THE DOMINANT TIME CONSTANT FOR DISTILLATION COLUMNS

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DEDICATION

This article is dedicated to the memory of Richard R. Hughes, a dear friend and colleague. He was a continuous source of the type of engineering insight we are seeking in this paper.

Abstract—It is shown that the dominant part of the dynamic composition response of two-product distillation columns can be approximated by a linear first-order response. This applies also for *large* perturbations to the column. The numerical value of this dominant time constant (τ_c) can be obtained from steady-state simulations. A simple analytical expression for small perturbations is derived which provides insight into the variation of τ_c with operating conditions. The time constant τ_c does not apply when there are changes in the internal flows only.

1. INTRODUCTION

Analytical models

Simple analytical models are useful for understanding and analyzing the behavior of complex systems. In this paper we present such a model for the composition dynamics of distillation columns. We stress that it is *not* our goal to develop models for simulation; detailed column models which can be easily solved on a digital computer have been available for at least 30 yr. The main purpose of simple analytical models is to provide insight. For example, we might want to answer the following questions—Under what conditions do we find the very large time constants which have been observed in the simulations of some columns (e.g. Fuentes and Luyben[1])? Why does the *nonlinear* dynamic composition response of distillation columns resemble often closely a *linear* first-order response? Does a change in reboiler holdup, condenser holdup or column holdup have the largest effect on the time constant for the composition response? For gaining such valuable insights a simple analytical model can be more useful than running hundreds of tray-by-tray simulations.

Furthermore for the modern robust control system design techniques, simple models are preferred which reflect the main dynamic characteristics of the system. The most important characteristics are those which limit the performance achievable by feedback control. An analytic model can be very helpful for pinpointing these limiting characteristics.

Dynamic composition response

The dynamics of most distillation columns are

dominated by one large time constant, which is nearly the same, regardless of where a disturbance is introduced or where composition is measured. This is well known both from plant measurements[2] and from theoretical studies[3–5].

A distillation column is described by a large number of differential equations. For each tray, i, a differential equation may be formulated for (a) the material balance of each component (composition dynamics):

$$\frac{d}{dt}(M_i x_i) = L_{i+1}x_{i+1} + V_{i-1}y_{i-1} - L_i x_i - V_i y_i,$$

where, from the VLE: $y_i = K_i(x_i, T)$,

(b) the overall material balance (flow dynamics):

$$\frac{d}{dt}M_i = L_{i+1} + V_{i-1} - L_i - V_i,$$

where, (tray hydraulics) $L_i = f_1(V_i, M_i, \Delta p_i)$,

(pressure drop) $V_i = f_2(M_i, \Delta p_i)$,

and (c) the energy balance:

$$\frac{d}{dt}(M_i U_i) = L_{i+1}H^L_{i+1} + V_{i-1}H^V_{i-1} - L_i H^L_i - V_i H^V_i,$$

where,

$$H^L_i = f_3(x_i, p_i), \quad H^V_i = f_4(y_i, p_i).$$

We only want to outline the *structure* of the equations and not concern ourselves with the details. Viewed against the background of the large number of nonlinear differential equations, the simple low-order responses (often first-order) observed for most distillation columns are somewhat surprising. For a specific example Levy *et al.*[6] showed through modal analysis that the slowest mode involves primarily the

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composition effects and is nearly unaffected by the flow dynamics (if we assume constant molar flows, then the flow dynamics are decoupled from the composition dynamics and it is trivial to show that the eigenvalues for the modes corresponding to the composition dynamics are unaffected by flow dynamics). This leads to the conjecture that the dominant part of the dynamics can be captured by modelling only the composition dynamics. This is the approach taken in this paper.

The simplest approach is to consider the *total* holdup of each component in the column. Assuming that all trays have the same response, a first-order model is found directly and the dominant time constant can be estimated. According to Rademaker *et al.*([7] p. 280) this idea dates back to the beginning of the century (Lord Raleigh) and seems to get rediscovered every few years. Moczek *et al.*[3] used it to introduce the "inventory time constant" for a column going from one steady-state (subscript 0) to another (subscript f):

$$T_{inv} = \frac{\Delta(\Sigma M_i x_i)}{\Delta(Fz_F) - y_{D0}\Delta D - x_{B0}\Delta B}. \qquad (1)$$

Here $\Delta D = D_f - D_0$ and $\Delta B = B_f - B_0$ are the changes in distillate and bottoms flow rate, $\Delta(\Sigma M_i x_i)$ is the change in holdup in the column of any component, $\Delta(Fz_F)$ is the change in feed rate of this component and y_{D0} and x_{B0} are the initial product mole fractions of this component.

