

SHORTCUT MODELS FOR DISTILLATION COLUMNS -

I. STEADY-STATE BEHAVIOR

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Abstract

Jafarey et al. (1979) derived a simple analytical expression for the separation factor S . This paper provides a simpler and more instructive derivation of this expression, and also evaluates its validity for estimating steady-state gains and RGA-values. The results show that the expression gives a good estimate of how S changes with internal flows, but describes poorly its variation with external flows. Fortunately, when computing the steady-state gains, this error is often not important.

1. INTRODUCTION

Shortcut models. Simple “shortcut” models are useful for analyzing and understanding the strongly nonlinear behavior of distillation columns. For robust distillation column control, for example, it is important to know the correlation between the transfer matrix elements as they vary with operating conditions. The essential part of this behavior may be predicted from simple analytical models.

This paper presents a derivation and evaluation of analytical expressions for the separation factor S which is useful for steady-state calculations. In Part II (Skogestad and Morari, 1987a) we discuss the dynamic behavior and present an analytical expression for the dominant time constant. Though our main goal is to develop shortcut models for use in control system design, the results presented in these two papers are useful for obtaining general insight into distillation column behavior. For example, simple analytical models are invaluable as a teaching tool; a basic understanding of distillation columns is much more easily acquired by analyzing simple analytical models than by running tray-by-tray simulation programs.

We stress that the shortcut models presented are not intended to replace tray-by-tray simulations; for design purposes we recommend that more accurate models are obtained using simulation programs.

Steady-state behavior. A simple nonlinear steady-state model is useful for deriving analytical expressions for the gains g_{ij} between the process inputs (e.g., reflux L and boilup V for the LV-configuration) and the controlled outputs (top and bottom compositions, y_D and x_B).

$$\begin{aligned} dy_D &= g_{11}dL + g_{12}dV \\ dx_B &= g_{21}dL + g_{22}dV \end{aligned} \tag{1}$$

To derive these gains analytically, two equations relating y_D and x_B to L and V and other operating variables for the column are needed. One is given by the overall

material balance for the light component

$$Fz_F = Dy_D + Bx_B \quad (2)$$

and the other is conveniently written in terms of the separation factor S (Shinskey, 1984)

$$S = \frac{y_D/1 - y_D}{x_B/1 - x_B} \approx \frac{1}{x_B(1 - y_D)} \quad (3)$$

(the approximation holds for high-purity separations with $y_D \approx 1$ and $(1 - x_B) \approx 1$).

S is in general a complex function of the operating and design variables for the column (flow rates, feed composition, VLE-data for system, number of trays, feed location, etc.). There are three reasons for choosing to express the column behavior in terms of S :

- (1) Reasonably simple and reliable expressions may be derived for S . This is motivated by Fenske's total reflux equation $S = \alpha^N$ which is exact for mixtures with constant relative volatility α .
- (2) Usually S does not change much with operating conditions. The essential part of the variation of the gains g_{ij} with operating conditions may therefore be captured by assuming S is constant.
- (3) S as defined by (3) is a function of y_D and x_B only. This makes it simple to derive analytical expressions for the steady-state gains.

There are other ways of expressing shortcut models for distillation columns, besides using S . For example, Gilliland's empirical correlation relates $\frac{R - R_{min}}{R + 1}$ to $\frac{N - N_{min}}{N + 1}$, and analytical equations have been derived to fit the correlation. However, this form is not convenient for obtaining analytical expressions for the gains, since it does not satisfy (2) and (3) above.

The separation factor S has been used extensively by Shinskey (1984) for predicting the steady-state value of the RGA. The 1-1 element of the RGA is

$$\lambda_{11} = \left(1 - \frac{g_{12}g_{21}}{g_{11}g_{22}} \right)^{-1} \quad (4)$$

For columns with both products of high purity Skogestad and Morari (1987b) derived the following approximations for the LV - and DV - configurations

$$\lambda_{11}(G_{LV}) \approx \frac{1}{D(1 - y_D) + Bx_B} \frac{1}{(\partial \ln S / \partial L)_D} \quad (5)$$

$$\lambda_{11}(G_{DV}) \approx \frac{1}{1 + \frac{Bx_B}{D(1 - y_D)}} \quad (6)$$

Consequently, a good model for S is needed to evaluate the RGA for the LV-configuration, but is less important for the DV-configurations. Also note that λ_{11} for the LV-configuration may be very large if both products are of high purity, while the value for the DV- configuration is always between 0 and 1.

Shinskey uses the simple analytical model for S developed by Jafarey et al. (1979) to estimate the RGA. In their paper, Jafarey et al. only checked the validity of the model for predicting the total number of theoretical trays. However, to estimate steady-state gains (g_{ij}) and RGA-values, *derivatives* of the model are needed. The objective of our paper is to check the models validity for estimating gains and the RGA.

We also feel that the derivation by Jafarey et al. does not provide much insight. They start from Smokers exact analytical solution, derive a simplified model which is not very good, delete some terms in this model, and finally arrive at a better model. Another goal of this paper is therefore to rederive Jafarey's model in a more direct manner which yields more insight. Our derivation yields a slightly different form of the model, but it reduces to Jafarey's expression if the assumption $D/F \approx z_F$ is made.

Assumptions. All the results in this paper are for a two-product column, binary mixture with constant relative volatility (α) and constant molar flows. The extension to multicomponent mixtures is discussed at the end of the paper.

2. CASE STUDY EXAMPLES

In this section we present steady-state data for seven high-purity distillation columns which may be used as case study examples in this and future work. The columns were selected to include a wide range of operating conditions. Data for the columns are given in Table 1, together with computed values for R/R_{min} , L/F and D/F .

