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Understanding the Dynamic Behavior of Distillation Columns

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The dynamic behavior of a distillation column is approximated with a two time constant model. The response to changes in the external flows is approximately first order with time constant τ_1 . This dominant time constant can be estimated by using a simple mixing tank model for the column. The response to changes in the internal flows is also first order, but its time constant τ_2 is generally significantly smaller than τ_1 . The condition number and the RGA are smaller at high frequency than at steady state. Most models presented in the literature do not take this into account. The two time constant model does predict this behavior, and τ_2 can be estimated by matching the RGA at high frequency. Finally, it is shown that the effect of nonlinearity is almost eliminated if logarithmic compositions $\ln x_B$ and $\ln(1 - y_D)$ are used. In particular, this applies to the initial response which is of primary importance for feedback control.

1. Introduction

This paper is mainly concerned with understanding the composition response of distillation columns (Figure 1). Modeling the dynamic response of distillation columns is conceptually straightforward. Consider the simplest case with binary separation, constant relative volatility (α), 100% tray efficiency, constant molar flows, and constant vapor or liquid holdups. The dynamic behavior of a column with N theoretical trays and a total condenser is then described by $N + 1$ first-order differential equations (see Appendix). For tray i (which is not a feed tray, reboiler or condenser),

$$M_i dx_i/dt \equiv M_i \dot{x}_i = Lx_{i+1} + Vy_{i-1} - Lx_i - Vy_i \quad (1)$$

where

$$y_i = \alpha x_i / (1 + (\alpha - 1)x_i) \quad (2)$$

Solving this set of differential and algebraic equations on a digital computer is also straightforward (although computer times may be excessive for columns with a large number of trays and components). An early discussion on this is found in Rosenbrock (1957). However, even though the governing equations themselves are well-known, the understanding of the overall behavior of this set of equations is not. It is known that the response is dominated by one large time constant, τ_1 , which may be estimated by some "mixing tank" approach (Davidson, 1956; Moczek et al., 1963, 1965; Wahl and Harriot, 1970; Skogestad and Morari, 1987a). However, this dominant time constant generally does not apply when we make changes in the internal flows only (simultaneous increase in L and V). This will become evident from the discussion in section 3. Furthermore, because of the nonlinear VLE relationship (eq 2), the response turns out to be strongly nonlinear, in particular for high-purity separations, and the value of the dominant time constant τ_1 may change drastically with

operating conditions (e.g., Skogestad and Morari (1987a)).

The main objective of this paper is to gain insight into the dynamic behavior of distillation columns by developing simple analytical models. For feedback control, an accurate model of the plant is usually not needed. Rather, a model which includes the factors most important for feedback control (inverse responses, multivariable effects, and sensitivity to model uncertainty) is desired. Pinpointing these factors is most easily accomplished with simple analytical models. We stress that these models are by no means intended to replace nonlinear simulations. Also, we stress that it is desirable that these models be analytic. Consequently, the models are not intended to replace low-order models which may be obtained by employing standard model reduction techniques (including residualization, balanced realization, collocation methods, etc.).

Internal and External Flows. Throughout the paper, we make use of the terms external and internal flows. A change in external flows is any change which changes the ratio D/B , for example, an increase in flux L with constant boilup V . An increase in internal flows is accomplished by a simultaneous increase in L and V , while keeping the product rates, D and B , constant.

Linear Input-Output Model. For feedback control, we need an overall model that describes the effect of the inputs (flows) on the outputs (product compositions, y_D and x_B). All results in this paper (gains, RGA values, etc.) are with reflux (L) and boilup (V) as inputs (LV configuration). We assume perfect level control. Distillate (D) and bottom flows (B) are then manipulated to keep constant holdups in the condenser (accumulator) and the reboiler (column base). With the additional assumption of constant molar flows and with no feed disturbances ($dF = 0$) this yields

$$dD = dV - dL \quad dB = -dD \quad (3)$$

This does not imply that the LV configuration is the preferred choice for control purposes. The choice is made because L and V have a direct effect on compositions and their effect is therefore only weakly dependent on the

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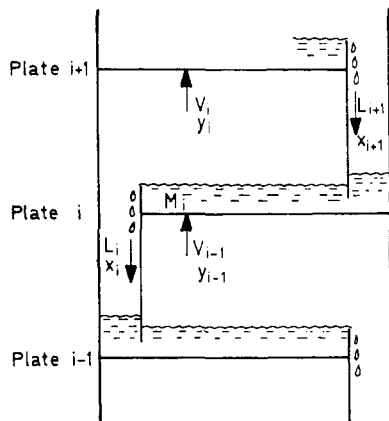
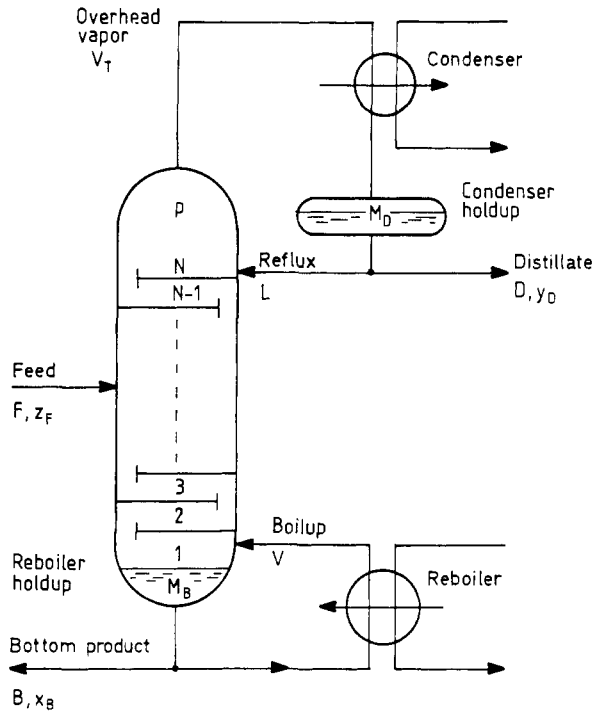


Figure 1. Two product distillation column with single feed and total condenser. Details are shown of the flows and holdups on a plate.

tuning of the level loops. This makes it most natural to write the column model in terms of L and V as manipulated inputs. In the paper, we make extensive use of linearized models at different operating points. These models are most conveniently written in terms of Laplace transforms

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G_{LV}(s) \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (4)$$

$$G_{LV}(s) = C(sI - A)^{-1}B \quad (5)$$

where the matrices A , B , and C are obtained by linearizing the nonlinear model as shown in the Appendix. The frequency response of the plant is obtained by setting $s = j\omega$.

Low- and High-Frequency Behaviors. The uncontrolled (open-loop) response of, for example, the top composition, y_D , to a step disturbance in boilup, V (possibly caused by a disturbance in steam pressure), can be divided into an initial response, followed by a slow settling to the new steady state. When feedback control is used, the initial response to the disturbance is still the same, but then the control system takes action and brings y_D back to its desired value. Therefore, for feedback control, the initial part of the open-loop response, and in particular that

part corresponding to the closed-loop time constant, is of primary interest. The initial part of the time response corresponds to the high-frequency behavior ($\omega \rightarrow \infty$) and the slow settling to the new steady state corresponds to the low-frequency behavior ($\omega \rightarrow 0$) of $G(j\omega)$.

Scaling and Logarithmic Compositions. It is convenient to scale the plant such that the expected variations in each output (or input) are comparable. Let y_D° and x_B° denote the nominal product compositions. To get outputs (i.e., deviations in y_D and x_B from their nominal values) of comparable magnitude, scale each composition with respect to the amount of impurity. For a binary separation, the scaled outputs are

$$\Delta y_D^S = \frac{\Delta y_D}{1 - y_D^\circ} \quad \Delta x_B^S = \frac{\Delta x_B}{x_B^\circ} \quad (6)$$

where $\Delta y_D = y_D - y_D^\circ$, etc. Similarly, the inputs (ΔL and ΔV) are scaled with respect to the nominal feed flow rate. In terms of these scaled variables, the linear model (eq 4) becomes

$$\begin{pmatrix} dy_D^S \\ dx_B^S \end{pmatrix} = \begin{pmatrix} dy_D / (1 - y_D^\circ) \\ dx_B / x_B^\circ \end{pmatrix} = G_{LV}^S(s) \begin{pmatrix} dL / F^\circ \\ dV / F^\circ \end{pmatrix} \quad (7a)$$

where the scaled transfer matrix is

$$G_{LV}^S(s) = \begin{pmatrix} \frac{F^\circ}{1 - y_D^\circ} & 0 \\ 0 & \frac{F^\circ}{x_B^\circ} \end{pmatrix} G_{LV}(s) \quad (7b)$$

(Throughout this paper, we shall use $F^\circ = 1$.) The logarithmic (relative) composition is defined as the logarithm of the amount of impurity of key component in each product. For the case of a binary separations, we define the logarithmic top and bottom compositions as

$$Y_D = \ln(1 - y_D) \quad X_B = \ln x_B \quad (8)$$

Note that the desired output scaling (eq 7) is automatically obtained if we use logarithmic compositions since

$$d \ln(1 - y_D) = -\frac{dy_D}{1 - y_D} \quad d \ln x_B = \frac{dx_B}{x_B} \quad (9)$$

Ryskamp (1981) has proposed the use of logarithmic compositions as a simple means of making the plant less nonlinear. An analysis of eq 1 for the initial response provides theoretical justification for Ryskamp's proposal. This is discussed in section 5.

Example Columns. Throughout the paper, we make use of the seven example columns A–G introduced by Skogestad and Morari (1987a). Steady-state data for these columns are given in Table I. For all examples, we assume constant molar flows, no flow dynamics (constant holdup), and binary mixtures with constant relative volatility. The steady-state gain matrices $G_{LV}(0) = -CA^{-1}B$ are given in Table II. The poles of $G_{LV}(s)$ are equal to the eigenvalues of A . The time constants τ_{1e} and τ_{2e} , which are equal to the inverse of the two smallest eigenvalues of A , are given in Table III. The assumed holdup on the trays is $M_i/F = 0.5$ min in all examples. The holdups in the reboiler and condenser are also $M_D/F = M_B/F = 0.5$ min, unless stated otherwise.