Later, Wahl and Harriot[4] and Waller *et al.* (Toijala[8]) introduced similar concepts (T_s and T_{eq}), but they considered only the time constant of the linearized system (called the "linearized time constant" in the following). Moczek *et al.* introduced (1) through somewhat intuitive arguments; we will return with a complete derivation and interpretation below.

In spite of the excellent agreement found for high-purity separations[3,9] between (1) and the actual time response of the column, the usefulness of (1) does not appear to be appreciated by the chemical engineering community. For example, Shinskey([10] p. 157) claims that the only general relationship that seems to hold for the dominant time constant is that it is proportional to $\Sigma M_i/F$. In fact, this follows

directly from (1), but (1) certainly contains much more information. The limited use of (1) is probably caused by the following two *misconceptions*:

(i) equation (1) provides the value of the linearized time constant, that is, it is only useful for small perturbations from steady-state,

(ii) the linearized time constants are substantially in error (much larger) when compared to either the actual or the simulated response.

Both these claims are incorrect. Misconception (i) is probably based on the work by Wahl and Harriot[4] and Toijala[8] who derived (1) for small pertubations. In fact, (1) can be used to estimate the "average" time constant between any two steady-states. Misconception (ii) is due to the unfortunate assumption of equal product purities $(1 - y_D = x_B)$ used in the majority of the academic case studies. It turns out, as we will show, that the time constant has its peak value for approximately $1 - y_D = x_B$. In general, however, the estimated linearized time constant is *not* necessarily larger than the actual time constant (e.g. see Fig. 2). In fairness we should add that the criticism in (ii) is correct if *both* products are of high purity. The reason is that in this case the perturbations to the column will bring the column to a new steady state where one of the products is less pure. Since the time constant is determined by the *least pure* product this implies that the actual time constant will be smaller than the linearized one (see Section 3).

A major source of misconception (ii) is probably the work of Wahl and Harriot[4]. They present a figure (Fig. 7 in their paper) for estimating the linearized time constant as a function of operating variables for the column. Although not stated in the paper, these values apply *only* to the special case $1 - y_D = x_B$. The figure is therefore of very limited practical value and will generally yield too large values for the time constant. (Similar figures, which are misleading, for the same reason, are presented by Tyreus *et al.*[11].) Wahl and Harriot[4] also claim that the time constant is relatively constant for a large perturbation in the loads; this is not correct for high-purity columns as seen from Fig. 1.
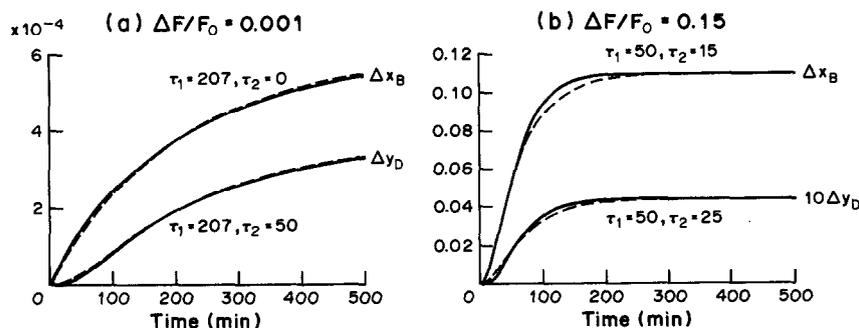

Fig. 1. Column A. Nonlinear open-loop response to small (a) and large (b) change in feed rate F with L and V constant. Dotted line: approximation with second-order response $k/(\tau_1 s + 1)(\tau_2 s + 1)$. ($M_i/F = 0.5$ min, $M_D/F = 32.1$ min, $M_B/F = 11.1$ min).

Misconception (ii) is also present in a recent work by Kapoor et al.[12]. They claim that "published tower time constants based on linear analysis have been substantially in error when compared to actual responses for many cases. The reason for this error is a . . . positive feedback loop produced by the re-cycle tower structure . . . (for which the) gain drops sharply for small perturbations from steady state". Firstly, the results based on linear analysis are not "in error". (The range of validity may be very limited however if both products are of high purity.) Sec-ondly, the simple mixing-tank model (1) explains in at least as simple a fashion as the "positive feedback loop concept" when and why the linearized time constant is "in error". This is discussed in detail below.