Steady-state gains. The exact steady-state gain matrices for the seven columns were obtained by linearizing the material balance for each tray. For tray i with no feed

$$L(x_{i+1} - x_i) + V(y_{i-1} - y_i) = 0, \quad y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i} \quad (7)$$

Linearizing (7) for small perturbations

$$(x_{i+1} - x_i)dL + (y_{i-1} - y_i)dV + Ldx_{i+1} + (-L - K_iV)dx_i + K_{i-1}Vdx_{i-1} = 0 \quad (8)$$

where K_i is the linearized VLE-constant on each tray

$$K_i = \frac{dy_i}{dx_i} = \frac{\alpha}{(1 + (\alpha - 1)x_i)^2} \quad (9)$$

In matrix form (8) becomes

$$Ax + Bu + Ed = 0, \quad y = Cx \quad (10)$$

Here $x = (dx_1 \dots dx_N)^T$ are the tray compositions, $u = (dL \ dV)^T$ are the inputs, $d = (dF \ dz_F)^T$ are the disturbances, and $y = (dy_D \ dx_B)^T$ are the outputs. Solving these equations give

$$y = -CA^{-1}Bu - CA^{-1}Ed$$

and the steady-state gain matrix and disturbance matrix are

$$G = -CA^{-1}B \quad \text{and} \quad G_d = -CA^{-1}E \quad (11)$$

These matrices are given for the seven columns in Table 2. They are given both for the LV - and the DV -configurations:

$$\text{LV - configuration : } \begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G_{LV} \begin{pmatrix} dL \\ dV \end{pmatrix} + G_{dLV} \begin{pmatrix} dF \\ dz_F \end{pmatrix} \quad (12a)$$

$$\text{DV - configuration : } \begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G_{DV} \begin{pmatrix} dD \\ dV \end{pmatrix} + G_{dDV} \begin{pmatrix} dF \\ dz_F \end{pmatrix} \quad (12b)$$

Note that G_{LV} and G_{DV} are not independent. Because of the assumption of constant molar flows we have $dL = dV - dD$ which yields

$$\begin{pmatrix} dL \\ dV \end{pmatrix} = M \begin{pmatrix} dD \\ dV \end{pmatrix} \text{ where } M = \begin{bmatrix} -1 & 1 \\ 0 & 1 \end{bmatrix}$$

and we derive

$$G_{DV} = G_{LV}M \quad (13)$$

Similar relationships are easily derived for other choices of manipulated inputs (Skogestad and Morari, 1987b). The matrix G_{LV} is very sensitive to small relative errors in the elements (as is seen from the large value of λ_{11} (Skogestad and Morari, 1987c)), while G_{DV} is insensitive to such errors. The reader should therefore find G_{LV} from $G_{LV} = G_{DV}M^{-1}$ rather than using the G_{LV} -matrix given in Table 2. The disturbance matrices G_{dLV} and G_{dDV} are in general different, but happen to be equal in this case since the feed is liquid.

3. A SIMPLE EXPRESSION FOR S

Previous Work

For mixtures with constant relative volatility (α) the following exact expressions for N_{min} and R_{min} hold (e.g., Henley and Seader, 1981).

$$R \rightarrow \infty : S = \alpha^{N_{min}} \quad (\text{Fenske}) \quad (14)$$

$$N \rightarrow \infty : R_{min} = \frac{1}{\alpha - 1} \left(\frac{y_D}{x_F} - \alpha \frac{1 - y_D}{1 - x_F} \right) \approx \frac{1}{\alpha - 1} \frac{1}{x_F} (y_D \approx 1) \quad (15)$$

x_F is the composition of the flashed feed. Simple extensions to multicomponent mixtures exist (e.g., Henley and Seader). Jafarey, Douglas and McAvoy (1979)

derived a simple expression for S which has also been adopted by Shinskey (1984).

For liquid feed we have $x_F = z_F$ and Jafarey's expression becomes

$$q_F = 1 : \quad S = \alpha^N \left(\frac{1}{1 + 1/(Rz_F)} \right)^{N/2} \quad (16)$$

The expression (16) gives the correct limiting value (14) as $R \rightarrow \infty$, but its value of R_{min}

$$N \rightarrow \infty : \quad R_{min} = \frac{1}{(\alpha^2 - 1)z_F} \quad (17)$$

is lower than the correct one (15). Jafarey et al. used (16) for design purposes to find the number of theoretical stages N needed to accomplish a given separation. For 24 cases studied the average error in N was 5.3% compared to 2.5% for the Gilliland correlation.

Derivation of Expression for S

The main reason for including this section is that the derivation given here is much simpler and more instructive than the one given by Jafarey et al. Furthermore, extension to multicomponent mixtures is straightforward. We will initially linearize the vapor-liquid equilibrium (VLE) curve in the top and bottom parts of the column.

$$\text{Above feed :} \quad (1 - y_i) = \frac{1}{\alpha_T}(1 - x_i) \quad (18a)$$

$$\text{Below feed :} \quad y_i = \alpha_B x_i \quad (18b)$$

Here α_T and α_B denote the relative volatility in the top and bottom part of the column. The assumption of linear VLE will clearly make the separation in the middle of the column simpler as seen from Fig. 1. Note that for high-purity columns, most of the stages will be at the column ends in the regions of high purity where the linear approximation is good. The operating lines (material balance of light component for each tray) are

$$\text{Above feed :} \quad V_T y_{i-1} = L_T x_i + D y_D \quad (19a)$$

$$\text{Below feed : } \quad L_B x_{i+1} = B_B y_i + B x_B \quad (19b)$$

Since the equilibrium and operating lines are assumed linear it is simple to derive exact relationships between the feed tray composition and y_D and x_B . Consider the top part of the column. The vapor composition of the heavy component $(1 - y_j)$ on the j th tray from the top is found by repeated use of (18a) and (19a) (Kremser equations, see McCabe and Smith, 1976).