Many results in this paper are derived from binary separations, and $x_i(y_i)$ is the mole fraction of light component. The results generally hold for multicomponent mixtures if in the bottom section of the column $x_i(y_i)$ is the mole fraction of light key component, and in the top

Table I. Steady-State Data for Distillation Column Examples. All Columns Have Liquid Feed ($q_F = 1$)

column	z_F	α	N	N_F	$1 - y_D$	x_B	D/F	L/F	N_{\min}	$(L/F)_{\min}$
A	0.5	1.5	40	21	0.01	0.01	0.500	2.706	22.7	1.95
B	0.1	1.5	40	21	0.01	0.01	0.092	2.329	22.7	1.82
C	0.5	1.5	40	21	0.10	0.002	0.555	2.737	20.7	1.66
D	0.65	1.12	110	39	0.005	0.10	0.614	11.862	66.1	7.76
E	0.2	5	15	5	0.0001	0.05	0.158	0.226	7.55	0.197
F	0.5	15	10	5	0.0001	0.0001	0.500	0.227	6.80	0.0971
G	0.5	1.5	80	40	0.0001	0.0001	0.500	2.635	45.4	2.00

Table II. Steady-State Values of the Scaled Gain Matrix, the Condition Number, and the 1,1 Element of the RGA

column	$G_{LV}^S(0)$	$\gamma(G_{LV}^S(0))$	$\lambda_{11}(G_{LV}^S(0))$
A	$\begin{pmatrix} 87.8 & -86.4 \\ 108.2 & -109.6 \end{pmatrix}$	141.7	35.1
B	$\begin{pmatrix} 174.79 & -171.7 \\ 90.191 & -90.5 \end{pmatrix}$	229.2	47.5
C	$\begin{pmatrix} 16.023 & -16.0 \\ 9.29 & -10.7 \end{pmatrix}$	31.3	7.53
D	$\begin{pmatrix} 24.585 & -24.2 \\ 21.270 & -21.3 \end{pmatrix}$	234.9	58.7
E	$\begin{pmatrix} 203.4 & -131.5 \\ 22.47 & -22.5 \end{pmatrix}$	36.7	2.82
F	$\begin{pmatrix} 10740 & -10730 \\ 9257 & -9267 \end{pmatrix}$	2014	499
G	$\begin{pmatrix} 8648.94 & -8646 \\ 11347.06 & -11350 \end{pmatrix}$	6939	1673

Table III. Time Constants τ_1 and τ_2 (in Minutes) Used in Example 3. For Comparison Are Shown τ_{1e} (Estimated from (16) for a Small Perturbation in L) and τ_{2e}

column	$\tau_1 = \tau_{1e}$	τ_{1e}	τ_2	τ_{2e}
A	194	193	15	12
B	250	252	15	11
C	24	29	10	8
D	154	150	30	23
E	82	71	30	8
F	2996	2996	4	5
G	20333	20332	30	20

section $1 - x_i(1 - y_i)$ is the mole fraction of heavy key component.

2. Singular Values, the Condition Number, and the RGA

From a control point of view distillation columns are usually highly "interactive". This means that a change in any input (e.g., L or V), generally affects both outputs (y_D and x_B). Furthermore, for multivariable plants, we generally have the property that the outputs are more sensitive to some combination of inputs than to others. For example, for high-purity distillation columns, the product compositions y_D and x_B are very sensitive to changes in external flows but much less sensitive to changes in internal flows (Rosenbrock, 1962). We say that such a plant is ill-conditioned or equivalently has a strong degree of directionality. The objective of this section is to introduce some tools which are commonly used when evaluating interactions and directionality of multivariable systems. Readers who are mostly interested in the physics of distillation column dynamics might want to skip to section 3 at this point.

Singular Values. Let the plant model be $y(s) = G(s)u(s)$, where u denotes the plant inputs and y the outputs. The maximum and minimum singular values are the maximum and minimum gains of the plant as the direction of the input (u) is varied:

$$\bar{\sigma}(G) = \max_{u \neq 0} \frac{\|Gu\|_2}{\|u\|_2} \quad (10a)$$

$$\underline{\sigma}(G) = \min_{u \neq 0} \frac{\|Gu\|_2}{\|u\|_2} \quad (10b)$$

(Both of these are functions of frequency, but this is not shown explicitly to simplify notation.) $\|\cdot\|_2$ denotes the usual Euclidean norm, e.g., $\|u(j\omega)\|_2 = (\sum_k u_k(j\omega)^2)^{1/2}$. For distillation columns, Skogestad and Morari (1986) have shown that at steady state the most sensitive direction of the input, u (corresponding to the maximum gain), is obtained by changing the external flows, and the least sensitive input direction is obtained by changing the internal flows. Consequently, with L and V as manipulated inputs, the most sensitive direction is found for $dL = -dV$ and the least sensitive direction is obtained for $dL = dV$. This also holds at higher frequencies as we show in section 6.

Condition Number. The condition number is defined as the ratio between the plant's maximum and minimum gain:

$$\gamma(G(j\omega)) = \bar{\sigma}(G(j\omega)) / \underline{\sigma}(G(j\omega)) \quad (11)$$

(It is possible to define $\gamma(G)$ in terms of other norms, but the induced 2-norm (singular values) used in (11) is most common.) A plant with a large value of $\gamma(G)$ is called ill conditioned. Physically this means that the gain of the plant is strongly dependent on the input direction.

The singular values and condition number are scaling dependent. For correct interpretation of these quantities, the plant should be scaled such that outputs are of comparable magnitude and the inputs are of comparable magnitude (this is obtained with the suggested scaling in (6) and (7)). The two measures defined next are scaling independent.

Minimum Condition Number. The minimum condition number is the value of $\gamma(G)$ obtained when minimized over all possible input and output scalings:

$$\gamma^*(G) = \min_{S_1, S_2} \gamma(S_1 G S_2) \quad (12)$$

Here S_1 and S_2 are diagonal matrices with real, positive entries. A large value of $\gamma^*(G)$ has been suggested to imply a plant which is fundamentally difficult to control (Grosdidier and Morari, 1985). However, obtaining $\gamma^*(G)$ numerically is not simple. Fortunately, there is a very close relationship between $\gamma^*(G)$ and the magnitude of the elements in the Relative Gain Array. The RGA is defined below and is easy to compute. Thus, for practical computations, we recommend using the RGA rather than $\gamma^*(G)$.

RGA (Bristol, 1966). For 2×2 plants, the RGA is defined as

$$\text{RGA} = \begin{bmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{bmatrix} = \begin{bmatrix} \lambda_{11} & 1 - \lambda_{11} \\ 1 - \lambda_{11} & \lambda_{11} \end{bmatrix} \quad (13a)$$

where

$$\lambda_{11} = \frac{1}{1 - \kappa} \quad \kappa(j\omega) = \frac{g_{12}g_{21}}{g_{11}g_{22}}(j\omega) \quad (13b)$$

We define the 1-norm of the RGA as the sum of the absolute values of the elements:

$$\|\text{RGA}\|_1 = \sum_{i,j} |\lambda_{ij}| = 2|\lambda_{11}| + 2|1 - \lambda_{11}| \quad (14)$$

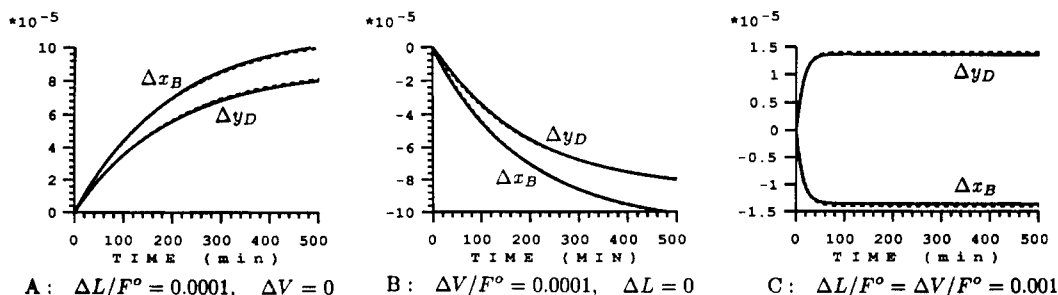


Figure 2. Column A. Responses to small changes in external (A and B) and internal (C) flows. Dotted lines for A and B: first-order model (eq 17) with time constant $\tau_1 = 194$ min. Dotted line for C: first-order model (eq 19) with time constant $\tau_2 = 15$ min.

For 2×2 plants, $\|RGA\|_1$ and $\gamma^*(G)$ are always close in magnitude as seen from the following inequalities (Nett and Manousiouthakis, 1987; Grosdidier and Morari, 1985):

$$\|RGA\|_1 - \frac{1}{\gamma^*(G)} \leq \gamma^*(G) \leq \|RGA\|_1 \quad (15)$$

Thus, the difference between $\|RGA\|_1$ and $\gamma^*(G)$ is at most one (since $\gamma^*(G) \geq 1$) and goes to zero as $\gamma^*(G) \rightarrow \infty$.

A plant with large RGA elements is fundamentally difficult to control (e.g., Skogestad and Morari (1987c)): To have tight control of a multivariable plant, it is desirable to use a controller that inverts the plant. However, such a controller is extremely sensitive to uncertainty with respect to the magnitude of the inputs when the RGA elements are large. In particular, control problems are expected if the RGA has large elements around the crossover frequency (the frequency corresponding to the closed-loop time constant). Consequently, the high-frequency behavior of the RGA is as important for evaluating potential control problems as its steady-state value.

3. Observations Regarding the Composition Response

The dynamic response of most distillation columns is dominated by one large time constant, τ_1 , which is nearly the same, regardless of where an input or disturbance is introduced or where composition is measured. This is well-known both from plant measurements (McNeill and Sachs, 1969) and from theoretical studies (Moczek et al., 1963, 1965). Furthermore, the value of this time constant is largely unaffected by the flow dynamics.

It is somewhat surprising that the response of a distillation column with, for example, 100 trays, corresponding to at least a 100th-order model, may be adequately described by a simple first-order model. Skogestad and Morari (1987a) and others (Davidson, 1956; Moczek et al., 1963, 1965; Wahl and Harriot, 1970) have studied this in more detail. They found that the main reason for the low-order behavior is the interactions between the trays which cause all trays to have essentially the same composition response. This leads to the conclusion that the distillation column can be approximated by one large mixing tank, for which the dominant time constant, τ_{1c} (subscript c denotes *change*), is given by

$$\tau_{1c} \approx \frac{\sum_{i=1}^{N_T} M_i x_i}{D^f \Delta y_D + B^f \Delta x_B} = \frac{\text{change in holdup of one component (kmol)}}{\text{imbalance in supply of this component (kmol min}^{-1}\text{)}} \quad (16)$$

Here Δ represents the difference between the final (su-

perscript f) and initial (superscript o) steady state. For example, $\Delta y_D = y_D^f - y_D^o$.

Example 1. Linear Responses for Column A. The agreement between (16) and observed responses is very good for columns with both products of high purity (Skogestad and Morari, 1987a). This is illustrated by Figure 2, where parts A and B show the response to small increases in reflux L (V constant) and boilup V (L constant) for column A. This column has 40 theoretical trays plus a condenser, and the exact model is 41st order. This response is compared with a first-order response with time constant of 194 min corresponding to the linear model (the steady-state gains are taken from Table II):

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \frac{1}{1 + 194s} \begin{pmatrix} 0.878 & -0.864 \\ 1.082 & -1.096 \end{pmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (17)$$

The agreement is so good that the dotted line corresponding to this approximation is hardly visible. The value of the time constant (194 min) was found by using (16), and in this case it is almost identical with the inverse of the smallest eigenvalue of the linearized model (τ_{1e} , Table III).

If we make small changes (disturbances) in the feed rate or feed composition for this column, we again find that the response is dominated by a first-order response with time constant $\tau_1 = 194$ min. This confirms the initial statements made in this section that all inputs and disturbances yield similar dynamic responses. The only exception to this rule seems to be changes in *internal* flow. To illustrate this, consider the response to a simultaneous increase in L and V (D and B constant). If the model (eq 17) was correct, we would expect the following response (use $dL = dV$):

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \frac{1}{1 + 194s} \begin{pmatrix} 0.878 & -0.864 \\ 1.082 & -1.096 \end{pmatrix} \begin{pmatrix} dL \\ dL \end{pmatrix} = \frac{1}{1 + 194s} \begin{pmatrix} 0.014 \\ -0.014 \end{pmatrix} dL \quad (18)$$

This predicted response should be compared to the actual simulated response in Figure 2C. We see that the values of the steady-state gains (0.014 and -0.014) are correct. However, the time response is much faster than predicted from (18). In fact, an excellent fit is obtained with a first-order response with time constant $\tau_2 = 15$ min (rather than the expected $\tau_1 = 194$ min), corresponding to the linear model

$$\text{internal flows, } \begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \frac{1}{1 + 15s} \begin{pmatrix} 0.014 \\ -0.014 \end{pmatrix} dL \quad (19)$$

There is a fundamental difference in column behavior for changes in external and internal flows: changes in external flows have a large steady-state effect on compositions, but the dynamic response is slow (time constant

$\tau_1 = 194$ min). Changes in internal flows have smaller effects on compositions, but the response is faster (time constant $\tau_2 = 15$ min). The difference between external and internal flows with respect to their steady state effect (gains) has been known for a long time (Rosenbrock, 1962). However, somewhat surprisingly, the difference in their dynamic behavior does not seem to have been reported previously. The reason is probably that the "direction" corresponding to changes in the internal flows is very difficult to observe because of the small gain. For example, we showed in the simulations that it is almost impossible to detect this effect when we make changes in L and V one at a time (Figure 2, A and B)—a simultaneous change $\Delta L = \Delta V$ was needed (Figure 2C). Furthermore, in a real column it is highly unlikely that we would even be able to observe the predicted (Figure 2C) effect of changes in internal flows: it is almost impossible, in practice, to increase L and V by the same amount, and any imbalance from $\Delta L = \Delta V$ will yield a change in external flows ($\Delta D = \Delta V - \Delta L$) which has a much higher gain and will therefore dominate the response.