2. DERIVATION OF EXPRESSION FOR τ_c

Consider a column which initially ($t = 0$) is at steady state (subscript 0). At $t = 0$ a step change is introduced to the column which eventually ($t \to \infty$) moves the column to a new steady-state (subscript f). The nature of this step change is not important as long as: (i) the new steady-state is known; and (ii) it leads to a change in the total holdup in the column of one or more component. This includes most disturbances and inputs except changes in the internal flows (changes in L and V keeping product rates constant).

Assumption 1. The flow dynamics are immediate, i.e. for $t > 0$: $M_i(t) = M_{if}$, $D(t) = D_f$, $B(t) = B_f$.

This assumption is also used in all simulations in this paper. It is reasonable for the composition dynamics, provided the flow response is much faster than the composition response. Using Assumption 1 the overall material balance for any component be-comes for $t > 0$:

$$\frac{d}{dt}\left[\sum_{i=1}^{N+1} M_{if}x_i(t)\right] = F_f z_{Ff} - D_f y_D(t) - B_f x_B(t). \quad (2)$$

Subtracting the final steady state ($0 = F_f z_{Ff} - D_f y_{Df} - B_f x_{Bf}$) and introducing $\Delta y_L(t) = y_D(t) = y_{Df}$, yields:

$$\sum_{i=1}^{N+1} M_{if}\Delta \dot{x}_i(t) = -D_f \Delta y_D(t) - B_f \Delta x_B(t). \quad (3)$$

Assumption 2. All trays have the same dynamic responses, i.e. $\Delta x_i(t) = \Delta x_i k(t)$, $\Delta y_D(t) = \Delta y_D k(t)$, $\Delta x_B(t) = \Delta x_B k(t)$. [Here $k(0) = 1$ and $\Delta x_i = \Delta x_i(0)$, $\Delta y_D = \Delta y_D(0)$ and $\Delta x_B = \Delta x_B(0)$ denotes the differ-ence between the initial and final steady-state).

Assumption 2 corresponds to treating the column as a large mixing tank. This assumption is reasonable if the time constant for the internal mixing in the column, $\tau_M = M_I/L$, is much shorter than the domi-nant time constant. τ_M is approximately the time it takes for a composition change at the top of the column to travel to the bottom; for a composition change starting from the top each tray acts as a first

order lag with time constant M_i/L. The overall transfer function is the product of these lags which may be approximated by a time delay with time constant $\tau_M = M_I/L$. (τ_M was introduced by Wahl and Harriot[4] who called it the circulation time.)

Assumption 2 and equation (3) yield:

$$\left(\sum_{i=1}^{N+1} M_{if}\Delta x_i\right)\dot{k}(t) = (-D_f\Delta y_D - B_f\Delta x_B)k(t). \quad (4)$$

Solving (4) gives a linear first-order response:

$$k(t) = e^{-t/\tau_c},$$

where the time constant τ_c is defined as (subscript c denotes change in component holdup):

$$\tau_c = \frac{\sum_{i=1}^{N+1} M_{if}\Delta x_i}{\Delta S_i}, \quad \Delta S_i \stackrel{\text{def}}{=} D_f\Delta y_D + B_f\Delta x_B, \quad (5)$$

(ΔS_i is the supply imbalance). A simple interpretation of (5) is:

$$\tau_c = \frac{\text{"change in holdup of one component" (kmol)}}{\text{"imbalance in supply of this component" (kmol min}^{-1})}.$$

Note that:

$$\Delta S_i = D_f\Delta y_D + B_f\Delta x_B$$
$$= \Delta(Fz_F) - y_{D0}\Delta D - x_{B0}\Delta B \quad (6)$$

and τ_c defined by (5) is therefore equal to T_{inv} defined by (1) if we assume that the holdup on each tray is constant, i.e. $M_{if} = M_i$. This assumption is used in the rest of the paper; its effect on the value of τ_c is clearly insignificant.

Comments on (5)

1. The column model was *not* linearized and (5) applies to any finite change provided that Assump-tions 1 and 2 hold.

2. The time constant depends on the *magnitude* and *direction* (negative or positive change) of the step change introduced.