$$(1 - y_j) = (1 - y_D) \left(A_T^j + \frac{(A_T^j - 1)(1 - L_T/V_T)}{A_T - 1} \right) \quad (20)$$

where A_T is the absorption factor

$$A_T = \frac{L_T/V_T}{1/\alpha_T} \quad (21)$$

Since $A_T > 1$ we have $A_T^j \gg 1$ for j large. Using this assumption for the feed tray we derive

$$(1 - y_{NF}) \approx (1 - y_D) A_T^{N_T} \left(\frac{A_T - L_T/V_T}{A_T - 1} \right) \quad (22)$$

where N_T is the number of theoretical stages above the feed. Similarly, we derive for the bottom section of the column an expression for the liquid composition on the feed tray

$$\begin{aligned} x_{NF} &= x_B \left(A_B^{-N_B} + \frac{(A_B^{-N_B} - 1)(1 - V_B/L_B)}{A_B^{-1} - 1} \right) \\ &\approx x_B A_B^{-N_B} \left(\frac{A_B^{-1} - V_B/L_B}{A_B^{-1} - 1} \right) \end{aligned} \quad (23)$$

Here N_B is the number of theoretical trays below the feed and $A_B < 1$ is the absorption factor in the bottom part of the column

$$A_B = \frac{L_B/V_B}{\alpha_B} \quad (24)$$

Multiplying equations (22) and (23) gives an approximate expression for the separation factor S :

$$S \approx \frac{1}{x_B(1 - y_D)} = \frac{\alpha_B^{N_B} \alpha_T^{N_T}}{(1 - y_{NF}) x_{NF}} \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \cdot c \quad (25)$$

$$c = \frac{(\alpha_T - 1)(\alpha_B - 1)}{(\alpha_T - V_T/L_T)(\alpha_B - L_B/V_B)}$$

In most cases c is close to one; in particular, this is the case if the reflux is high. Assuming constant relative volatility $\alpha = \alpha_B = \alpha_T$ and using $\alpha = \frac{y_{NF}/1 - y_{NF}}{x_{NF}/1 - x_{NF}}$ and $N = N_B + N_T + 1$ we derive from (25)

$$S = \frac{\alpha^N}{y_{NF}(1 - x_{NF})} \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \cdot c \quad (26)$$

We know that S predicted by (26) is too large because of the linearized VLE. However, (26) may be corrected to satisfy the exact relationship $S = \alpha^N$ at infinite reflux simply by dropping $1/y_{NF}(1 - x_{NF})$ from (26). By assuming in addition $c = 1$ we get

$$S = \alpha^N \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \quad (27)$$

This expression is somewhat misleading since it suggests that the separation may always be improved by transferring stages from the bottom to the top section if $(L/V)_T > (L/V)_B$. This is clearly not generally true, and to avoid this problem we follow Jafarey et al. (1979) and choose $N_T \approx N_B \approx N/2$ and derive the alternative expression

$$S = \alpha^N \left(\frac{(L/V)_T}{(L/V)_B} \right)^{N/2} \quad (28)$$

If the feed is liquid then $V_B = V_T$ and

$$q_F = 1 : \quad S = \alpha^N \left(\frac{L_T}{L_B} \right)^{N/2} = \alpha^N \left(\frac{L}{L + F} \right)^{N/2} \quad (28a)$$

Since $L/F = \frac{L}{D} \frac{D}{F}$, this reduces to Jafarey's expression (16) if the additional assumption $\frac{D}{F} \approx z_F$ is made. Jafarey et al. derived (16) as a design equation and the assumption $\frac{D}{F} \approx z_F$ is reasonable in this case. However, the assumption is not so easy to justify for control purposes where D is a variable which may take on values different from $D = z_F F$. The assumption seems particularly misleading if the model is used to compute gains for disturbances in z_F . Table 3 gives the estimated

number of trays in the seven example columns obtained from (28) and (16). The two formulas yield almost identical values since the columns have $\frac{D}{F} \approx z_F$.

The main shortcoming of (28) is obvious from the derivation: The model is poor if a pinch zone appears around the feed plate such that the assumption that most of the trays are in the region of high or low purity which led to (26) is no longer valid. A pinch zone occurs around the feed plate if the reflux is near minimum; this explains why (16) gives a value of R_{min} (17) which is too low. More importantly, pinch zones appear above or below the feed plate if the feed location is not optimal. This is likely to happen during operation of the column. The use of (28) implicitly assumes that the feed location is optimal. Finally, for columns with large differences between N_T and N_B , (27) should be used instead of (28). We will study the validity of the models (16) and (28) for estimating steady-state gains in Section 5.

4. WHY ARE DISTILLATION COLUMNS NONLINEAR?

For the simple case of constant molar flows and constant relative volatility considered in this paper, there are two possible sources of nonlinearity

(A) Nonlinear VLE

$$y_i = \frac{\alpha x_i}{1 + (\alpha + 1)x_i} \quad (29)$$

(B) Bilinear terms (Lx_i, Vy_i , etc). in the material balance for each tray

$$Lx_{i+1} + Vy_{i-1} = Lx_i + Vy_i \quad (30)$$

None of these nonlinearities seem very strong, and the strongly nonlinear behavior observed for (high-purity) distillation columns is therefore somewhat surprising. The main reason for the nonlinear behavior is, as we will show, the nonlinear VLE.

Consider changes in product compositions (y_D and x_B) caused by a change in feed composition (z_F), when all flows, including reflux L and boilup V , are constant. In this case the material balance (30) is linear, and the only possible source of nonlinearity is the VLE.

