrac	This work	RadFrac	This work	RadFrac
Methanol	0.999	1	10^{-8}	2 PPM	0.033	0.054
Isopropanol	0.0007	5 PPB	0.0099	0.007	0.5538	0.593
Water	0.0003	trace	0.9901	0.993	0.4132	0.353
Side-stream above the feed						
Acetone	0.9922	0.958	0.0034	Trace	0.348	0.36
Chloroform	0.0078	0.04	0.0066	0.005	0.5739	0.567
Benzene	10^{-8}	0.001	0.99	0.995	0.0781	0.072

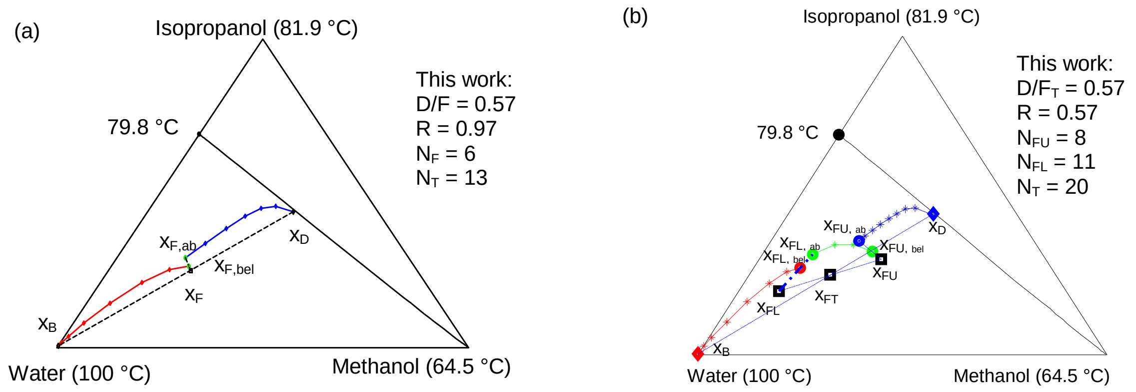

Figure 6. Design results of the separation of the mixture of methanol, isopropanol and water: (a) simple configuration, (b) 2-feed column

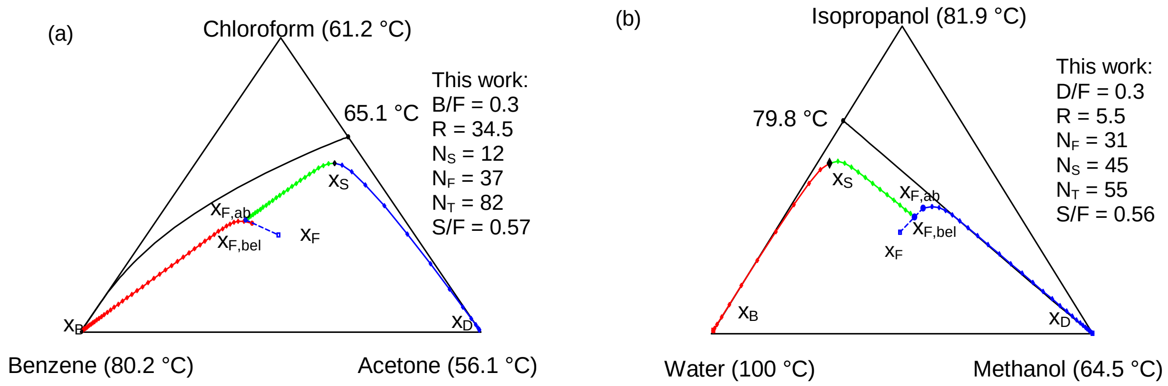

Figure 7. Design results of the separation of azeotropic mixtures in: (a) column with one side stream above the feed location, (b) column with one side stream below the feed location

5. Conclusions

Short-cut methods for the design of simple and complex distillation columns are proposed. The developed algorithms are based on the design tools for ideal systems and on the geometrical analysis of a given separation. Furthermore, the mass balance around each feed section has been taken into account. The new short-cut methods are completely numerical and provide optimal design parameters with a minimum number of specifications for simple and complex configurations.

The proposed short-cut methods have been tested with highly non-ideal azeotropic mixtures and they proved to be very efficient in comparison with rigorous simulation methods. In conclusion, the new short-cut methods discussed in this paper are well suited for the synthesis of multicomponent distillation processes[10], particularly if complex configurations are involved.

Acknowledgements

The authors gratefully acknowledge financial support of the German Academic Exchange Service (DAAD).

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