3. The expression for τ_c applies to any component in a multicomponent mixture.

4. Equation (5) applies to any change which changes the *external* material balance, i.e. which has $\Delta S_i \neq 0$. Equation (5) does *not* apply for changes in the *internal* flows (changing L and V while keeping D and B constant) because the denominator $\Delta S_i = 0$ in this case [see (6)]. Furthermore, in this case there is very little change in component holdup and the entire holdup approach is not appropriate. Methods for estimating the time constant for changes in the internal flows are discussed in another paper[13].

5. To compute τ_c according to (5) a *steady-state* model of the column is needed. For obtaining accu-rate numerical values a nonlinear simulation program should be used. Such programs are usually readily available. For any given step change only two simu-lations are required to compute τ_c. To simplify the

Table 1. Steady-state data for distillation column examples. $\lambda_{11}(0)$ denotes the 1-1-element in the RGA for the LV-configuration

Column	z_F	α	N	N_F	y_D	x_B	D/F	L/F	$\lambda_{11}(0)$
A	0.5	1.5	40	21	0.99	0.01	0.500	2.706	35.1
B	0.1	1.5	40	21	0.99	0.01	0.092	2.329	47.5
C	0.5	1.5	40	21	0.90	0.002	0.555	2.737	7.53
D	0.65	1.12	110	39	0.995	0.10	0.614	11.862	58.7
E	0.2	5	15	5	0.9999	0.05	0.158	0.226	2.82
F	0.5	15	10	5	0.9999	0.0001	0.500	0.227	499
G	0.5	1.5	80	40	0.9999	0.0001	0.500	2.635	1673
WH	0.5	2.0	26	13	0.995	0.005	0.500	1.477	41.6

computations the program should be modified to print out $\Sigma_{i=1}^{N+1} M_i x_i$.

6. Very large time constants are found for *small* perturbations to columns with *both* products of high purity. This agrees with the observations of Wahl and Harriot[4], Tyreus *et al.*[11] and Fuentes and Luyben[1]. The reason is that the compositions inside the column may change significantly (resulting in a large change in component holdup), while the change in product compositions may be very small (resulting in a small imbalance ΔS_i to cause the change in component holdup).

7. The expression for τ_c can be split into three contributions (caused by holdup inside column, in condenser and in reboiler):

$$\tau_c = \tau_{cI} + \tau_{cD} + \tau_{cB}, \qquad (7a)$$

$$\tau_{cI} = \frac{M_I \Delta \bar{x}_I}{\Delta S_i},$$

$$\tau_{cD} = \frac{M_D \Delta y_D}{\Delta S_i} \leqslant \frac{M_D}{D_f}, \quad \tau_{cB} = \frac{M_B \Delta x_B}{\Delta S_i} \leqslant \frac{M_B}{B_f}, \quad (7b)$$

where $M_I = \Sigma_{i=2}^{N} M_i$ is the total holdup and $\bar{x}_I = \Sigma_{i=2}^{N} x_i M_i / M_I$ is the average composition *inside* the column. The contribution to τ_c from the change in holdup inside the column (τ_{cI}) is often dominating. Furthermore, the reboiler and condenser are to some degree "decoupled" from the rest of the column and their contribution to τ_c may be less than what is indicated by (7) (see Example 4 below).

8. One disadvantage of (5) is that the compositions on all trays are needed to compute τ_c. We will therefore later derive an *analytical* expression for τ_c, based on a very simple model, which involves

only the product compositions (y_D and x_B). This expression is useful for gaining insight into the non-linear behavior of distillation columns.

Comparison with nonlinear simulations

Moczek *et al.*[3] reported excellent agreement between (5) and the observed nonlinear response for a high-purity BTX-column. Weigand *et al.*[9] studied six different columns and found very good agreement for the high-purity column (Column V in their paper) and reasonably good agreement for the five low-purity columns. The agreement was found to be best for small perturbations to high-purity columns, which is expected, since this gives large time constants and Assumption 1 and 2 are likely to hold. For columns with only one product of high purity, τ_c was found to apply to the low-purity end, while the time constant for the high-purity end was often significantly smaller.