Linear VLE. If the VLE were assumed to be linear (e.g., by linearizing (29) on each tray; $y_i = a_i x_i + b_i$), all equations describing the column behavior are linear, and a linear relationship between the product compositions and z_F results

$$y_D = k_1 z_F, \quad x_B = k_2 z_F$$

Here the gains $(\partial y_D / \partial z_F)_{L,V} = k_1$ and $(\partial x_B / \partial z_F)_{L,V} = k_2$ are constant and independent of the feed composition.

Nonlinear VLE. A completely different result is found, however, when the VLE is not linearized. The simplified model (27) for S was derived using the nonlinear VLE model (29). (Actually, the VLE was first linearized, but the final expression was corrected to match $S = \alpha^N$ at total reflux.) This model predicts that S is constant for changes in feed composition provided L and V are unchanged. Consider a column which nominally has $z_F^o = 0.5$ and $1 - y_D^o = x_B^o = 0.01$. For S constant the following two equations give y_D and x_B as a function of z_F

$$\frac{y_D(1 - x_B)}{(1 - y_D)x_B} = \frac{y_D^o(1 - x_B^o)}{(1 - y_D^o)x_B^o} = 9801 \quad (31)$$

$$z_F = \frac{D}{F} y_D + \frac{B}{F} x_B \quad (32)$$

(The second equation is the overall material balance for light component.) Note that all flows are constant, so $D/F = B/F = 0.5$ is constant. (31) and (32) clearly result in a nonlinear relationship between y_D and x_B , and z_F . The steady-state gains found by combining these equations are strongly dependent on the operating point. For example,

$$S \text{ constant : } \left(\frac{dy_D}{\partial z_F} \right)_{L,V} = \frac{1}{\frac{D}{F} + \frac{B}{F} \frac{x_B(1-x_B)}{y_D(1-y_D)}} \quad (33)$$

At the nominal operating point $(\partial y_D / \partial z_F)_{L,V} = 1$. However, for $z_F = 0.55$, (31) and (32) give $x_B = 0.10$ and $1 - y_D = 0.0092$, and the linearized gain at this

operating point is $(\partial y_D / \partial z_F)_{L,V} = 0.0202$. This is 50 times smaller than the nominal value.

The conclusion is that the nonlinear VLE results in a strongly nonlinear behavior for high-purity columns. The bilinear terms in (30) are of much less importance for the observed nonlinearity of distillation columns.

5. STEADY-STATE GAINS FROM EXPRESSION FOR S

Consider any input or disturbance ζ (for example $\zeta = L, V, B, F, z_F$, etc.). The steady-state gains $\partial y_D / \partial \zeta$ and $\partial x_B / \partial \zeta$ may be found by differentiating the material balance (2) and using the defining expression for the separation factor (3)

$$D \frac{\partial y_D}{\partial \zeta} + B \frac{\partial x_B}{\partial \zeta} = e_\zeta \quad (34)$$

$$\frac{\partial \ln S}{\partial \zeta} = \frac{1}{y_D(1-y_D)} \frac{\partial y_D}{\partial \zeta} - \frac{1}{x_B(1-x_B)} \frac{\partial x_B}{\partial \zeta} \quad (35)$$

Here e_ζ is defined as

$$e_\zeta = -(y_D - x_B) \frac{\partial D}{\partial \zeta} + F \frac{\partial z_F}{\partial \zeta} + (z_F - x_B) \frac{\partial F}{\partial \zeta} \quad (36)$$

Solving for the gains give

$$\frac{1}{(1-y_D)y_D} \frac{\partial y_D}{\partial \zeta} = \frac{1}{I_s} \left(e_\zeta + Bx_B(1-x_B) \frac{\partial \ln S}{\partial \zeta} \right) \quad (37a)$$

$$\frac{1}{(1-x_B)x_B} \frac{\partial x_B}{\partial \zeta} = \frac{1}{I_s} \left(e_\zeta - Dy_D(1-y_D) \frac{\partial \ln S}{\partial \zeta} \right) \quad (37b)$$

where I_s is the "sum" of impurities leaving the column

$$I_s = Bx_B(1-x_B) + Dy_D(1-y_D) \quad (38)$$

For high-purity separations $I_s \approx Bx_B + D(1-y_D)$. There are two contributions to the gains in (37): The e_ζ -term and the contribution from changes in the separation factor S . The e_ζ -term physically represents the effect on the gains of changing the external material balance. This is clear since $\partial D / \partial \zeta = 0$ and $e_\zeta = 0$ is obtained

when we change the internal flows in the column only (change L and V keeping D and B constant).

For changes in the external flows (which represent most disturbances and inputs) the e_ζ -term in (37) is usually dominating - at least when both products are high-purity. This means that the major contribution to the gains in this case may be obtained by assuming S constant and the exact value of $\partial \ln S / \partial \zeta$ is of minor importance in this case.

On the other hand, a good model for S is important for obtaining the gains for changes in the internal flows : In this case the gains, for example $(\partial y_D / \partial L)_D$, are directly proportional to $(\partial \ln S / \partial L)_D = (\partial \ln S / \partial V)_D$ and a good estimate of this quantity is required for estimating the correct value of the gain.

Estimating $\partial \ln S / \partial \zeta$ from shortcut models

Equations (37) are exact. I_s is a given constant and e_ζ is trivial to find for the case of constant molar flows. The only “unknown” in (37) is $\partial \ln S / \partial \zeta$, which may be estimated from the shortcut models (28) or (16). Analytic expressions for $\partial \ln S / \partial \zeta$ obtained with these models for different choices of ζ are given in Table 4. Estimated numerical values of $\partial \ln S / \partial \zeta$, and of the gains and the RGA for the LV-configuration are compared with exact values for the seven columns in Table 5-7 and Fig.2. The results are discussed below for each shortcut model.