The observation that (16) does not apply to changes in internal flows is not too surprising from its derivation (Skogestad and Morari, 1987a). In fact, for changes in the internal flows ($\Delta D = \Delta B = 0$), the denominator in (16)

$$D^f \Delta y_D + B^f \Delta x_B = \Delta(Fz_F) - y_D^o \Delta D - x_D^o \Delta B$$

is identically zero, and (16) clearly does not apply.

4. A Simplified Dynamic Model Based on Internal and External Flows

In this section we propose a simple two time constant model based on the observations above regarding the fundamental difference in time responses for changes in internal and external flows. We neglect flow dynamics by assuming constant holdups. However, the flow dynamics may simply be added on to the model (see section 9) if it is written in terms of reflux (L) and boilup (V) as inputs. The reason is that the flow dynamics are independent of the composition response (this is not quite true for non-ideal mixtures where the assumption of constant molar flows does not apply), and conversely, the composition dynamics are only weakly dependent on the flow dynamics when L and V are used as inputs.

The steady-state model with L and V as manipulated inputs is

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (20)$$

In order to model explicitly the difference in dynamic behavior between internal and external flows, we will for the moment consider V and D as manipulated inputs. Assuming perfect level control and constant molar flows (eq 3), we find

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \begin{pmatrix} dV - dD \\ dV \end{pmatrix} = \begin{pmatrix} g_{11} + g_{12} & -g_{11} \\ g_{21} + g_{22} & -g_{21} \end{pmatrix} \begin{pmatrix} dV \\ dD \end{pmatrix} \quad (21)$$

To get a dynamic model, make the following assumption:

Modeling Assumption. The response to changes in the external flows (D in (21)) is first order with time constant τ_1 . The response to changes in internal flows (V in (21)) is first order with time constant τ_2 .

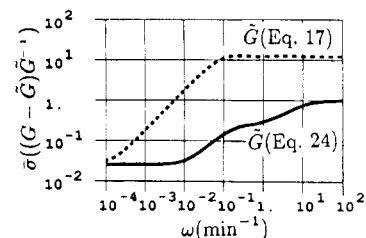


Figure 3. Column A. Relative difference between low-order approximations \tilde{G} and 41st-order plant G (eq 5).

With this assumption, we derive the following dynamic model from (21):

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \begin{pmatrix} g_{11} + g_{12} & -g_{11} \\ g_{21} + g_{22} & -g_{21} \end{pmatrix} \begin{pmatrix} dV/(1 + \tau_2 s) \\ dD/(1 + \tau_1 s) \end{pmatrix} \quad (22)$$

Switching back to L and V as manipulated inputs, and assuming $dD(s) = dV(s) - dL(s)$ (eq 3), we finally derive

$$\begin{aligned} dy_D &= \frac{g_{11}}{1 + \tau_1 s} dL + \left(\frac{g_{11} + g_{12}}{1 + \tau_2 s} - \frac{g_{11}}{1 + \tau_1 s} \right) dV \\ dx_B &= \frac{g_{21}}{1 + \tau_1 s} dL + \left(\frac{g_{21} + g_{22}}{1 + \tau_2 s} - \frac{g_{21}}{1 + \tau_1 s} \right) dV \end{aligned} \quad (23)$$

This two time constant model requires three pieces of information: The steady-state gains (g_{ij}) and the time constants τ_1 and τ_2 . This simple model is obviously not an accurate description of all distillation columns, but may be adequate for controller design. The model is most accurate when the reboiler and condenser holdups are small as discussed in section 9. Note that a slightly different form of the model (eq 23) is obtained if, for example, L and D are used instead of V and D in (21). These differences are believed not to have any significance.

Example 2. Two Time Constant Model for Column A. With the values $\tau_1 = 194$ min and $\tau_2 = 15$ min proposed in section 3, eq 23 becomes

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \frac{1}{1 + 194s} \begin{pmatrix} 0.878 & -0.864 \frac{1 + 12.1s}{1 + 15s} \\ 1.082 & -1.096 \frac{1 + 17.3s}{1 + 15s} \end{pmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (24)$$

The agreement between this model and the exact 41st-order model is excellent for small perturbations, as we showed with the simulations in Figure 2. The relative error $\bar{\sigma}((G - \tilde{G})\tilde{G}^{-1})$ between the two time constant model (eq 24) (denoted by \tilde{G}) and the full linear 41st-order model (denoted by G) is shown as a function of frequency in Figure 3. It is clear that \tilde{G} (eq 24) is an excellent approximation of G up to about a frequency of 1 min^{-1} . On the other hand, the one time constant model (eq 17), which corresponds to the choice $\tau_1 = \tau_2 = 194$ min, gives a very poor approximation (dotted line in Figure 3).

Note that without the seemingly negligible "correction terms" $(1 + 12.1s)/(1 + 15s)$ and $(1 + 17.3s)/(1 + 15s)$ the response to changes in the internal flows would have a time constant of 194 min instead of the observed 15 min. In the literature, each transfer matrix element in (23) is often approximated by a first-order lag with time delay ($ge^{-\theta s}/(1 + \tau s)$) where g is obtained by matching steady-state data. It is clear that, unless special care is taken, it is very unlikely that such a model will be able to capture the difference in time constants between external and internal flows.

Example 3. Singular Values and RGA for Columns A-G. "Full" linear models of the seven example columns

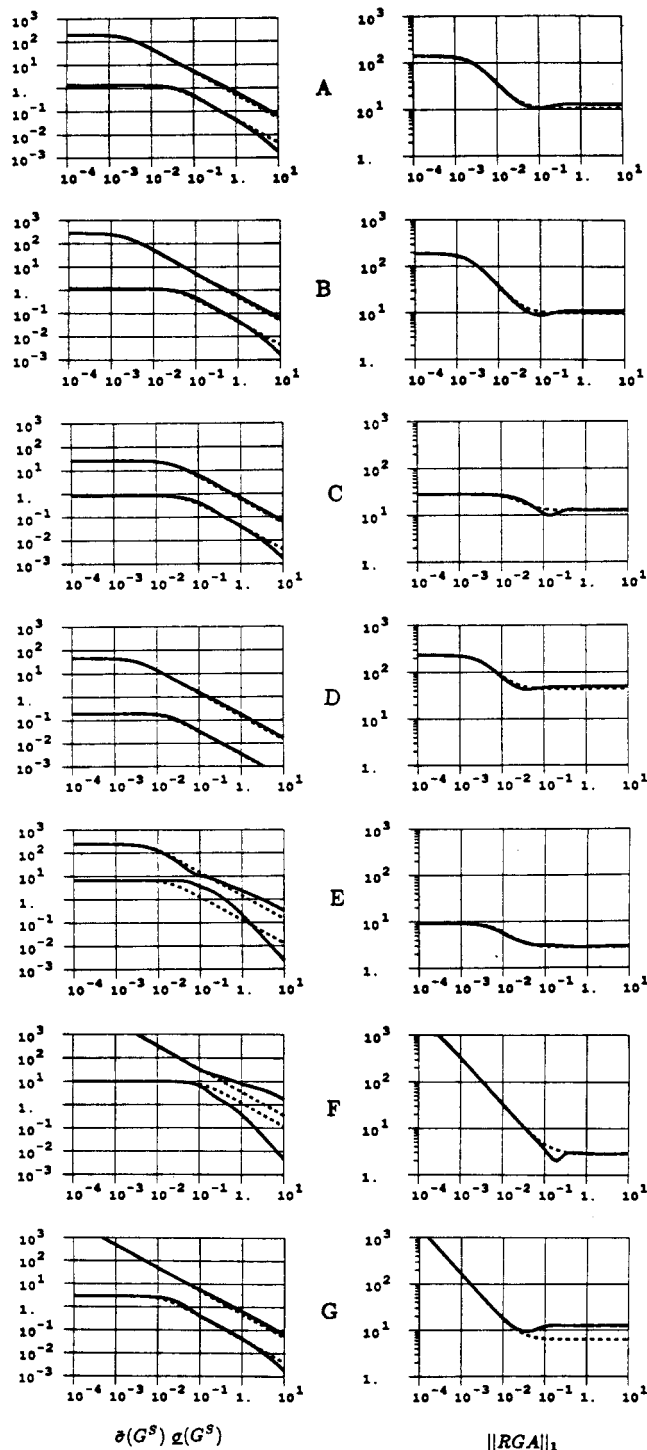


Figure 4. Singular values and $\|RGA\|_1$ as a function of frequency ($1/\text{min}^2$) for columns A-G. Dotted lines: approximation using two time constant model (eq 23) with data from Tables II and III.

were obtained by linearizing the tray-by-tray model as shown in the Appendix. Figure 4 shows the singular values (using *scaled* compositions, eq 6) and $\|RGA\|_1$ as a function of frequency. (The condition number $\gamma(G^S)$ is not shown, but its value is equal to the difference between the curves of $\bar{\sigma}(G^S)$ and $\underline{\sigma}(G^S)$ and it is close to $\|RGA\|_1$ for our examples.) In all cases, the condition number and the RGA are lower at high frequencies than at steady state. The dotted lines in Figure 4 are the approximate values obtained with the simple two time constant model (eq 23). The steady-state gain matrices needed in (23) were taken from Table II (these are the exact linearized gains), and the time constants τ_1 and τ_2 used are given in Table III.

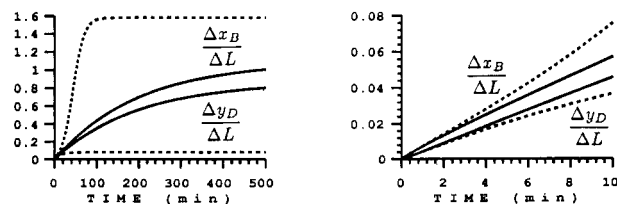


Figure 5. Column A. Unit responses to a small and large increase in reflux, L .

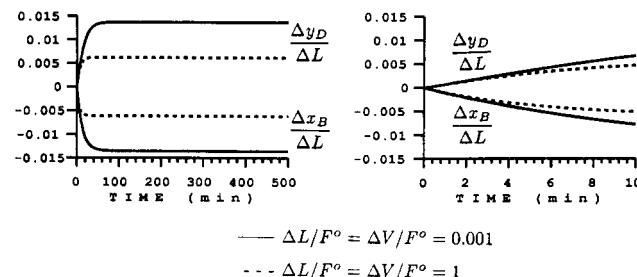


Figure 6. Column A. Unit responses to a small and large increase in internal flows.