In this paper the eight columns (A–WH) in Table 1 are used as examples. In all examples we assume constant molar flows, constant liquid and vapor holdup (i.e. instantaneous flow responses), constant relative volatility, liquid feed, 100% tray efficiency, total condenser and equal holdup, N_i, on all trays inside the column.

Example 1. Column A. ($M_i/F = 0.5$ min, $M_D/F = 32.1$ min, $M_B/F = 11.1$ min). Table 2 compares τ_c with the actual time constant τ_1 observed for nonlinear responses to small and large changes in F, V and L. Each nonlinear response was fitted by eye to a second-order linear response $1/(1 + \tau_1 s)(1 + \tau_2 s)$ as shown in Fig. 1. (We do not propose this as a good column model, but it gives the reader an idea of the shape of the nonlinear response.) The agreement

Table 2. Column A. Time constants for inputs of various magnitude. Note that (7) often overestimates the magnitude of τ_{cD} and τ_{cB} (see *Example 4*). ($M_I/F = 0.5$ min, $M_D/F = 32.1$ min, $M_B/F = 11.1$ min)

Input	Holdup model (7)			τ_c = Sum	Fit of nonlinear response to $\dfrac{1}{(\tau_1 s + 1)(\tau_2 s + 1)}$			
	τ_{cI}	τ_{cD}	τ_{cB}		τ_1 (y_D)	τ_2 (y_D)	τ_1 (x_B)	τ_2 (x_B)
$\Delta F/F_0 = 0.001$	190	24.6	13.7	228	207	50	207	0
$\Delta V/F_0 = 0.001$	194	30.6	11.6	236	210	50	210	0
$\Delta L/F_0 = 0.001$	190	26.4	13.1	229	228	20	228	0
$\Delta L/F_0 \to 0$	191	28.7	12.3	232				
$\Delta F/F_0 = 0.150$	41.1	1.9	16.6	59.6	50	25	50	15
$\Delta V/F_0 = 0.200$	29.6	45.2	0.5	75.3	50	25	14.5	0
$\Delta V/F_0 = -0.20$	25.7	1.5	15.6	42.8	43	0	25	20
$\Delta L/F_0 = 0.200$	26.5	1.5	15.6	43.7	40	0	25	20

between τ_c and τ_1 is good for small perturbations. For the larger perturbations τ_c agrees better with $\tau_1 + \tau_2$. The only large deviation is found for the response in x_B to a large increase in $\Delta V/F_0 = 0.20$ (L constant); this change takes the column from the initial steady-state with $y_D = 0.99$ and $x_B = 0.01$ to a new steady-state with $y_D = 0.714$ and $x_B = 0.0006$. For the pure bottom product we find $\tau_1 + \tau_2 = 14.5$ min which is much smaller than $\tau_c = 75.3$ min. However, as observed by Weigand *et al.*[9] the agreement is very good for the less pure top product ($\tau_1 + \tau_2 = 75$ min).

Example 2. Column D. ($M_i/F = M_D/F = M_B/F =$ 1 min). To show that the linearized time constant is not necessarily larger than the actual "nonlinear" time constant, we considered a feed composition disturbance to column D. The linearized time constant for a small disturbances in z_F found using (5) is $\tau_c = 319$ min. This compares nicely with the actual response which has a time constant of about 388 min for y_D and 341 min for x_B (Fig. 2a). Next, we studied a 7.7% decrease in z_F (Fig. 2b):

initial steady state:
$z_F = 0.65$, $\quad y_D = 0.9950$,
$x_B = 0.1000$, $\quad \bar{x}_I = 0.714$,

final steady state (all flows unchanged):
$z_F = 0.60$, $\quad y_D = 0.9578$,
$x_B = 0.0296$, $\quad \bar{x}_I = 0.495$,

We find for this change:

$$\tau_{cI} = \frac{(N-1)M_i\Delta\bar{x}_I}{\Delta(Fz_F)} = \frac{109 \times 1 \times 0.219}{0.05} = 477 \text{ min},$$

$$\tau_{cB} = \frac{M_B\Delta x_B}{\Delta(Fz_F)} = 1.4 \text{ min}, \quad \tau_{cD} = \frac{M_D\Delta y_D}{\Delta(Fz_F)} = 0.7 \text{ min}.$$

Consequently, for this large disturbance in z_F, (5) gives $\tau_c = 479$ min, which is *higher* than the linearized value of 319 min. This is also confirmed by the simulations in Fig. 2; the response of y_D to the large disturbance in z_F is clearly more sluggish ($\tau_1 \approx \tau_2 \approx 400$ min) than for the small disturbance.