Using the model (28) for $\ln S$. From Table 5 we see that, with the exception of $(\partial \ln S / \partial V)_D$, the estimates of $\partial \ln S / \partial \zeta$ are extremely poor. Note that because of the assumption of constant molar flows we have

$$\left(\frac{\partial \ln S}{\partial V} \right)_D = \left(\frac{\partial \ln S}{\partial V} \right)_L + \left(\frac{\partial \ln S}{\partial L} \right)_V \quad (39)$$

and even though the two terms $(\partial \ln S / \partial V)_L$ and $(\partial \ln S / \partial L)_V$ individually are estimated very poorly with (28), the estimate of the sum $(\partial \ln S / \partial V)_D$ is in reasonable agreement (Fig.2). Also note from Fig. 2 that $(\partial \ln S / \partial V)_L$ and $(\partial \ln S / \partial L)_V$

are very sensitive to the feed point location, while their sum $(\partial \ln S / \partial V)_D$ is nearly constant. The conclusion is that the model (28) is only useful for estimating the effect of changing the internal flows on S

$$\left(\frac{\partial \ln S}{\partial V}\right)_D = \left(\frac{\partial \ln S}{\partial L}\right)_D \quad (40)$$

Fortunately, as pointed out above, this corresponds exactly to the case when the term $\partial \ln S / \partial \zeta$ in (37) is most important. Therefore, in spite of the generally poor estimates of $\partial \ln S / \partial \zeta$, the model (28) can be useful for estimating steady-state gains and the RGA (recall Eq. (5)). This will in particular be the case for columns with both products of high purity. In other cases the errors may be significant. This is evident by comparing the estimated steady-state gain matrices in Table 7 with the exact values in Table 2.

Using Jafarey's model (16) for $\ln S$. As seen from Table 5 and 6, the estimated values for $(\partial \ln S / \partial V)_D$ are very similar to those found using (28). The estimated values for $\partial \ln S / \partial \zeta$ with respect to changes in the external material balance are again poor. Surprisingly, the values are also very different from what is obtained using (28). The estimated steady-state gain matrices are also very different for the two models in some cases as seen from Table 7. Shinskey (1984) uses the model (16) to estimate the RGA. This estimate can be quite poor as seen from Table 8. The model (28) seems to be somewhat better than (16) for estimating the RGA.

Choice of Model for $\ln S$

The two seemingly very similar shortcut models (16) and (28) for $\ln S$ may result in quite different estimates for the steady-state gain matrices (Table 7). None of the models give very accurate results, but they may still be useful for obtaining a first estimate. Based on the numerical results presented above, there is no reason to give preference to one of the models (16) or (28). However, the assumption $D \approx z_F F$ which led to (16) does not seem to be justified from a theoretical point of

view, and we therefore recommend using (28), which also gives simpler analytical expressions for $\partial \ln S / \partial \zeta$ (Table 4).

6. A NEW FORMULA FOR THE OPTIMAL FEED LOCATION

Equations (22) and (23) are reasonably accurate if most of the trays are located in the region of high and low purity. Divide equation (22) by (23) and assume the feed plate is optimally located such that $x_{N_F} = x_F$ and $y_{N_F} = y_F$

$$\frac{1 - y_F}{x_F} = \frac{1 - y_D}{x_B} \alpha^{N_T - N_B} \frac{(L/V)_T^{N_T}}{(V/L)_B^{N_B}} \frac{\alpha - (L/V)_B}{\alpha - (V/L)_T} \quad (41)$$

As a crude approximation neglect the last two terms. This approximation is reasonable if N_T and N_B are not too different since $(L/V)_T$ and $(V/L)_B$ are often reasonably close in magnitude. (41) then gives

$$N_T - N_B = \frac{\ln \frac{1 - y_F}{x_F} \frac{x_B}{1 - y_D}}{\ln \alpha} \quad (42)$$

x_F and y_F are functions of z_F, q_F and α and are obtained by flashing the feed. The optimal feed tray location is then given by

$$N_F = N_B + 1 = \frac{N + 1 - (N_T - N_B)}{2} \quad (43)$$

(N is the total number of theoretical stages.) Estimated and exact values of the optimal feed stage locations are shown for the seven columns in Table 9. The exact value is found using Stoppel (1946) (for the feed as liquid $N_F = n_2 + 1$, where n_2 is found from Stoppel's paper). The average error $|\Delta N_F|$ in percent of $N/2$ for the seven columns using (42) is 7.0%. This compares to 12.2% when using the Fenske ratio (Henley and Seader, 1981)

$$\frac{N_T}{N_B} = \frac{\ln \left(\frac{y_D}{1 - y_D} \frac{1 - z_F}{z_F} \right)}{\ln \left(\frac{1 - x_B}{x_B} \frac{z_F}{1 - z_F} \right)} \quad (44)$$

and 18.0% when using the empirical Kirkbride formula (Henley and Seader, 1981)

$$\frac{N_T}{N_B} = \left[\frac{1 - z_F}{z_F} \frac{B}{D} \left(\frac{x_B}{1 - y_D} \right)^2 \right]^{0.206} \quad (45)$$

(The crude estimate $N_F = N/2$ gives an average error of 20.0%). We also computed the optimal feed point location for the 24 columns given by Jafarey et al. (1979). (There is a misprint in this paper, and R/R_{min} should be 1.75 for case b). The following average errors were found

	$\frac{ \Delta N_F }{N/2}$
This work (42)	4.4%
Fenske ratio (44)	15.7%
Kirkbride (45)	12.8%