τ_1 was chosen to be equal to τ_{1e} (the inverse of the smallest eigenvalue), and τ_2 was adjusted by trial and error to get a good fit to the singular value and $\|RGA\|_1$ plots in Figure 4. We see from Figure 4 that the agreement between the full-order model and the simple two time constant model (eq 23) is generally very good. This provides further justification for the validity of this simple model. Note that if a one time constant model were used ($\tau_1 = \tau_2$), then we would predict constant values of the condition number and the RGA as a function of frequency, which is clearly not correct.

5. The Effect of Nonlinearity

We found in the examples above that the simple two time constant model (eq 23) provides a very good approximation of the full-order *linear* model. However, distillation columns are known to be strongly nonlinear (e.g., Moczek et al. (1963, 1965) and Fuentes and Luyben (1983)), and one might question the usefulness of a linear model such as (23). The results in this section show that the use of logarithmic compositions effectively counteracts the nonlinearity and that a linear model may still be adequate if it is written in terms of logarithmic compositions.

5.1. Observations. The effect of nonlinearity is illustrated by the following two examples.

Example 4. Nonlinear Responses for Column A.

Figures 5 and 6 show the unit responses $\Delta y_D/\Delta L$ and $\Delta x_B/\Delta L$ to small and large changes in external ($\Delta L \neq 0$, $\Delta V = 0$, Figure 5) and internal flows ($\Delta L = \Delta V$, Figure 6). If the column were linear, these unit responses would be independent of the magnitude of ΔL . This is clearly not the case for large simulation times (steady state), but note that the initial unit responses are almost independent of the magnitude of ΔL .

However, there are also other sources of nonlinearity; the most important is probably a change in operating conditions. Within a linear framework, one way of studying the effect of changing operating conditions is to study how the *linearized model* changes.

Example 5. Operating Points A and C. Columns A and C actually represent the same column, but at two entirely different operating points. The product compositions for column A are $1 - y_D = x_B = 0.01$. Column C

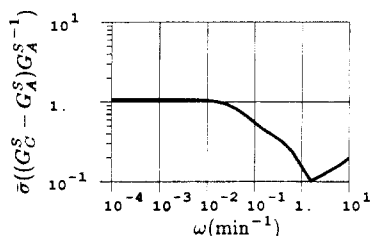


Figure 7. Relative difference between scaled linear models for columns A and C.

is obtained by changing D/F from 0.500 to 0.555, which yields $1 - y_D = 0.10$ and $x_B = 0.002$. We found in example 3 that the linear model at these two operating points is adequately described by the two time constant model (eq 23) with data for the gains and time constants as given in Tables II and III. We have for column A $\tau_1 = 194$ min and $\tau_2 = 15$ min, and for column C $\tau_1 = 24$ min and $\tau_2 = 10$ min. Consider the linear model for the steady state (low frequency, $\omega = 0$) and for the initial response (high frequency, $\omega \rightarrow \infty$). For the case with unscaled (absolute) compositions (y_D and x_B) as outputs, we find

	steady state $G_{LV}(0) =$	initial response $G_{LV}(\infty) =$
A:	$0.01 \begin{pmatrix} 87.8 & -86.4 \\ 108.2 & -109.6 \end{pmatrix}$	$\frac{0.01}{s} \begin{pmatrix} 0.45 & -0.36 \\ 0.56 & -0.65 \end{pmatrix}$
C:	$0.01 \begin{pmatrix} 160.2 & -160.0 \\ 1.87 & -2.15 \end{pmatrix}$	$\frac{0.01}{s} \begin{pmatrix} 6.5 & -6.5 \\ 0.08 & -0.10 \end{pmatrix}$

We see that the steady-state gains change by almost 2 orders of magnitude from operating point A to C. The transfer function elements for the initial response change by about 1 order of magnitude. With such large changes, it would seem almost impossible to find a single linear controller that yields acceptable responses at both operating points. In particular, the large change in the initial response is disturbing, because this part is generally most important for feedback control.

Next, consider using logarithmic compositions (Y_D and X_B) as outputs (corresponds to scaling the gain elements as shown in (7b)). This is suggested by Ryskamp (1981) as a means to make the responses less nonlinear. Indeed, we do find that this is the case, as seen from the following data:

	steady state $G_{LV}^S(0) =$	initial response $G_{LV}^S(\infty) =$
A:	$\begin{pmatrix} 87.8 & -86.4 \\ 108.2 & -109.6 \end{pmatrix}$	$\frac{1}{s} \begin{pmatrix} 0.45 & -0.36 \\ 0.56 & -0.65 \end{pmatrix}$
C:	$\begin{pmatrix} 16.0 & -16.0 \\ 9.3 & -10.7 \end{pmatrix}$	$\frac{1}{s} \begin{pmatrix} 0.65 & -0.65 \\ 0.38 & -0.52 \end{pmatrix}$

There is still a large change in the steady-state behavior from operating point A to C, but the change is reduced about 10 times compared to the case with absolute compositions. At high frequency, there is almost no change in the plant model as we go from A to C. This is also seen from Figure 7 which shows the relative difference between the linearized *scaled* models for columns A and C; the models are almost identical at higher frequencies. This implies that, even though the steady-state behavior is quite different, the initial response in terms of logarithmic compositions is similar. This, in turn, indicates that, when logarithmic compositions are used for control, a single linear controller may yield acceptable performance at both

operating points. This is indeed confirmed in a simulation study by Skogestad and Morari (1988).

The above example indicates that the use of logarithmic compositions effectively eliminates nonlinearity at high frequency. The objective of the remainder of this section is to prove that this is a general result that holds for any column.

5.2. Predicted Nonlinear Initial Responses. In this section we want to prove the following claims:

(1) The initial unit response of Δx_i (Δx_i may be the composition on any tray) is independent of the magnitude of ΔL and ΔV .

(2) The initial unit response of Δx_i is independent of the operating point if relative (logarithmic) compositions are used.

Proof of (1). Assume constant molar flows and constant holdup. The component material balance for tray i at steady state is (tray i is any tray except a feed tray, reboiler, or condenser)

$$M_i \dot{x}_i = 0 = L_i^o(x_{i+1}^o - x_i^o) + V_i^o(y_{i-1}^o - y_i^o) \quad (25)$$

Assume a step change is made in L_i and V_i such that the flows for $t > 0$ are $L_i^o + \Delta L_i$ and $V_i^o + \Delta V_i$. We have

$$M_i \dot{x}_i = (L_i^o + \Delta L_i)(x_{i+1} - x_i) + (V_i^o + \Delta V_i)(y_{i-1} - y_i) \quad (26)$$

Immediately following this change, we may neglect second-order effects and assume the tray compositions to be unchanged; i.e., $x_i = x_i^o$. Subtracting the steady state (eq 25) then yields (Rademaker et al., 1975, p 129)

($t = 0^+$):

$$M_i \dot{x}_i = (x_{i+1}^o - x_i^o)\Delta L_i - (y_i^o - y_{i-1}^o)\Delta V_i \quad (27a)$$

Similarly, using $\Delta B = \Delta L_B - \Delta V_B$, we derive for the reboiler ($x_B = x_1$)

($t = 0^+$):

$$M_B \dot{x}_1 = (x_2^o - x_1^o)\Delta L_B - (y_1^o - x_1^o)\Delta V_B \quad (27b)$$

and using $\Delta D = \Delta V_T - \Delta L_T$, we derive for the total condenser (note that $y_T^o = y_D^o$ at steady state)

($t = 0^+$):

$$M_D \dot{y}_D = (y_D^o - y_D^o)\Delta L_T - (y_D^o - y_T^o)\Delta V_T = 0 \quad (27c)$$

Note that eq 27 are linear in ΔL_i and ΔV_i . This explains why the initial unit responses in example 4 were independent of the magnitude of L and V .

Comment. Equations 27 show that the response at high frequency is essentially first order. Furthermore, we know that for a column with N trays there are N poles if only the composition dynamics are considered. Consequently, each transfer function must have exactly $N - 1$ zeros (Kim and Friedly, 1974).

Proof of (2). Use the steady-state relationship (eq 25) to eliminate $(y_{i-1}^o - y_i^o)$ in (27a). We find the initial response

($t = 0^+$):

$$\dot{x}_i = \frac{1}{M_i}(x_{i+1}^o - x_i^o) \left(\Delta L_i - \frac{L_i}{V_i} \Delta V_i \right) \quad (28)$$

The initial response in terms of x_i is strongly dependent on the operating point. This follows since the term $(x_{i+1}^o - x_i^o)$ is strongly dependent on the operating point. However, from example 5 we expect the response to be much less dependent on operating conditions if logarithmic compositions are used. To this end rewrite (28) as follows:

for the bottom section of column ($t = 0^+$):

$$\frac{\dot{x}_i}{x_i} = \frac{d \ln x_i}{dt} = \frac{1}{M_i} \left(\frac{x_{i+1}^0}{x_i^0} - 1 \right) \left(\Delta L_i - \frac{L_i}{V_i} \Delta V_i \right) \quad (29a)$$

Similarly, for the top section ($t = 0^+$):

$$\frac{\dot{x}_i}{1 - x_i} = - \frac{d \ln (1 - x_i)}{dt} = \frac{1}{M_i} \left(1 - \frac{1 - x_{i+1}^0}{1 - x_i^0} \right) \left(\Delta L_i - \frac{L_i}{V_i} \Delta V_i \right) \quad (29b)$$

Our observations from example 5 must imply that the ratio x_{i+1}^0/x_i^0 is only weakly dependent on operating conditions in the bottom part of the column and that the ratio $(1 - x_{i+1}^0)/(1 - x_i^0)$ is nearly constant near the top of the column. This is indeed correct as is shown below.

Consider the bottom section of the column. Assume that the equilibrium and operating lines are linear in this section:

$$y_i^0 = K_B x_i^0 \quad (30)$$

$$x_{i+1}^0 = (V/L)_B y_i^0 + \frac{B}{L_B} x_B^0 \quad (31)$$

These assumptions are reasonable for most columns, in particular near the bottom for high-purity columns. Combining (30) and (31) yields

$$\frac{x_{i+1}^0}{x_i^0} = \left(\frac{V}{L} \right)_B K_B + \frac{B}{L_B} \frac{x_B^0}{x_i^0} \quad (32)$$

The second term is negligible as we go up the column, and it is also small near the bottom for columns with $V/B > 1$. We get

$$x_{i+1}^0/x_i^0 \approx (V/L)_B K_B \quad (33)$$

We see from (33) that in the bottom section x_{i+1}^0/x_i^0 is (a) independent of the tray location and (b) only weakly dependent on the operating point (since K_B and $(V/L)_B$ are only weakly dependent on the operating point). Substituting (33) into (29a) yields

bottom section ($t = 0^+$):

$$\frac{\dot{x}_i}{x_i} \approx \frac{1}{M_i} \left(\left(\frac{V}{L} \right)_B K_B - 1 \right) \left(\Delta L_i - \left(\frac{L}{V} \right)_B \Delta V_i \right) \quad (34a)$$

A similar expression is derived for the top section where for binary mixtures $(1 - y_i) \approx K_T(1 - x_i)$

top section ($t = 0^+$):

$$\frac{\dot{x}_i}{1 - x_i} \approx \frac{1}{M_i} \left(1 - \left(\frac{V}{L} \right)_T K_T \right) \left(\Delta L_i - \left(\frac{L}{V} \right)_T \Delta V_i \right) \quad (34b)$$

Note that for the case of constant relative volatility, α , we have $K_B = K_T^{-1} = \alpha$. The terms on the right-hand side in eq 34 are only weakly dependent on operating conditions. This proves claim 2. Furthermore, we note that the initial response in terms of logarithmic compositions is almost the same for any tray in the top (or bottom) part of the column.

