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TECHNICAL NOTE

Transfer Units and Nonkey Component Distributions in Packed Columns at Total Reflux

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ABSTRACT

Analytical equations for the number of transfer units (NTU) for multicomponent packed column systems at total reflux have been derived. These expressions are the packed column equivalents of Fenske's equation for staged columns. Two cases are considered in this paper: 1) all mass transfer resistance is assumed to occur in the vapor phase and 2) all mass transfer resistance is assumed to occur in the liquid phase. Using a characterizing parameter (C), it is seen that the distribution ratios of the nonkey components in a given system differ for both packed column cases, which in turn differ from the staged column case. Finally, it is shown that some nonvolatile component may be overheaded in the case where all mass transfer resistance is in the vapor phase, while some component of infinite volatility may be bottomed in the case where all mass transfer resistance is in the liquid phase.

INTRODUCTION

Fenske's equation (1) for the minimum number of theoretical equilibrium stages required to obtain a given separation between two key components, the light (in volatility) key (LK) and the heavy key (HK), in a multicomponent system is well-known as a useful tool to those working in the field of distillation column design. Fenske's equation also yields the distribution ratios of the nonkey components at total reflux, which approximate the actual distribution ratios found near typical optimum reflux ratios (2).

As King (3) states: "In the continuous-contact process, equilibrium is not attained. . . ." Thus, packed columns are not equilibrium devices, and we suggest that they should not generally be calculated by theoretical equilibrium stage methods. It would be useful for designers to have available equations similar to the Fenske equation to properly handle multicomponent packed column systems. These expressions would be used to establish the minimum number of transfer units required for a given separation as well as estimates for the distribution ratios of any nonkey components in the system. However, even in this day of renewed interest in using various packing materials as vapor/liquid contacting devices, there do not appear to be any equations for minimum transfer units and nonkey component distributions available for multicomponent systems. An equation for the minimum number of transfer units for binary systems does exist (4–6), but only for the case where all mass transfer resistance is in the vapor phase.

DISCUSSION

A general model, applicable at total reflux for stages, trays (trays are not discussed in this Technical Note), and packing, can be derived from the Murphree vapor efficiency equations (7) as written for the two key components in a multicomponent system at total reflux. Solving the model for Murphree vapor efficiencies of unity for the key components yields the Fenske equation:

$$N(\mathrm{MIN}) = \frac{\ln[\mathrm{DR(LK)}/\mathrm{DR(HK)}]}{\ln[\alpha(\mathrm{LK,HK})]} \tag{1}$$

where DR(I) is the distribution ratio, D(I)/B(I), of a component between top (D) and bottom (B) products, for the two key components, and α(LK,HK) is the constant relative volatility between the key components.

It is seen that N(MIN), the minimum number of theoretical equilibrium stages, depends only on the separation specifications of the two key components; the nonkey components do not enter into Eq. (1). The distribution ratios of the nonkey (NK) components are calculated from the relationship

$$\mathrm{DR(NK)} = \mathrm{DR(LK)}^{C(\mathrm{NK,S})} \cdot \mathrm{DR(HK)}^{[1 - C(\mathrm{NK,S})]} \tag{2}$$

where S refers to stages. The characterizing parameter C(NK,S) is different for each component and is given by

$$C(\mathrm{NK,S}) = \frac{\ln[\alpha(\mathrm{NK,HK})]}{\ln[\alpha(\mathrm{LK,HK})]} \tag{3}$$

Solving the model for packed column conditions (infinite trays at infinitesimal Murphree vapor efficiency for the key components), permits the derivation of the equation for the minimum number of transfer units required to obtain a given separation of two key components in a multicomponent packed column system at total reflux.

$$\mathrm{NTU(OV,MIN)} = \frac{\ln\left[\dfrac{\mathrm{DR(LK)}}{\mathrm{DR(HK)}}\,\alpha(\mathrm{LK,HK})\right]}{\alpha(\mathrm{LK,HK}) - 1} + \ln\left(\frac{\mathrm{D}}{\mathrm{B}}\right) \tag{4}$$

where NTU(OV,MIN) is the minimum number of transfer units for the case where all mass transfer resistance is in the vapor phase. The other variables are as described for Eq. (1).