7. EXTENSIONS TO MULTICOMPONENT MIXTURES

Define separation in terms of two key components (L and H), and define the pseudo-binary values of composition and flows (superscript ') by considering only these key components. For example

$$y' = y'_L = \frac{y_L}{y_L + y_H} \quad , \quad V' = V(y_L + y_H) \quad (46)$$

(as usual the subscript L has been dropped for the light component). The nonkey components are assumed to be non-distributing; the heavy nonkey (HN) is assumed to have much lower relative volatility than the heavy key (H). Also, the light nonkey (LN) is assumed to have much higher relative volatility than the light key (L). Under these assumptions (27) still holds if a pseudo-binary basis is used (Appendix):

$$S = \frac{y'_D/1 - y'_D}{x'_B/1 - x'_B} = \alpha^N \frac{(L'/V')_T^{N_T}}{(L'/V')_B^{N_B}} \quad (47)$$

where as before

$$\alpha = \frac{y_L/y_H}{x_L/x_H} = \frac{y'/1 - y'}{x'/1 - x'} \quad (48)$$

The material balance may also be written on a pseudo-binary basis

$$F' z'_F = B' x'_B + D' y'_D \quad (49)$$

Consequently, all the gain equations (34)-(38) derived above still apply when a pseudo-binary basis is used.

Similarly, Eq. (42) for the optimal feed point location applies if x_B, y_D, y_F and x_F are replaced by the pseudo-binary values x'_B, y'_D, y'_F and x'_F .

8. CONCLUSION

It is convenient to express the column behavior in terms of the separation factor

$$S = \frac{y_D(1 - x_B)}{(1 - y_D)x_B} \quad (3)$$

S is often nearly constant for varying operating conditions. For columns with constant relative volatility and constant molar flows, Fenske's exact equation applies at total reflux

$$S = \alpha^N \quad (4)$$

For finite reflux the following generalization is useful

$$S = \alpha^N \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \quad (27)$$

This model gives a good description of how S changes with the internal flows, but describes poorly the effect of changes in the external material balance. Fortunately, it turns out that this is of less importance if the model for S is used to obtain estimates for the steady state gains.

Finally, a new formula for estimating the optimal feed stage location is proposed

$$N_T - N_B = \frac{\ln \frac{1-y_F}{x_F} \frac{x_B}{1-y_D}}{\ln \alpha} \quad (42)$$

From its derivation we know that this formula may give poor results if N_T and N_B are very different, but it gave better results than other proposed methods for the seven columns in Table 1 and for the 24 columns studied by Jafarey et al. (1979).

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NOMENCLATURE

B - bottom product rate

D - distillate (top product) rate

F - feed rate

$L_T = L$ - liquid flow in top section of column

$L_B = L + q_F F$ - liquid flow in bottom section of column

N_B - number of theoretical trays below feed (incl. reboiler)

$N_F = N_B + 1$ - feed tray location

N_T - number of theoretical trays above feed

$N = N_B + N_T + 1$ - total number of theoretical trays in column

q_F - fraction of liquid in feed

$R = L/D$ - reflux ratio

$S = \frac{y_D(1-x_B)}{(1-y_D)x_B}$ - separation factor

$V_B = V$ - vapor flow in bottom section of column

$V_T = V + (1 - q_F)F$ - vapor flow in top part of column

x_B - mole fraction of light component in bottom product

x_i - liquid mole fraction of light component on stage i

x_F, y_F - mole fraction in feed at feed stage pressure

x_{N_F}, y_{N_F} - mole fractions on feed tray

$y_D = x_D$ - mole fraction of light component in distillate (top product)

y_i - vapor mole fraction of light component on stage i

Subscripts

B - bottom part of column, bottom product

D - distillate product

T - top part of column

i - tray no. numbered from bottom ($i=1$ for reboiler, $i=2$ for first tray,
 $i=N$ for top tray, $i=N+1$ for condenser)

Superscript

' - pseudo-binary basis is used

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APPENDIX

Extensions to multicomponent mixtures

The relative volatility between the key components is defined as (subscript i for the tray is dropped)

$$\alpha = \frac{y_L/x_L}{y_H/x_H} = \frac{y'(1-x')}{x'(1-y')} \quad (48)$$

Bottom section. From (48) we get

$$y_L = \left(\alpha_B \frac{y_H}{x_H}\right)x_L = \hat{\alpha}_B x_L \quad (A1)$$

In Section 3 we linearized the VLE by assuming $y_H \approx 1$ and $x_H \approx 1$, but the last approximation does not hold in presence of heavy nonkey-components (HN). Assuming $y_{HN} \approx 0$ (i.e., the heavy nonkey has very low relative volatility) we get

$$x_{HN} \approx \frac{z_{HN}F}{L_B}$$

and we find $y_H \approx 1$ and $x_H \approx 1 - x_{HN} = 1 - \frac{z_{HN}F}{L_B}$, i.e.,

$$\hat{\alpha}_B = \alpha_B \left(1 - \frac{x_{HN}F}{L_B}\right) \quad (A2)$$

and we have a linear VLE relationship for the bottom section. This leads to an expression for x_{LN_F} similar to (23) but with α_B replaced by $\hat{\alpha}_B$.

Top section. From (48) we get

$$y_H = \left(\frac{1}{\alpha_T} \frac{y_L}{x_L}\right)x_H = \frac{1}{\hat{\alpha}_T} x_H \quad (A3)$$

A derivation similar to the one for the bottom section yields

$$\hat{\alpha}_T = \frac{\alpha_T}{1 - z_{LN}F/V_T} \quad (A4)$$

This leads to an expression for y_{HN_F} as a function of y_{HD} similar to (22), but with α_T replaced by $\hat{\alpha}_T$.