Range of Validity of (34). Second-order effects were neglected when deriving (34). However, from (34a) and (34b), we see that all trays in a column section have similar initial responses. This implies that the terms $(x_{i+1} - x_i)$ and $(y_i - y_{i-1})$ in (26) are kept approximately constant, and the interactions between the trays will prolong the slope of the initial response predicted by (26) (and (34)). This

effect makes the overall time constant τ_1 much larger than the composition time constant $\tau_x = M_i/(L_i + K_i V_i)$ of an individual tray.

Reboiler and Condenser. Equations 34 do not apply to the reboiler and condenser. Assume perfect level control and total condenser. We derive from (27b) and (27c) ($t = 0^+$)

reboiler:

$$\frac{\dot{x}_B}{x_B} = \frac{K_B - 1}{M_B} \left(\frac{V}{L} \right)_B \left(\Delta L_B - \left(\frac{L}{V} \right)_B \Delta V_B \right) \quad (35a)$$

condenser:

$$\frac{\dot{y}_D}{1 - y_D} = \theta \left(\Delta L_T - \left(\frac{L}{V} \right)_T \Delta V_T \right) \quad (35b)$$

Note that \dot{x}_B predicted from (35a) is larger than from (34a) with $M_i = M_B$. From (35b) we predict that \dot{y}_D is initially zero because a change in L and V has no direct effect on the composition in the condenser. However, note from Figure 5B that the observed initial slope for y_D is *not* zero (at least not for $t > \tau_x \approx 0.1$ min). The reason for the discrepancy is the "second-order effects" (change in y_T) which are neglected when deriving (35b). For columns with *small* reboiler and condenser holdup, the following example shows that the interactions with the other trays dominate and (34) may in fact also give a good approximation of the initial response in the reboiler and condenser. (However, if the holdup is large, then the response for y_D is approximately second order and the initial slope is indeed zero; see example 8 below).

Example 6. Column A (Small Condenser and Reboiler Holdup, $M_D/F = M_B/F = M_i/F = 0.5$ min). The slopes of the initial unit response to a change in reflux obtained from (34a) and (34b) are

$$\frac{\dot{x}_B}{\Delta L} = \frac{x_B}{M_i} \left(\left(\frac{V}{L} \right)_B \alpha - 1 \right) = \frac{0.01}{0.5} \left(\frac{3.21}{3.71} 1.5 - 1 \right) = 0.0060 \quad (36a)$$

$$\frac{\dot{y}_D}{\Delta L} = \frac{1 - y_D}{M_i} \left(1 - \frac{(V/L)_T}{\alpha} \right) = \frac{0.01}{0.5} \left(1 - \frac{3.21/2.71}{1.5} \right) = 0.0042 \quad (36b)$$

These are very close to the observed values in Figure 5.

6. III Conditioning at High Frequency

The expressions (eq 34) for the initial response assuming constant molar flows may be used to obtain some very interesting insights into the plant behavior at high frequency.

6.1. Most Sensitive Direction. Consider small changes in reflux and boilup; i.e., let $\Delta L_i = dL$ and $\Delta V_i = dV$. Recall that at steady state the maximum gain is found when $dL = -dV$, corresponding to changing the external flows, and the minimum gain is found when $dL = dV$, corresponding to changing the internal flows. The same also holds at high frequency for most columns as is shown next. In the bottom section of the column, we see from (34a) and (35a) that the minimum initial effect on composition (zero effect) is found when $dL/dV = (L/V)_B$. Similarly, from (34b) and (35b) we see that the minimum effect on composition in the top section is obtained with $dL/dV = (L/V)_T$. Since $(L/V)_T < 1$ and $(L/V)_B > 1$, the minimum gain (combined effect on y_D and x_B) is obtained for

$$(L/V)_T < dL/dV < (L/V)_B \quad (37)$$

For liquid feeds $(L/V)_B = (L/V)_T + F/V$. Thus, with the possible exception for columns with large values of F/V (small reflux), we will always find the minimum gain for $dL \approx dV$. (This proves that $dL = -dV$ corresponds to the maximum gain since $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ are orthogonal.) Since the simple two time constant model (eq 23) yields indeed the minimum gain for $dL = dV$ at all frequencies, this provides a further justification for using (23).

6.2. Variation of RGA with Frequency. The frequency dependence (set $s = j\omega$) of λ_{11} predicted by the two time constant model (eq 23) is

$$\lambda_{11}(s) = \lambda_{11}(0) \frac{1 + \tau_2 s}{1 + \tau_1 s} (1 + \epsilon) \quad (38a)$$

where

$$\epsilon = \left(\frac{g_{21}}{g_{22}} + 1 \right) \frac{(\tau_1 - \tau_2)s}{1 + \tau_2 s} \quad (38b)$$

For columns with a pure top product, $g_{21}/g_{22} \approx -1$ (Skogestad and Morari, 1987d), and $\epsilon \approx 0$. Indeed, Figure 4 shows that eq 38a with $\epsilon = 0$ is a good approximation for most columns.

Low Frequency. The RGA values at low frequency are mainly determined by the purity of the least pure product. This follows from the following approximation for $\lambda_{11}(0)$ for the LV configuration which applies to binary mixtures with both products of high purity and liquid feed (Skogestad and Morari, 1987d):

$$\lambda_{11}(0) \approx \frac{2L}{NI_s} \left(1 + \frac{L}{F} \right) \quad (39)$$

Here the "impurity sum"

$$I_s = Bx_B(1 - x_B) + Dy_D(1 - y_D) \quad (40)$$

depends strongly on operating conditions, and its value is determined by the purity of the least pure product. $I_s \rightarrow 0$ and $\lambda_{11}(0) \rightarrow \infty$ when both products are of high purity.

High Frequency. We want to estimate $\lambda_{11} = (1 - \kappa)^{-1}$ at high frequency. Here $\kappa(j\omega) = (g_{21}/g_{22})/(g_{11}/g_{12})(j\omega)$ and

$$\frac{g_{21}}{g_{22}} = \frac{(\partial x_B / \partial L)_V}{(\partial x_B / \partial V)_L} \quad \frac{g_{11}}{g_{12}} = \frac{(\partial y_D / \partial L)_V}{(\partial y_D / \partial V)_L} \quad (41)$$

At high frequency these ratios are given by the ratio between the slopes of the initial response of x_B (and y_D) to changes in L and V . From (34a) and (34b), we get (these apply to the entire bottom and top part of the column)

$$(g_{21}/g_{22})(\infty) = -(V/L)_B \quad (g_{11}/g_{12})(\infty) = -(V/L)_T \quad (42)$$

and we derive

$$\kappa(\infty) = (L/V)_T / (L/V)_B \quad (43)$$

This derivation does not depend on the amount of holdup, and therefore we expect $\lambda_{11}(\infty)$ to be almost independent of condenser and reboiler holdup. For the case of constant molar flows and feed as liquid ($L_B = L_T + F$, $V_T = V_B$), we find $\kappa(\infty) = L_T/L_B$ and the RGA becomes

feed liquid:

$$\lambda_{11}(\infty) = 1 + L/F \quad (44)$$

which gives

$$\| \text{RGA}(\infty) \|_1 = 4 \frac{L}{F} + 2 \quad (45)$$

For the seven examples, the agreement between the RGA values estimated from (45) and those obtained from the

Table IV. Estimate (Equation 45) of $\| \text{RGA} \|_1$ at High Frequency ($\omega = \infty$)

column	$\ \text{RGA}(\infty) \ _1$, obsd	$4(L/F) + 2$ (eq 45)
A	12.83	12.82
B	11.32	11.32
C	12.95	12.94
D	49.10	49.44
E	2.90	2.90
F	2.91	2.91
G	12.54	12.54

full linearized model is excellent (maximum error is less than 1% for the seven cases; see Table IV). From (44) we conclude that large reflux ($L/F \gg 1$) is necessary for the column to have large RGA values at high frequency.

Is it possible to have larger RGA values at high frequency than at low frequency? This would require $\tau_2 > \tau_1$ in the model (eq 23) and thus does not seem likely. In fact, we have not been able to find any examples of columns which exhibit $\lambda_{11}(0) < \lambda_{11}(\infty)$. (One column which has $\lambda_{11}(0)$ and $\lambda_{11}(\infty)$ close together is the following: $z_F = 0.65$, $y_D = 0.9$, $x_B = 0.002$, $\alpha = 1.12$, $N = 110$, and $N_F = 39$. This yields $L/F = 49.6$, $\lambda_{11}(0) = 57.7$, and $\lambda_{11}(\infty) = 1 + L/F = 50.6$.)

6.3. Implications for Control Purposes. For control purposes, it is bad if the RGA values are large either at low or high frequencies. We conclude from (39) and (44) that the *worst* columns to control using the LV configuration are those with large reflux *and* with both products of high purity. For most well-designed columns, the reflux L/F is about 5–50% higher than $(L/F)_{\min}$. For binary mixtures with constant relative volatility and feed liquid, the minimum reflux ratio is approximately $(L/D)_{\min} \approx (1/(\alpha - 1))(1/z_F)$ (e.g., Henley and Seader (1981)). For most columns, $D \approx Fz_F$, and we derive

$$\left(\frac{L}{F} \right)_{\min} \approx \frac{1}{\alpha - 1} \quad (46)$$

This means that, in industrial columns (which hopefully are reasonably optimal), large RGA values at high frequency are observed only for columns with relative volatility, α , close to one. Furthermore, such separations usually require a large number of trays (e.g., column D). This follows since most well-designed columns have $N \approx 2N_{\min}$ where

$$N_{\min} = \ln S / \ln \alpha \quad (47)$$

and $\ln \alpha$ is small for α close to one. To observe large RGA values throughout the frequency range in a *university* column, which usually has few trays, one should use systems with *high* relative volatility (to get high-purity products) and operate (nonoptimally) at high reflux.

7. Estimates of Time Constants τ_1 and τ_2

7.1. Estimate of Dominant Time Constant, τ_1 . There are at least five methods for estimating the dominant time constant, τ_1 : (i) plant data, (ii) simulations, (iii) eigenvalue of linearized model, (iv) simple mixing tank model, and (v) initial response. It is relatively easy to observe τ_1 from plant data (method i), but simulations (method ii) are preferable because they give a consistent set of values for the gains and τ_1 . When simulations are employed, steady-state plant data should be employed to estimate the number of theoretical trays (N), and dynamic plant data could be used to estimate tray holdups. Method iii relies on a linearized model, and τ_1 is approximately equal to the inverse of the smallest eigenvalue of the state matrix **A**. A linear model may be obtained analytically for simple cases (e.g., constant relative volatility and constant molar

flows; see Appendix) but must generally be obtained by numerical differentiation.

Mixing Tank Model (Method iv). The mixing tank approach yields the estimate (eq 16) for the dominant time constant. In addition to holdup data, steady-state data for the initial (o) and final (f) states are required. These steady-state data may be obtained from a simulation program. However, to gain insight into the expected variations in τ_1 , an analytical expression is preferable. On the basis of (16), Skogestad and Morari (1987a) have derived an analytical expression which is valid for high-purity binary separations and *small* perturbations to the column:

$$\tau_{1c} \approx \frac{M_I}{I_s \ln S} + \frac{M_D y_D (1 - y_D)}{I_s} + \frac{M_B x_B (1 - x_B)}{I_s} \quad (48)$$

Here M_I is the total holdup *inside* the column, M_D and M_B are the condenser and reboiler holdups, and S is the separation factor. The first term in (48), which represents the contribution from changing the component holdup *inside* the column, dominates for columns with both products of high purity ($1 - y_D$ and x_B both small). Note that I_s may be extremely small in such cases, resulting in very large values of τ_{1c} . This agrees with the observations of Fuentes and Luyben (1983). The reader is encouraged to study the paper by Skogestad and Morari (1987a), who discuss (16) and (48) in detail.