Linearized time constant

The linearized time constant is derived from (7) by replacing the Δ's by differentials:

$$\tau_{cI} = \frac{M_I \, d\bar{x}_I/dx_B}{B + D \, dy_D/dx_B},$$

$$\tau_{cD} = \frac{M_D}{D + B \, dx_B/dy_D}, \quad \tau_{cB} = \frac{M_B}{B + D \, dy_D/dx_B}. \quad (8)$$

These values are in general different depending on the disturbance or input because the linearized gains (dy_D/dx_B) are different. The values of τ_{cD} and τ_{cB} are easily obtained from the steady-state gain matrix.

Example 3. Column A. ($M_i/F = 0.5$ min, $M_D/F = 32.1$ min, $M_B/F = 11.1$ min). The steady-state gain matrix [equal to $-CA^{-1}B$, see equation (11) below] for this column is:

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = \begin{pmatrix} 0.878 & -0.864 \\ 1.082 & -1.096 \end{pmatrix} \begin{pmatrix} dL \\ dV \end{pmatrix}.$$

For a small change in L with V constant this gives $(dy_D/dx_B)_V = 0.878/1.082 = 0.811$ which yields $\tau_{cD} = 28.7$ min and $\tau_{cB} = 12.3$ min. The value of $(d\bar{x}_I/dx_B)_V = 8.85$ for a small change in L is obtained numerically. This gives:

$$\tau_{cI} = \frac{39 \times 0.5 \times 8.85}{0.5 + 0.5 \times 0.811} = 191 \text{ min},$$

$$\tau_c = \tau_{cI} + \tau_{cD} + \tau_{cB} = 232 \text{ min}$$

Very similar values are obtained for a small change in V (L constant) since $(dy_D/dx_B)_L = 0.864/1.096 = 0.799$ and $(d\bar{x}_I/dx_B)_L = 8.74$ are almost unchanged. Note that the 1–1 element in the RGA for the LV-configuration is given by[10]:

$$\lambda_{11} = \left(1 - \frac{(dy_D/dx_B)_L}{(dy_D/dx_B)_V} \right)^{-1}. \quad (9)$$

Therefore columns with large RGA-elements (which corresponds to columns with both products of high purity) are expected to yield similar values for τ_c for small perturbations in L or V.
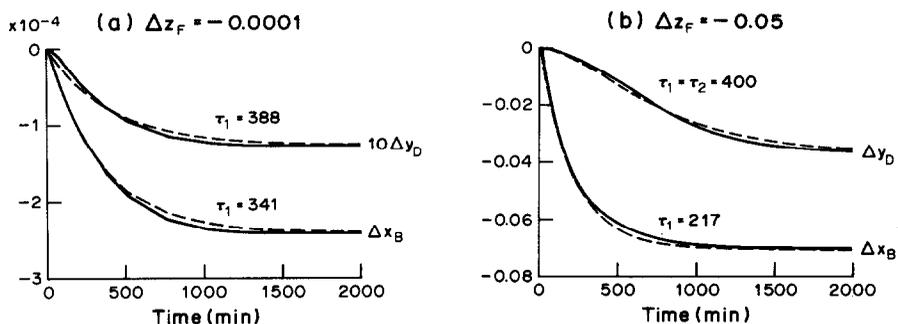

Fig. 2. Column D. Nonlinear open-loop response to small (a) and large (b) change in feed composition z_F. Dotted line: approximation with second-order response $k/(\tau_1 s + 1)(\tau_2 s + 2)$, $\tau_2 = 0$ if not specified. ($M_i/F = M_D/F = M_B/F = 1$ min).

Comparison with eigenvalues

To find the linearized dynamics more accurately, linearize the material balance and *VLE* on each tray:

$$M_i \dot{x}_i = L \, dx_{i+1} - (L + K_i V) \, dx_i + K_{i-1} V \, dx_{i-1}$$
$$+ (x_{i+1} - x_i) \, dL - (y_i - y_{i-1}) \, dV.$$

Here K_i is the linearized VLE-constant:

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

Written in the standard state-variable form in terms of deviation variables:

$$\dot{x} = Ax + Bu + Ed, \quad y = Cx. \tag{10}$$

Here $x = (dx_1, \ldots, dx_{N+1})^T$ are the tray compositions, $u = (dL, dV)^T$, $d = (dF, dz_F)^T$ and $y = (dy_D, dx_B)^T$. Written in transfer matrix form:

$$y = C(sI - A)^{-1}(Bu + Ed). \tag{11}$$

The poles (eigenvalues of A) are the same for *any* input or disturbance and independent of where composition is measured (y_D, x_B, x_i). However, the zero locations are different which may yield entirely different responses.