Note that Fenske's expression for S at infinite influx is exact also when there are nonkey components.

$$S = \frac{y_{LD}/x_{LD}}{y_{HD}/x_{HD}} = \frac{y'_D(1-x'_B)}{x'_B(1-y'_D)} = \alpha^N \quad (A5)$$

Multiplying (22) with (24) as before, and correcting with the exact expression (A5) we derive

$$S = \alpha^N \left(1 - \frac{z_{HN}F}{L_B}\right)^{N_B} \left(1 - \frac{z_{LN}F}{V_T}\right)^{-N_T} \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \quad (A6)$$

Since the nonkey components are non-distributing we have

$$L'_T = L_T, \quad V'_T = V_T - z_{LN}F$$

$$L'_B = L_B - x_{HN}F, \quad V'_B = V_B$$

Substituting this into (A6) we finally derive

$$S = \alpha^N \frac{(L'/V')_T^{N_T}}{(L'/V')_B^{N_B}} \quad (47)$$

Column	z_F	α	N	N_F	y_D	x_B	$\frac{D}{F}$	$\frac{L}{F}$	$\frac{N}{N_{min}}$	$\frac{R}{R_{min}}$
<i>A</i>	0.5	1.5	40	21	0.99	0.01	0.500	2.706	1.76	1.388
<i>B</i>	0.1	"	"	"	"	"	0.092	2.329	"	1.301
<i>C</i>	0.5	"	"	"	0.90	0.002	0.555	2.737	1.93	1.645
<i>D</i>	0.65	1.12	110	39	0.995	0.10	0.614	11.862	1.66	1.529
<i>E</i>	0.2	5	15	5	0.9999	0.05	0.158	0.226	1.99	1.144
<i>F</i>	0.5	15	10	5	0.9999	0.0001	0.500	0.227	1.47	3.183
<i>G</i>	0.5	1.5	80	40	0.9999	0.0001	0.500	2.635	1.76	1.318

Table 1. Steady-state data for distillation column examples. All columns have liquid feed ($q_F = 1$).

Column	G_{LV}	G_{DV}	$G_d (F, z_F)$
<i>A</i>	$\begin{pmatrix} 0.878 & -0.864 \\ 1.082 & -1.096 \end{pmatrix}$	$\begin{pmatrix} -0.878 & 0.014 \\ -1.082 & -0.014 \end{pmatrix}$	$\begin{pmatrix} 0.394 & 0.881 \\ 0.586 & 1.119 \end{pmatrix}$
<i>B</i>	$\begin{pmatrix} 1.748 & -1.717 \\ .9023 & -.9054 \end{pmatrix}$	$\begin{pmatrix} -1.748 & .03088 \\ -0.9023 & -.00312 \end{pmatrix}$	$\begin{pmatrix} 0.0858 & 1.636 \\ 0.0904 & 0.936 \end{pmatrix}$
<i>C</i>	$\begin{pmatrix} 1.604 & -1.602 \\ .01865 & -.02148 \end{pmatrix}$	$\begin{pmatrix} -1.604 & .00227 \\ -.01865 & -.00283 \end{pmatrix}$	$\begin{pmatrix} 0.8822 & 1.790 \\ 0.0197 & 0.0170 \end{pmatrix}$
<i>D</i>	$\begin{pmatrix} 0.1231 & -0.1211 \\ 2.126 & -2.129 \end{pmatrix}$	$\begin{pmatrix} -0.1231 & .00192 \\ -2.126 & -.00307 \end{pmatrix}$	$\begin{pmatrix} 0.0516 & 0.1252 \\ 1.344 & 2.395 \end{pmatrix}$
<i>E</i>	$\begin{pmatrix} .02033 & -.01315 \\ 1.124 & -1.126 \end{pmatrix}$	$\begin{pmatrix} -.02033 & .00719 \\ -1.124 & -.00135 \end{pmatrix}$	$\begin{pmatrix} .00045 & .00949 \\ 0.1780 & 1.186 \end{pmatrix}$
<i>F</i>	$\begin{pmatrix} 1.074 & -1.073 \\ 0.9257 & -0.9267 \end{pmatrix}$	$\begin{pmatrix} -1.074 & .000998 \\ -0.9257 & -.000998 \end{pmatrix}$	$\begin{pmatrix} 0.5362 & 1.073 \\ 0.4636 & 0.9269 \end{pmatrix}$
<i>G</i>	$\begin{pmatrix} 0.8649 & -0.8646 \\ 1.135 & -1.135 \end{pmatrix}$	$\begin{pmatrix} -0.8649 & .000294 \\ -1.135 & -.000294 \end{pmatrix}$	$\begin{pmatrix} 0.4315 & 0.8647 \\ 0.5683 & 1.135 \end{pmatrix}$

Table 2. Steady-state gain matrices for examples obtained using (11). $G_{DV} = G_{LV}M$ (13). Unscaled product compositions (y_D and x_B) are used as defined in (12).

Column	Actual N	Estimated N	
		This work (28)	Jafarey (16)
A	40	37.02	37.02
B	40	40.51	38.41
C	40	33.67	35.73
D	110	102.81	99.89
E	15	15.92	14.17
F	10	9.88	9.88
G	80	75.32	75.32
Average Error		6.3%	6.3%

Table 3. Estimated number of theoretical trays in columns.