Matching Initial Response (Method v). Recall that the simple two time constant model (eq 23) predicts that each transfer function element by itself is approximately first order with time constant τ_1 . Assume that the simple model (eq 23) is valid also for the initial response. Then τ_1 can be estimated by equating (23) with the initial response derived in (34). The initial slope ($t = 0^+$) derived from (23) is (use $\mathcal{L}^{-1}\{s dy_D\} = \dot{y}_D$ and let $s \rightarrow \infty$):

$$\begin{pmatrix} \dot{y}_D \\ \dot{x}_B \end{pmatrix} = \begin{bmatrix} \frac{g_{11}}{\tau_1} & \frac{g_{11} + g_{12}}{\tau_2} - \frac{g_{11}}{\tau_1} \\ \frac{g_{21}}{\tau_1} & \frac{g_{21} + g_{22}}{\tau_2} - \frac{g_{21}}{\tau_1} \end{bmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (49)$$

Note that (23) is most accurate for the case with small reboiler and condenser holdup (see section 8). This is exactly the case for which (34) gives a good estimate of \dot{x}_B and \dot{y}_D (recall example 6). Equations 34 yield ($t = 0^+$)

$$\begin{pmatrix} \dot{y}_D \\ \dot{x}_B \end{pmatrix} = \frac{1}{M_i} \begin{bmatrix} (1 - y_D)k_T & -(1 - y_D)k_T(L/V)_T \\ x_B k_B & -x_B k_B(L/V)_B \end{bmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (50)$$

where $k_T = 1 - (V/L)_T/\alpha$ and $k_B = (V/L)_B/\alpha - 1$.

Example 7. Column A. Equation 49 yields

$$\begin{pmatrix} \dot{y}_D \\ \dot{x}_B \end{pmatrix} = \begin{pmatrix} 0.0045 & -0.0036 \\ 0.0056 & -0.0065 \end{pmatrix} \quad (51)$$

From (50) with $M_i/F = 0.5$ min

$$\begin{pmatrix} \dot{y}_D \\ \dot{x}_B \end{pmatrix} = \begin{pmatrix} 0.0042 & -0.0036 \\ 0.0060 & -0.0069 \end{pmatrix} \quad (52)$$

The consistency between (51) and (52) is excellent for this particular example. This shows that the simple two time constant model (eq 23) is indeed valid at high frequency for this column. Skogestad (1987) has shown that this is generally true for high-purity columns with large reflux (L/V close to one).

Table V. Two Estimates of the Dominant Time Constant (Minutes)

column	τ_{1e}	τ_{1i} (eq 54)
A	194	206
B	250	284
C	24	40
D	154	202
E	82	154
F	2996	6827
G	20333	20858

τ_1 may now be estimated by matching (49) and (50). This approach is also suggested by Rademaker et al. (1975, p 137). For example, matching \dot{y}_D/dL in (49) and (50) yields

$$\frac{g_{11}}{\tau_1} = \frac{1 - y_D}{M_i} \left(1 - \frac{(V/L)_T}{\alpha} \right) \quad (53)$$

In terms of scaled gains ($g_{11}^S = g_{11}/(1 - y_D)$)

$$\tau_{1i} = \frac{g_{11}^S M_i}{1 - \frac{(V/L)_T}{\alpha}} \quad (54)$$

(The subscript i on τ_1 denotes that it is derived by matching the initial responses.) Note from (54) that the ratio τ_{1i}/g_{11}^S is almost independent of operating conditions (although τ_1 and g_{11}^S individually may change significantly). Other relationships result if we try to match other elements in (49) and (50), but the resulting τ_{1i} is about the same. Because condenser holdup was neglected when deriving (50), M_i in (54) represents the holdup on a *tray* inside the column. τ_{1i} computed from (54) is compared to τ_{1e} (the dominant time constant corresponding to the largest eigenvalue) in Table V. As expected, τ_{1i} and τ_{1e} are very similar for columns with high purity and/or large reflux. For these columns (A, B, D, and G), we conclude that the *entire* composition response is indeed well approximated by a first-order model. For cases with $\tau_{1i} > \tau_{1e}$, the initial response is somewhat slower than expected from τ_{1e} , indicating a more complicated behavior than a pure first-order response. However, the difference between τ_{1i} and τ_{1e} is at most a factor of 2 for the seven columns, and the assumption regarding first-order response is justified.

7.2. Estimate of Internal Time Constant, τ_2 . We suggest two methods for obtaining τ_2 : (i) simulations and (ii) initial response. τ_2 may be obtained from *simulations* of changes in the internal flows (Figure 2C). It is *not* recommended to obtain τ_2 from plant data since it is almost impossible, in practice, to carry out test runs for changes in the internal flows without changing the external flows (because of flow uncertainty and disturbances in feed rate, boilup, etc.). Also recall from parts A and B of Figure 2 that the small time constant (τ_2) was not detectable from the individual responses to changes in reflux (L) and boilup (V).

τ_2 by Matching Initial Response. In addition to τ_1 , we may also estimate τ_2 by matching (49) and (50). One way of doing this is to match the RGA of (49) and (50). The 1,1 element of the RGA is $\lambda_{11} = (1 - \kappa)^{-1}$. Equation 49 yields

$$\kappa(\infty) = \frac{\frac{g_{21}}{\tau_1} \left(\frac{g_{11} + g_{12}}{\tau_2} - \frac{g_{11}}{\tau_1} \right)}{\frac{g_{11}}{\tau_1} \left(\frac{g_{21} + g_{22}}{\tau_2} - \frac{g_{21}}{\tau_1} \right)} = \frac{\left(1 + \frac{g_{12}}{g_{11}} \right) - \frac{\tau_2}{\tau_1}}{\left(1 + \frac{g_{22}}{g_{21}} \right) - \frac{\tau_2}{\tau_1}} \quad (55)$$

Table VI. Comparison of Ratio τ_1/τ_2 Used in Examples 3 and Estimate (Equation 56) Obtained by Matching the High-Frequency Behavior

column	τ_2/τ_1 (Table III)	$(\tau_2/\tau_1)_i$ (eq 56)
A	0.077	0.092
B	0.060	0.069
C	0.408	0.420
D	0.195	0.218
E	0.364	0.434
F	0.00133	0.00139
G	0.00147	0.00192

Equation 50 yields $\kappa(\infty)$ as given in (43). The ratio τ_1/τ_2 may now be estimated by equating (55) and (43):

$$\left(\frac{\tau_2}{\tau_1}\right)_i = \frac{\left(\frac{L}{V}\right)_B \left(1 + \frac{g_{12}}{g_{11}}\right) - \left(\frac{L}{V}\right)_T \left(1 + \frac{g_{22}}{g_{21}}\right)}{\left(\frac{L}{V}\right)_B - \left(\frac{L}{V}\right)_T} \quad (56a)$$

For the special case of liquid feed,

$$\left(\frac{\tau_2}{\tau_1}\right)_i = \frac{L}{F} \left(\frac{g_{12}}{g_{11}} - \frac{g_{22}}{g_{21}}\right) + \left(1 + \frac{g_{12}}{g_{11}}\right) \quad (56b)$$

(subscript i denotes initial). This ratio is shown in Table VI for our seven examples and is compared with the actual value used in example 3 (Figure 4). The agreement is obviously good since τ_2 in example 3 was derived partially based on matching the RGA values.

An explicit formula for τ_{2i} is obtained as follows: (55) yields for the case $g_{21}/g_{22} \approx -1$ (holds for columns with a pure top product):

$$\lambda_{11}(\infty) = \lambda_{11}(0) \frac{\tau_2}{\tau_1} \quad (57)$$

Substituting the approximations (eq 39 and 44) for $\lambda_{11}(0)$ and $\lambda_{11}(\infty)$ into (57) and using $\tau_1 \approx M_I/I_s \ln S$ (eq 48) yields

feed liquid:
$$\tau_{2i} \approx \frac{N}{2 \ln S} \frac{M_I}{L_T} \quad (58)$$

(replace L_T by L_B for columns with a pure bottom product, i.e., for $Bx_B < D(1 - y_D)$). Well-designed columns have L/F about 1.25 times higher than $(L/F)_{\min}$ and $N/N_{\min} \approx 2$. Using (46) and (47) we then get that for well-designed columns

$$\tau_{2i} \approx 0.8(\alpha - 1)/(\ln \alpha)(M_I/F) \quad (58a)$$

or

$$\tau_{2i} \approx M_I/F \quad (58b)$$

when α is less than about two. The analytical formula (eq 58) applies to columns with both products of high purity. The agreement between (58) and the values for τ_2 in Table III is good. However, for practical calculations we recommend using (56) to estimate τ_2 , rather than (58), in order to get consistent values for τ_1 and τ_2 . One important point to note about (58) is that it predicts τ_2 to be only weakly dependent on operating conditions.

8. The Effect of Reboiler and Condenser Holdup

Example 8. Column A. All examples considered so far have had negligible reboiler and condenser holdups. However, the responses may depend strongly on the amount of holdup as seen from Figure 8: Curve 1 shows the initial response in y_D to a small change in reflux, L , for a column with $M_i/F = 0.5$ min on all trays including the condenser. This response is closely approximated by (17): $dy_D = 0.878/(194s + 1) dL$. Curve 2 shows the

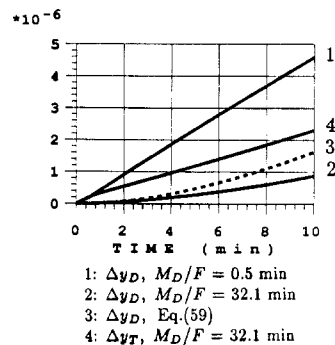


Figure 8. Column A. Effect of condenser holdup, M_D , on initial response of y_D to a small increase in reflux ($\Delta L/F^o = 0.0001$).

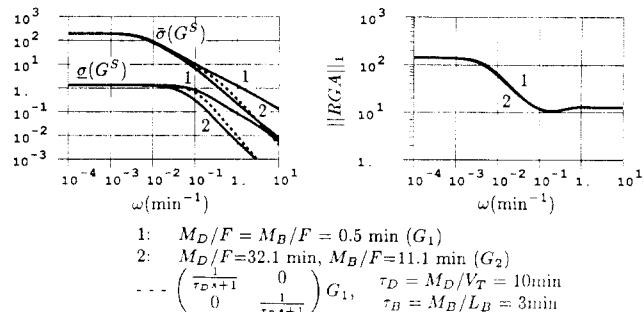


Figure 9. Column A. Effect of reboiler and condenser holdup on singular values and RGA.

response with the same holdups inside the column, but with M_D/F increased from 0.5 to 32.1 min. The initial response is significantly more sluggish than estimated from (17). To derive a better approximation, we argue as follows: The composition y_D in the condenser is not directly affected by the reflux, L (recall eq 27c), but the composition y_T in the overhead vapor is. The effect of y_T on y_D is given by a first-order response with time constant $\tau_D = M_D/V_T = 10$ min. The following approximation to curve 2 is then derived (shown as curve 3)

$$dy_D = \frac{0.878}{(10s + 1)(194s + 1)} dL \quad (59)$$

Figure 8 shows that this is a much better approximation than curve 1.