The first term on the right-hand side of Eq. (4) depends only on the specifications of the two key components as in Eq. (1). This term normally dominates NTU(OV,MIN). There is, additionally, a second term that depends on the feed composition and the α(NK,HK) values of the nonkey components. This is the top product/bottom product molar ratio. There is no corresponding term in Eq. (1). When D equals B, this second term vanishes. Note that NTU does not vanish at infinite α(LK,HK) value as *N*(MIN) does in Eq. (1).

The D/B ratio for a packed column is not the same as for a staged column, but may be calculated from equations similar in form to Eqs. (2) and (3). For Eq. (4), the required equations as derived from the total reflux model are:

$$\mathrm{DR(NK,OV)} = \mathrm{DR(LK)}^{\mathrm{C(NK,OV)}} \cdot \mathrm{DR(HK)}^{[1 - \mathrm{C(NK,OV)}]} \tag{5}$$

with

$$\mathrm{C(NK,OV)} = \frac{\alpha(\mathrm{NK,HK}) - 1}{\alpha(\mathrm{LK,HK}) - 1} \tag{6}$$

The DR(NK) are calculated for the nonkey components and the D/B ratio obtained from Eq. (7), where the summation is over all (nc) components, and Eq. (8). For a unit feed and two-product column, we have for the tops rate

$$\mathrm{D} = \sum_{\mathrm{I}=1}^{\mathrm{nc}} \left[\frac{\mathrm{DR(I)} \cdot \mathrm{X(I,F)}}{1 + \mathrm{DR(I)}}\right] \tag{7}$$

where X(I,F) denotes the feed composition. The bottom rate is

$$\mathrm{B} = 1 - \mathrm{D} \tag{8}$$

Once the DR(I) are in hand, D/B can be calculated and then NTU(OV,MIN). Note from Eqs. (5) and (6) that a completely nonvolatile component will still distribute (slightly) to the top product, especially for small numbers of transfer units, when all the resistance to mass transfer is in the vapor phase.

Similarly, if the composition of both keys in both products is found through the use of Eqs. (5) through (8), then the D/B term vanishes and NTU(OV,MIN) can be determined from

$$\mathrm{NTU(OV,MIN)} = \frac{\ln\left\{\dfrac{\left[\dfrac{X(LK,D)}{X(LK,B)}\right]}{\left[\dfrac{X(HK,D)}{X(HK,B)}\right]}\alpha(LK,HK)\right\}}{\alpha(LK,HK) - 1} \tag{9}$$

This result, in various forms (4–6), is known for binaries, but apparently never has been extended to multicomponent systems. We see here that the binary equation can be used for multicomponent systems if the composition of the key components in the products is known and the α between the keys is used.

A similar model and analysis can be made for the case where all resistance to mass transfer is in the liquid phase. Here the Murphree liquid efficiency equation (7) is used. Efficiencies of unity for the key components again yield Eq. (1). When infinitesimal efficiencies for the key components and infinite trays are inserted into the model, the resulting relationships corresponding to Eqs. (4), (5), (6), and (9) are found to be

$$\mathrm{NTU(OL,MIN)} = \frac{\ln\left[\dfrac{DR(LK)^{\alpha(LK,HK)}}{DR(HK)}\right]}{\alpha(LK,HK) - 1} - \ln\left(\frac{D}{B}\right) \tag{10}$$

$$DR(NK,OL) = DR(LK)^{C(NK,OL)} \cdot DR(HK)^{[1 - C(NK,OL)]} \tag{11}$$

$$C(NK,OL) = C(NK,OV) \cdot \alpha(LK,HK)/\alpha(NK,HK) \tag{12}$$

$$\mathrm{NTU(OL,MIN)} = \frac{\ln\left\{\dfrac{\left[\dfrac{X(LK,D)}{X(LK,B)}\right]^{\alpha(LK,HK)}}{\left[\dfrac{X(HK,D)}{X(HK,B)}\right]}\right\}}{\alpha(LK,HK) - 1} \tag{13}$$

Again, NTU does not vanish at infinite α(LK,HK). Also, note from Eqs. (11) and (12) that a nonkey component of infinite volatility will still distribute (slightly) to the bottom product, especially at low numbers of transfer units, when all the resistance to mass transfer is in the liquid phase. When these two equations are compared to Eqs. (5) and (6), it is seen that the distribution ratios are different for the two packed column modes.

Equations (10) through (12) will generally give different values than Eqs. (4) through (6) as shown in the following example problem.