	This work (28)	Jafarey (16) (Feed liquid, $q_F = 1$)
$\ln S$	$N \ln \alpha + \frac{N(L/V)_T}{2(L/V)_B}$	$N \ln \alpha - \frac{N}{2} \ln \left(1 + \frac{1}{Rz_F} \right)$
$\left(\frac{\partial \ln S}{\partial L} \right)_V$	$\frac{N}{2} \frac{1}{L} \frac{q_F F}{L+q_F F}$	$\frac{N}{2} \frac{1}{L} \frac{R+1}{Rz_F+1}$
$\left(\frac{\partial \ln S}{\partial V} \right)_L$	$\frac{N}{2} \frac{1}{V} \frac{(1-q_F)F}{L+D}$	$-\frac{N}{2} \frac{1}{D} \frac{1}{Rz_F+1}$
$\left(\frac{\partial \ln S}{\partial V} \right)_D$	$(q_F = 1) : \frac{N}{2} \frac{1}{L} \frac{1}{L/F+1}$	$\frac{N}{2} \frac{1}{L} \frac{1}{Rz_F+1}$
$\left(\frac{\partial \ln S}{\partial z_F} \right)_{L,V}$	0	$\frac{N}{2} \frac{1}{z_F} \frac{1}{Rz_F+1}$
$\left(\frac{\partial \ln S}{\partial F} \right)_{L,V}$	$-\frac{N}{2} \left(\frac{q_F}{L+q_F F} + \frac{1-q_F}{L+D} \right)$	0
$\left(\frac{\partial \ln S}{\partial q_F} \right)_{L,V}$	$-\frac{N}{2} \left(\frac{1}{L/F+q_F} - \frac{1}{L/F+D/F} \right)$	$-\frac{N}{2} \left(\frac{1}{Rz_F+1} - \frac{1}{Rz_F+z_F} \right)$

Table 4. Analytical expressions for $\partial \ln S / \partial \zeta$ obtained from shortcut models (28) and (16). $(\partial \ln S / \partial V)_D$ for $q_F \neq 1$ is equal to $(\partial \ln S / \partial L)_V + (\partial \ln S / \partial V)_L$ (39).

	Column A			Column B		
	Exact	This work (28)	Jafarey (16)	Exact	Thiswork (28)	Jafarey (16)
$(\partial \ln S/\partial L)_V$	-21.1	1.99	12.8	85.3	2.58	64.0
$(\partial \ln S/\partial V)_L$	23.9	0	-10.8	-81.9	0	-61.6
$(\partial \ln S/\partial V)_D$	2.76	1.99	1.99	3.44	2.58	2.42
$(\partial \ln S/\partial z_F)_{L,V}$	-24.0	0	10.8	70.7	0	56.5
$(\partial \ln S/\partial F)_{L,V}$	-19.3	-5.4	0	-0.5	-6.0	0
$(\partial \ln S/\partial q_F)_{L,V}$	-22.7	0.8	0.8	84.8	2.3	1.9

Table 5. Estimated values for $\partial \ln S/\partial \zeta$ for columns A and B.

Column	Exact	Estimates	
		This work (28)	Jafarey (16)
A	2.76	1.99	1.99
B	3.44	2.58	2.43
C	1.44	1.96	2.11
D	0.42	0.36	0.34
E	71.9	27.1	25.8
F	20.0	18.0	18.0
G	5.87	4.18	4.18
Average error		29.2%	32.2%

Table 6. Estimates of $(\partial \ln S/\partial V)_D = (\partial \ln S/\partial L)_D$. This represents the effect of changing the internal flows on S .

Column	Exact	Estimated	
		This work (28)	Jafarey (16)
A	$\begin{pmatrix} 0.878 & -0.864 \\ 1.082 & -1.096 \end{pmatrix}$	$\begin{pmatrix} 0.990 & -0.980 \\ 0.970 & -0.980 \end{pmatrix}$	$\begin{pmatrix} 1.0434 & -1.0335 \\ 0.9166 & -0.9265 \end{pmatrix}$
B	$\begin{pmatrix} 1.748 & -1.717 \\ .9023 & -.9054 \end{pmatrix}$	$\begin{pmatrix} 1.0032 & -0.9800 \\ 0.9777 & -0.9800 \end{pmatrix}$	$\begin{pmatrix} 1.5554 & -1.5337 \\ 0.9218 & -0.9240 \end{pmatrix}$
C	$\begin{pmatrix} 1.604 & -1.602 \\ .01865 & -.02148 \end{pmatrix}$	$\begin{pmatrix} 1.5940 & -1.5909 \\ .03145 & -.03528 \end{pmatrix}$	$\begin{pmatrix} 1.6094 & -1.6061 \\ .01074 & -.01488 \end{pmatrix}$

Table 7. Estimates of G_{LV} for columns A, B and C obtained using (37) with shortcut models (28) and (16).

Column	λ_{11} , Exact	λ_{11} , Estimated	
		This work (28)	Jafarey (16)
A	35.1	50.3	50.0
B	47.5	39.3	61.0
C	7.53	9.06	3.58
D	58.7	66.7	85.9
E	2.82	1.87	3.35
F	499	558	558
G	1673	2394	2394
Average error		26.2%	36.5%

Table 8. Estimated and exact RGA-values for the LV-configuration. Note that the values of Jafarey are used in the book of Shinskey (1984).

Column	N	N_F , Exact		N_F , Estimated	
		Stoppel	This work (42)	Fenske ratio (44)	Kirkbride (45)
A	40	21.0	20.8	20.5	20.5
B	40	18.5	17.9	11.2	12.1
C	40	30.1	25.6	29.8	33.8
D	110	39.1	45.3	42.0	30.1
E	15	5.16	5.82	2.79	1.55
F	10	5.84	5.88	5.50	5.50
G	80	40.0	40.8	40.5	40.5
Average error, $\frac{ \Delta N_F }{N/2}$:			7.0%	12.2%	18.0%

Table 9. Optimal feed point locations.

Figure captions.

Fig. 1. VLE - curve for relative volatility $\alpha = 2.0$ and linear approximation with $y = \alpha x$ and $1 - y = \frac{1-x}{\alpha}$.

Fig. 2. Column A. Effect of feed point location N_F on derivatives of $\ln S$ with all other column data fixed (including $1 - y_D = x_B = 0.01$). Exact values are compared with shortcut model (28). Note that $(\partial \ln S / \partial L)_V + (\partial \ln S / \partial V)_L = (\partial \ln S / \partial V)_D$ and that $(\partial \ln S / \partial V)_L = 0$ for the shortcut model since $q_F = 1$ (see Table 4.).