From Figure 9 (right) we see that the value of the RGA is hardly affected at all by adding the reboiler and condenser holdups. This confirms the comments made following eq 43. On the other hand, the singular values do change significantly. Again, from the dotted line in Figure 9 we see that (59) provides a reasonable way of taking into account the effect of condenser holdup.

Approximate Model with Reboiler and Condenser Holdup. To include the real case with reboiler and condenser holdup, we propose to simply "add on" two lags for the condenser and reboiler to the model (eq 23)

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ \tau_D s + 1 & 0 \\ 0 & 1 \\ 0 & \tau_B s + 1 \end{pmatrix} G(s)_{(eq 23)} \begin{pmatrix} dL \\ dV \end{pmatrix} \quad (60)$$

where $\tau_D = M_D/V_T$ and $\tau_B = M_B/L_B$. In most cases, τ_D is larger than τ_B .

Overhead Vapor Responses. In practice, composition may not be measured in the condenser (y_D), but rather in the overhead vapor (y_T). Curve 4 on Figure 8 shows that the initial response for y_T is much faster than that of y_D (for the case with large condenser holdup) and that it is

reasonably approximated by curve 1 (eq 23).

Temperature Responses. Temperatures measured somewhere away from the top and the bottom are often used to infer compositions. These temperatures have a *dynamic* response that is only weakly dependent on M_D and M_B and which is often well approximated by (23). Consequently, for practical applications, the simplified model (eq 23), which neglects reboiler and condenser holdups, may be satisfactory for controller design.

9. Simplified Model Including Flow Dynamics

So far we have neglected the flow dynamics. However, the flow responses are very important for the initial dynamic response. These issues are discussed by Rademaker et al. (1975). If we make the simplifying assumption that the flow dynamics are essentially decoupled from the composition dynamics, we derive from (23) the following simplified column model when flow dynamics are included:

$$-dY_D = \frac{g_{11}^S}{1 + \tau_1 s} dL_T + \left(\frac{g_{11}^S + g_{12}^S}{1 + \tau_2 s} - \frac{g_{11}^S}{1 + \tau_1 s} \right) dV_T \quad (61a)$$

$$dX_B = \frac{g_{21}^S}{1 + \tau_1 s} dL_B + \left(\frac{g_{21}^S + g_{22}^S}{1 + \tau_2 s} - \frac{g_{21}^S}{1 + \tau_1 s} \right) dV_B \quad (61b)$$

Here L_T , V_T , L_B , and V_B are the "local" liquid and vapor flows at the top and bottom of the column. $g_{11}^S = g_{11}/1 - y_D^\circ$, $g_{12}^S = g_{12}/1 - y_D^\circ$, $g_{21}^S = g_{21}/1 - x_B^\circ$, and $g_{22}^S = g_{22}/1 - x_B^\circ$ are the scaled gains. g_{ij} , τ_1 , and τ_2 are evaluated at the nominal operating point (y_D° , x_B°).

Comments on (61). Logarithmic compositions $Y_D = \ln(1 - y_D)$ and $X_B = \ln x_B$ are used to reduce the effect of nonlinearity. Of course, if only small variations in the product compositions are expected, we may as well use the unscaled compositions y_D and x_B . For multicomponent mixtures, $Y_D = \ln y_{DH}$ and $X_B = \ln x_{BL}$ should be used. Here H and L denote the heavy and light key components.

g_{ij}^S in (61) represents the scaled steady-state gains for the LV configuration. The gains are easily obtained from steady-state simulations or from simple analytical models (for example, based on the separation factor, e.g., Skogestad and Morari (1987d)).

τ_1 and τ_2 should be evaluated at the same nominal operating points as the steady-state gains. τ_1 may be estimated by using (48) or (54); τ_2/τ_1 may be estimated by using (56).

Extra lags $1/1 + \tau_D s$ and $1/1 + \tau_B s$ should be added to the response in y_D and x_B if composition is measured in the condenser and reboiler (see eq 60).

Measurement and valve dynamics are not included in (61).

Local flows: Let L and V denote the manipulated values of the reflux and the boilup; i.e., let

$$dL_T = dL, \quad dV_B = dV \quad (62a)$$

Then the following approximations, which apply to case of constant molar flows, are useful (Rademaker et al., 1975):

$$dV_T = dV \quad (\text{assuming perfect pressure control}) \quad (62b)$$

$$dL_B \approx e^{-\theta_L s} dL + \lambda(1 - e^{-\theta_L s}) dV \quad (62c)$$

Here

$$\lambda = (\partial L_i / \partial V)_{M_i} \quad (63a)$$

$$\theta_L = N\tau_L, \quad \tau_L = (\partial M_i / \partial L)_V \quad (63b)$$

Equation 62c is derived by repeated combination of the following two equations for each tray (Rademaker et al., 1975)

$$dL_i = (\partial L_i / \partial V)_{M_i} dV + (\partial L_i / \partial M_i)_V dM_i = \lambda dV + \frac{1}{\tau_L} dM_i \quad (64a)$$

$$dM_i / dt = dL_{i+1} - dL_i \quad (64b)$$

and approximating the response of N equal lags in series by a dead time equal to the sum of the lags

$$\frac{1}{(1 + \tau_L s)^N} \approx e^{-\theta_L s} \quad (64c)$$

Preferably the values for θ_L and λ should be determined experimentally: θ_L is the time it takes for an increase in reflux to affect the reboiler level; λ represents the initial effect of a change in vapor flow on liquid flow. Its value may be obtained by observing the response in reboiler level to a change in boilup. The effect of nonzero λ 's was first discussed by Rijnsdorp (1965) and is often denoted as the K_2 effect because he used this symbol for λ .

Tray Columns. Let $M_i = M_{ui} + M_{oi}$ where M_{oi} represent the amount of liquid over the weir. According to the Francis weir formula, $M_{oi} = k_1 L_i^{2/3}$ and we derive

$$\tau_L = \left(\frac{\partial M_i}{\partial L_i} \right)_V = \left(\frac{\partial M_{oi}}{\partial L_i} \right)_V = \frac{2}{3} \frac{M_{oi}}{L_i} \quad (65)$$

Assuming all trays are identical, this yields the following value for θ_L

$$\theta_L = N\tau_L = \frac{2}{3} \frac{M_{oi}}{M_i} \frac{M_I}{L} \quad (66)$$

where $M_I = NM_i$ is the total holdup inside the column. Typical values for the holdups on each tray are $M_{oi}/M_i \approx 0.5$ and $M_i/F \approx 0.5$ min.

For most tray columns, λ is positive, but it may also be negative in some cases. A positive λ may be caused by vapor pushing liquid off the trays. For $\lambda > 0.5$, both x_B and the reboiler level will show an inverse response for an increase in boilup (Rademaker et al., 1975). Such behavior can be detrimental for control purposes.

Packed Columns. Equation 61 and 62 apply also to packed columns. The total liquid holdup inside the column (M_I) can be estimated for various packings from published correlations (e.g., Billet and Schultes (1987)). M_I increases with liquid load. We have $M_I = k_2 L^n$ where n is typically about 0.6 (Billet and Schultes, 1987). This yields

$$\theta_L = n \frac{M_I}{L} \quad n \approx 0.6 \quad (67)$$

At low vapor flow rates, the liquid holdup is nearly independent of V ; i.e., $\lambda = 0$. This applies up to the loading point where liquid entrainment becomes important, and we have $\lambda < 0$. Since λ is always negative for packed columns, we do not expect inverse response for changes in boilup.

Tray versus Packed Columns. Usually packed columns have smaller liquid holdups inside the column than do tray columns. This results in a faster dynamic response for packed columns, but it also makes flow and level responses more important. Firstly, the smaller holdup inside the column makes the condenser and reboiler holdups more important for packed columns. Secondly, the relative

importance of the flow response compared to the composition response inside the column is about twice as large for a packed column. The reason is that, whereas the entire liquid phase always contributes to the composition response, it is only the liquid above the weir (M_{oi}) that contributes to the flow response in a tray column (compare (66) and (67)).

Pressure Response. The pressure control was assumed perfect to derive $dV_T = dV$ (eq 62b). This is not quite true in practice, but a first-order response is probably adequate in most cases:

$$dV_T = \frac{1}{\tau_p s + 1} dV \quad (68)$$

The value of τ_p depends on the pressure control system. The open-loop pressure response is given by (note that the pressure is approximately proportional to the vapor holdup, i.e., $p = kM_V$)

$$dM_V(s) = \frac{1}{s + k_p} (dV - dV_T) \quad (69)$$

The constant k_p takes care of the pressure's self-regulating effect (for example, an increase in V increases pressure, which leads to condensation of vapor). Its value is often small and may usually be neglected for control purposes, i.e., $k_p = 0$. The control system manipulates dV_T (in some cases dV) for pressure control:

$$dV_T = c(s) dM_V(s) \quad (70)$$

If $c(s) = K_c$ (proportional control), then a first-order response (eq 67) with $\tau_p = 1/K_c$ is derived. In practice, $c(s)$ also includes some integral action, and there are dynamics included in order to actually change V_T (which is done indirectly by manipulating the cooling duty).

Level Control. The immediate effect of a change in one of the product flows (D and B) is to change the condenser or reboiler holdup (level) which has no direct effect on composition. Therefore, the response to changing D and B depends strongly on the tuning of the level loops. For configurations involving D or B for composition control, the level control system may have a significant effect on the performance of the composition control system. These issues are discussed by Shinsky (1984).

Decoupling at High Frequency. The flow dynamics have the effect of decoupling the response at high frequency. The reflux (L) has a direct influence on the compositions in the top of the column, but only a delayed influence on x_B . Similarly, the boilup directly influences x_B (at least for $\lambda \approx 0$), but has a smaller initial effect on the compositions in the top (because of (68)). This decoupling at high frequency yields $\lambda_{11}(\infty) = 1$, which may be beneficial for control purposes.

10. Discussion/Conclusion

It is well-known that the dynamic response for distillation columns is essentially first order, and we have presented results which justify this claim. The simple two time constant model (eq 23 or 61) was derived by considering the fundamental difference between external and internal flows, both at steady state and dynamically. The parameters in (23) are the steady-state gains, the dominant time constant τ_1 associated with the external flows, and the time constant τ_2 associated with the internal flows. τ_1 can be estimated from steady-state data by using (16) or (48) or by matching the predicted initial response by using (54). τ_2/τ_1 may also be estimated by matching the initial response using (56).

From the derivation and analysis of the model, it is clear that (23) is most likely to hold for high-purity columns with large reflux. This is exactly the case for which control is expected to be most difficult.

Disturbances in feed rate (F) and feed composition (z_F) have not been discussed in this paper. Their low-frequency response is approximately first order with time constant τ_1 (e.g., Skogestad and Morari (1987a)), but the initial response is of higher order, especially for a disturbance in z_F . For feedback control, the exact dynamics of the disturbances are not important. However, a good model is desirable if feedforward control is used.

One advantage of the simple analytical model (eq 23 or 61) is that it gives a good description of both the low- and high-frequency behaviors of distillation columns. The traditional approach has been to use a model which matches the steady-state gains, but which is not necessarily accurate for high frequencies. The other extreme is to match the high-frequency gains (Rademaker et al., 1975, p 137). Equation 23 provides a link between the low- and high-frequency regions. Another analytical model covering both the low- and high-frequency regions has been presented by Edwards and Jassim (1977). However, their model fails to identify the fundamental difference between internal and external flows.