ILLUSTRATIVE PROBLEM

Assuming total reflux, we will complete the material balance and determine the minimum steps required for the multicomponent distillation given below. We will consider the three cases of 1) theoretical equilibrium stages, 2) packing with all resistance to mass transfer in the vapor phase, and 3) packing with all resistance to mass transfer in the liquid phase. R refers to recovery fraction and here equals D(I)/X(I,F), the amount of component I in the top product divided by the amount of component I in the feed. R(I) is related to the distribution ratio by the relationship

$$R(I) = DR(I)/[1 + DR(I)]$$

Component	X(I,F)	(I,HK)	R(I)
1	0.1	2.5	
2(LK)	0.3	2.0	0.99
3	0.1	1.5	
4(HK)	0.3	1.0	0.01
5	0.1	0.5	
6	0.1	0.0	

Theoretical Equilibrium Stages

First, we calculate C(NK,S) from Eq. (3). Next we calculate DR(NK,S) from Eq. (2). After the R(NK,S) are calculated from the DR(NK,S), we complete the material balance as follows:

Component	(CI,S)	DR(I,S)	R(I,S)	X(I,F)	D(I,S)	B(I,S)
1	1.3219	9801	0.999476	0.1	0.099948	0.000052
2(LK)	(1.0)	99	0.990000	0.3	0.297000	0.003000
3	0.5850	1	0.685858	0.1	0.068586	0.031414
4(HK)	(0.0)	0.0101	0.010000	0.3	0.003000	0.297000
5	−1.0	1.0306E-6	1.0306E-6	0.1	1.0202E-7	0.100000
6	−inf.	0.0	0.0	0.1	0.0	0.100000
			Total	1.0	0.468534	0.531466

Finally, by Eq. (1), N(MIN) is 13.259. This value depends only on the two key components and could have been calculated before completing the material balance for all components.

Packing with All Mass Transfer Resistance in the Vapor Phase

First, we calculate C(NK,OV) from Eq. (6). Next, we calculate DR(NK,OV) from Eq. (5). After the R(NK,OV) are calculated from the DR(NK,OV), we complete the material balance as follows:

Component	C(I,OV)	DR(I,OV)	R(I,OV)	X(I,F)	D(I,OV)	B(I,OV)
1	1.5	9801	0.999898	0.1	0.09999	0.00001
2(LK)	(1.0)	99	0.990000	0.3	0.29700	0.00300
3	0.5	1	0.500000	0.1	0.05000	0.05000
4(HK)	(0.0)	0.0101	0.010000	0.3	0.00300	0.29700
5	−0.5	1.0202E-4	1.0202E-4	0.1	1.0202E-5	0.09999
6	−1.0	1.0306E-6	1.0306E-6	0.1	1.0306E-7	0.10000
			Total	1.0	0.45	0.55

Finally, we find NTU(OV,MIN) from Eq. (4) with:

$$D = 0.45$$

$$B = 0.55$$

$$DR(LK) = 99$$

$$DR(HK)\ 1/99$$

$$\alpha(LK,HK) = 2.0$$

Thus, NTU(OV,MIN) = 13.585. If the keys products compositions are calculated from the above table, then Eq. (9) gives the same results.

Packing with All Mass Transfer Resistance in the Liquid Phase

First, we calculate C(NK,OL) from Eq. (12). Next we calculate DR(NK,OL) from Eq. (11). After the R(NK,OL) are calculated from the DR(NK,OL), we complete the material balance as follows:

Component	C(I,OL)	DR(I,OL)	R(I,OL)	X(I,F)	D(I,OL)	B(I,OL)
1	1.2	622.14	0.998395	0.1	0.099840	0.000160
2(LK)	(1.0)	99	0.990000	0.3	0.297000	0.003000
3	2/3	4.626	0.822256	0.1	0.082226	0.017774
4(HK)	(0.0)	0.0101	0.010000	0.3	0.003000	0.297000
5	−2.0	1.052E-10	1.052E-10	0.1	0.0	0.1
6	−inf.	0.0	0.0	0.1	0.0	0.1
			Total	1.0	0.482065	0.517935

Finally, we find NTU(OL,MIN) from Eq. (10) with:

$$D = 0.482065$$

$$B = 0.517935$$

$$DR(LK) = 99$$

$$DR(HK) = 1/99$$

$$\alpha(LK,HK) = 2.0$$

Thus, NTU(OL,MIN) = 13.857. If the keys products compositions are calculated from the above table, then Eq. (13) gives the same results.

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