Wahl and Harriot[4] found very good agreement between the linearized value of τ_c and the time constant τ_{1e} corresponding to the smallest eigenvalue of A, and this is confirmed by our results. Wahl and Harriot found that the agreement was acceptable (errors less than 20%) even for some cases with $\tau_M/\tau_c < 1$.

Example 4. Column A. The value of the time constants corresponding to the three smallest eigenvalues of A are (all numbers in minutes, τ_c from *Example 1*):

M_i/F	M_D/F	M_B/F	τ_{1e}	τ_{2e}	τ_{3e}	τ_c
0.5	0	0	193	12	3.4	191
0.5	32.1	11.1	220	32	11.6	232

Note that τ_c and τ_{1e} are almost identical for the case $M_D = M_B = 0$. This indicates that Assumption 2 holds very well for what happens inside the column. However, with $M_D/F = 32.1$ min and $M_B/F = 11.1$ min the increase in τ_{1e} is only 27 min, while τ_c increases by 43 min. This indicates that Assumption 2 does not hold for the reboiler and condenser and that these are partially decoupled from the rest of the column. This is not surprising since the larger holdups in the reboiler and condenser make these less sensitive to "interactions" with the other trays. In addition, there is only one stream entering the reboiler and condenser, while the trays inside the column have two.

τ_{1e} and linearized values of τ_c (5) are compared for some other columns with small reboiler and condenser holdup in Table 3. The agreement is amazing for columns A,B,F,G and WH all of which have $\tau_M \ll \tau_c$ is generally very good. Also for the other cases the agreement is very good. The only exception is column E for which τ_c for a change in V is 42% smaller than τ_{1e}. This is not surprising because

Table 3. Linearized time constants (min). Values for τ_c (5) are given for small perturbations in L with V constant (and, if different, value for small change in V with L constant is in parentheses). Note that $\tau_M = M_i/L \ll \tau_c$ for Assumption 2 to hold. All columns: $M_i/F = M_D/F = M_B/F = 1$ min

Column	τ_c (5)	τ_{sc} (17)	Eigenvalues τ_{1e}	τ_{2e}	τ_M
A	387	427	388	24	15
B	504 (496)	428	500	23	18
C	58 (60)	91	49	16	15
D	300 (299)	385	308	47	9
E	142 (95)	29	165	16	71
F	5992	4886	5992	9	48
G	40664	42891	40667	40	31
WH	459	477	459	15	18

$\tau_c/\tau_M = 1.34$ in this case and Approximation 2 is not likely to be valid. The large difference in the linearized time constant τ_c for changes in L and V which is observed in this case is also expected because of the low values for the RGA for this column $(\lambda_{11} = 2.82)$ which implies that $(dy_D/dx_B)_L$ and $(dy_D/dx_B)_V$ are quite different.

Table 3 illustrates that the simple holdup model (5) gives strikingly accurate time constants for small pertubations to high-purity columns. According to (5) the reasons for the large time constants observed for high-purity columns is that there is a "large" change in component holdup inside the column, but only a small imbalance (change in product compositions) to bring about the change. Other explanations for the large time constants are given in the literature: Kapoor *et al.*[12] claim that they are caused by "positive feedback loops produced by the recycle structure". Fuentes and Luyben[1] claim that the cause is "small concentration changes from tray to tray (which) make some of the coefficients in the linearized equation very small, giving small eigenvalues". Both of these explanations seem unnecessarily complicated.

Note from Table 3 that very large linearized time constants may be encountered even for easy separations with few trays: Column F has 10 theoretical trays and $L/D = 0.45$, yet $\tau_c = \tau_{1e} = 5992$ min. The reason for the large value of the linearized time constant is the high purity of the products $(1 - y_D = x_B = 10^{-4})$. However, the time constant will be drastically smaller for any realistic perturbation to the column. This is discussed below.