The high-frequency behavior is generally much less affected by changing operating conditions than is the steady state. This partially explains why highly nonlinear distillation columns may be controlled satisfactorily using linear controllers. In particular, we showed that the initial response is almost independent of operating conditions if relative (logarithmic) compositions are used. This suggests that $\ln(1 - y_D)$ and $\ln x_B$ should be used as controlled outputs for columns where y_D or x_B may vary significantly.

It may be misleading to use steady-state data as an indicator of the expected control quality. In particular, this is the case for columns with both products of high purity. For such columns, the RGA values at high frequency are generally much smaller than at steady state. From (39) and (44), we conclude that the columns which are going to be most difficult to control are high-purity columns with large reflux.

In the paper we stress the fundamental difference between *external* and *internal* flows. The external flows are associated with the dominant time constant τ_1 and have a large effect on compositions. On the other hand, the response to changes in internal flows is faster (time constant τ_2), but the effect on compositions is much smaller and is probably not detectable from open-loop plant data. One might question if there is any need to model an effect which is almost impossible to observe in a real column. The answer is "yes". One reason is that this seemingly small effect does make a large difference with respect to the directionality of the plant at high frequency. For example, the condition number and RGA values are generally lower at high frequency than at steady state (whereas a model based on a single time constant τ_1 would yield a constant value). Furthermore, the effect of the internal flows turns out to be very important for columns under feedback control. Skogestad (1988) has studied single-loop PI control of column A. He found the optimal setting for the integral time τ_I to be about 194 min when he used the one time constant model (eq 17) (which has $\tau_1 = \tau_2 = 194$ min) as the column model. However, the optimal value for τ_I turned out to be less than 10 min when he used the accurate two time constant model (eq 24) (which has $\tau_1 = 194$ min and $\tau_2 = 15$ min). The reason for the large difference is that the interactions between the two com-

position loops, which are important under feedback control, are mostly associated with changes in the internal flows.

The traditional approach to modeling distillation columns is to approximate each transfer function by a first-order lag with time delay ($ge^{-\theta s}/(1 + \tau s)$) where g is obtained by matching the steady-state gains. It is very difficult to obtain a good model for high-purity columns which captures the difference between external and internal flows by using this approach. It is also unlikely that the correct behavior at high frequency (for example, the RGA) is obtained. Kapoor et al. (1986) have suggested to base the controller design on a model for the "perturbed" steady state. This approach is likely to yield a more reasonable high-frequency model. However, such "tricks" are unnecessary if one uses a model, for example, (23), that accurately describes both the low- and high-frequency behavior.

As a final remark we should point out that, although the simple two time constant model (eq 23) matches the dynamic response of a large class of columns, it does not always apply. Firstly, there is a large number of low-purity columns with low reflux where the difference between τ_1 and τ_2 is small and a one time constant model may be satisfactory. Secondly, there are some columns, in most cases of low purity, with large differences in response times between top and bottom composition. As an example, consider the following example column: $z_F = 0.27$, $y_D = 0.98$, $x_B = 0.02$, $\alpha = 1.36$, $N = 93$, and $N_F = 40$. This column has $L/F = 2.66$, $\lambda_{11}(0) = 4.05$, and $\lambda_{11}(\infty) = 3.66$. With $M_i/F = 0.5$ min on all trays, the dominant time constant corresponding to the smallest eigenvalue (τ_{1e}) is 320 min. From the small difference between the low- and high-frequency RGA values, we expect τ_1 and τ_2 to be close in magnitude. This is indeed confirmed by dynamic simulations which yield very similar response times (time constants) for small changes in internal and external flows. In both cases, the response in top composition (y_D) has a time constant of about 300 min. However, bottom composition (x_B) has a response time of about 50 min, which is much smaller than the dominant time constant. These effects have been studied by Weigand et al. (1972) who found that the dominant time constant generally applies to the column end with the largest absolute change in composition (thus requiring a large change in component holdup, recall eq 16), while the other end may respond significantly faster. Indeed, the above example confirms this rule since the gain for y_D is about 10 times that of x_B .

The above example shows that the simple two time constant model (eq 23) does not match all columns and points out the need for additional work. Still, we believe that a number of the results presented in this paper represent significant steps forward in understanding the dynamic behavior of distillation columns. These results include the fundamental difference in dynamic behavior between external and internal flows, the understanding and prediction of the initial response, the linearizing effect of logarithmic compositions, and the simple analytical two time constant model.

Acknowledgment

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Nomenclature

B = bottom product rate, kmol/min
 D = distillate (top product) rate, kmol/min
 F = feed rate, kmol/min

$G(s)$ = transfer function model of column (eq 5)
 g_{ij} = steady-state gains for column (eq 20)
 $I_s = Dy_D(1 - y_D) + Bx_B(1 - x_B)$, impurity sum
 $K_i = dy_i/dx_i$, linearized VLE constant
 $L = L_T$, reflux flow rate, kmol/min
 L_B = liquid flow rate into reboiler, kmol/min
 M_B = liquid holdup in reboiler, kmol
 M_D = liquid holdup in condenser, kmol
 M_i = liquid holdup on theoretical tray i , kmol
 $M_I = \sum_{i=2}^N M_i$, total holdup of liquid inside column, kmol
 M_{oi} = liquid holdup above weir on tray i , kmol
 N = total number of theoretical trays (including reboiler)
 N_F = feed tray location from bottom (feed enters above this tray)
 $N_T = N + 1$, total number of trays including total condenser
 q_F = fraction liquid in feed
 RGA = Relative Gain Array (eq 13a)
 $\|RGA\|_1$ = sum of magnitudes of elements in RGA (eq 14)
 $S = (y_D(1 - x_B))/((1 - y_D)x_B)$, separation factor
 t = time, min
 $V = V_B$, boilup from reboiler, kmol/min
 V_T = vapor flow rate on top tray, kmol/min
 x_B = mole fraction of light component in bottom product
 $X_B = \ln x_B$, logarithmic bottom composition
 x_i = liquid mole fraction of light component on stage i
 $y_D = x_D$, mole fraction of light component in distillate (top product)
 $Y_D = \ln(1 - y_D)$, logarithmic top composition
 y_i = vapor mole fraction of light component on stage i
 y_T = vapor mole fraction of light component on top tray
 z_F = mole fraction of light component in feed

Greek Symbols

$\alpha = (y_i/x_i)/((1 - y_i)/(1 - x_i))$, relative volatility
 $\kappa(s) = (g_{12}(s)g_{21}(s))/(g_{11}(s)g_{22}(s))$
 $\lambda = (\partial L_i/\partial V)_{M_i}$ (eq 63a)
 $\lambda_{11} = 1/(1 - \kappa)$, 1,1 element in RGA
 ω = frequency, min^{-1}
 $\bar{\sigma}(G)$, $\underline{\sigma}(G)$ = maximum and minimum singular values (eq 10)
 τ_1 = dominant time constant for external flows, min
 τ_2 = time constant for internal flows, min
 $\tau_{je} = -1/\lambda_j(A)$, time constant corresponding to the j th smallest eigenvalue of A in eq (5), min
 $\tau_L = (\partial M_i/\partial L)_V$, min (eq 63b)
 $\theta_L = N\tau_L$, overall lag for liquid response, min

Subscripts

B = bottom product or bottom part of column
 D = distillate product
 F = feed
 i = tray numbered from bottom ($i = 1$ for reboiler, $i = 2$ for first tray, $i = N$ for top tray, $i = N + 1$ for condenser)
 i = as subscript on τ : τ obtained by matching initial response
 I = inside column
 T = top part of column

Superscripts

o = nominal operating point
 S = scaled compositions (eq 6 and 7)

Appendix. Dynamic Model of Distillation Column

Assumptions. (1) Binary separation, constant molar flows, constant relative volatility; (2) vapor-liquid equilibrium (VLE) and perfect mixing on all stages; (3) no vapor holdup (i.e., immediate vapor response, $dV_T = dV_B$); (4) liquid holdup M_i on all trays constant (i.e., immediate liquid response, $dL_B = dL_T$); these assumptions imply in particular $\lambda = 0$ and $\tau_L = 0$ (no flow dynamics). This yields a $(N + 1)$ th-order model with one ordinary differential equation on each tray ($i = 1, N+1$).

Nonlinear Model. Material balances for change in holdup of light component on each tray:

$i = 2, N$ ($i \neq N_F, i \neq N_F + 1$)

$$M_i \dot{x}_i = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i$$

above feed location, $i = N_F + 1$

$$M_i \dot{x}_i = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i + F_V y_F$$

below feed location, $i = N_F$

$$M_i \dot{x}_i = L_{i+1} x_{i+1} + V_{i-1} y_{i-1} - L_i x_i - V_i y_i + F_L x_F$$

reboiler, $i = 1$

$$M_B \dot{x}_i = L_{i+1} x_{i+1} - V_i y_i - B x_i, \quad x_B = x_1$$

total condenser, $i = N + 1$

$$M_D \dot{x}_i = V_{i-1} y_{i-1} - L_i x_i - D x_i, \quad y_D = x_{N+1}$$

VLE on each tray ($i = 1, N$), constant relative volatility

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

Flow rates assuming constant molar flows:

$i > N_F$ (above feed) $L_i = L, \quad V_i = V + F_V$

$i \leq N_F$ (below feed) $L_i = L + F_L, \quad V_i = V$

$$F_L = q_F F, \quad F_V = F - F_L$$

$$D = V_N - L = V + F_V - L$$

(condenser holdup constant)

$$B = L_2 - V_1 = L + F_L - V \quad (\text{reboiler holdup constant})$$

Compositions x_F and y_F in the liquid and vapor phase of the feed are obtained by solving the flash equations:

$$F z_F = F_L x_F + F_V y_F$$

$$y_F = \frac{\alpha x_F}{1 + (\alpha - 1)x_F}$$

Linear Model. Linearized material balance on each tray ($dL_i = dL, dV_i = dV$)

$$M_i \dot{x}_i = L_{i+1} dx_{i+1} - (L_i + K_i V_i) dx_i + K_{i-1} V_{i-1} dx_{i-1} + (x_{i+1} - x_i) dL - (y_i - y_{i-1}) dV$$

where K_i is the linearized VLE constant:

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

and $y_i, x_i, L_i,$ and V_i are the steady-state values at the nominal operating point. Written in the standard state variable form in terms of deviation variables,

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \mathbf{B}\mathbf{u}, \quad \mathbf{y} = \mathbf{C}\mathbf{x}$$

Here $\mathbf{x} = (dx_1, \dots, dx_{N+1})^T$ are the tray compositions, $\mathbf{u} = (dL, dV)^T$ are the manipulated inputs and $\mathbf{y} = (dy_D, dx_B)^T$ are the controlled outputs. The state matrix $\mathbf{A} = \{a_{i,j}\}$ is tridiagonal:

$i \neq N + 1$

$$a_{i,i+1} = L_{i+1}/M_i \quad a_{i,i} = -(L_i + K_i V_i)/M_i$$

$i \neq 1$

$$a_{i,i-1} = K_{i-1} V_{i-1}/M_i$$

Input matrix $\mathbf{B} = \{b_{i,j}\}$ is

$i \neq N + 1$

$$b_{i,1} = (x_{i+1} - x_i)/M_i, \quad b_{N+1,1} = 0$$

$i \neq 1, i \neq N + 1$

$$b_{i,2} = -(y_i - y_{i-1})/M_i, \quad b_{N+1,2} = 0, \quad b_{1,2} = (y_1 - x_1)/M_1$$

Output matrix \mathbf{C} is

$$\mathbf{C} = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \end{pmatrix}$$

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