3. A SIMPLE FORMULA FOR τ_c

We will now use (5) to derive a simple formula for the *linearized* time constant for the case of a *binary* separation. The following additional assumptions are made.

Assumption 3. All trays $(i = 2, N)$ have equal and constant holdup (M_i).

Assumption 4. The average composition inside the column is (see Appendix):

$$\bar{x}_i = \left[1 + \frac{\ln \dfrac{1 - x_B}{x_B}}{\ln \dfrac{y_D}{1 - y_D}} \right]^{-1}. \tag{12}$$

Assumption 5. The steady-state gains may be estimated by assuming the separation factor $S = y_D(1 - x_B)/(1 - y_D)x_B$ is constant for any given change.

Equation (12) was derived by assuming the composition profile is the same as that of a column with total reflux, and Assumption 4 is therefore most likely to hold for columns with large reflux. Assumption 5 does not apply when there are changes in the internal flows, but this case is already excluded since (5) does not apply in this case. Assumption 5 is most likely to hold for high-purity columns because then the term involving the change of $\ln S$ in (15) is negligible.

In this section let y_D, x_B and x_i denote the mole fraction of the *light* component, and let ζ represent any input or disturbance to the column which changes the *external* material balance such that (5) holds. For a small perturbation, $d\zeta$, (5) yields:

$$\tau_c = \frac{M_I \dfrac{\partial \bar{x}_I}{\partial \zeta} + M_D \dfrac{\partial y_D}{\partial \zeta} + M_B \dfrac{\partial x_B}{\partial \zeta}}{D \dfrac{\partial y_D}{\partial \zeta} + B \dfrac{\partial x_B}{\partial \zeta}}. \qquad (13)$$

Differentiating the component material balance, $Fz_F = D_{yD} + Bx_B$, yields the following expression for the denominator of (13):

$$D \frac{\partial y_D}{\partial \zeta} + B \frac{\partial x_B}{\partial \zeta} = e_\zeta, \qquad (14a)$$

where e_ζ is defined as:

$$e_\zeta = -(y_D - x_B)\frac{\partial D}{\partial \zeta} + F\frac{\partial z_F}{\partial \zeta} + (z_F - x_B)\frac{\partial F}{\partial \zeta}. \quad (14b)$$

To evaluate the numerator, we need to find the linearized gains $\partial y_D/\partial \zeta$ and $\partial x_B/\partial \zeta$. (This will also yield $\partial \bar{x}_I/\partial \zeta$ because of Assumption 4.) For binary mixtures *exact* expressions for these gains are derived by combining (14a) with the definition of the separation factor S:

$$\frac{1}{(1 - y_D)y_D}\frac{\partial y_D}{\partial \zeta} = \frac{1}{I_s}\left[e_\zeta + Bx_B(1 - x_B)\frac{\partial \ln S}{\partial \zeta}\right], \quad (15a)$$

$$\frac{1}{(1 - x_B)x_B}\frac{\partial x_B}{\partial \zeta} = \frac{1}{I_s}\left[e_\zeta - Dy_D(1 - y_D)\frac{\partial \ln S}{\partial \zeta}\right]. \quad (15b)$$

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

$$I_s = Bx_B(1 - x_B) + Dy_D(1 - y_D). \qquad (16)$$

As pointed out by Shinskey[10] there is usually not too much error introduced by assuming the separation factor S is constant when considering changes in the external flows (e.g. D/F). Consequently, for upsets $d\zeta$ which change the external material balance ($e_\zeta \neq 0$), the term involving the change in separation factor S is usually of minor importance (in particular for high-purity separations with x_B and $1 - y_D$ small)

and a reasonable approximation is found by assuming S constant (Assumption 5). Equations (12) and (15) yield:

$$\left(\frac{\partial y_D}{\partial \zeta}\right)_s = \frac{(1 - y_D)y_D e_\zeta}{I_s}, \quad \left(\frac{\partial x_B}{\partial \zeta}\right)_s = \frac{(1 - x_B)x_B e_\zeta}{I_s},$$

$$\left(\frac{\partial \bar{x}_I}{\partial \zeta}\right)_s = \frac{\partial}{\partial \zeta}\left(\frac{\ln \dfrac{y_D}{1 - y_D}}{\ln S}\right)_s = \frac{1}{\ln S}\frac{\partial}{\partial \zeta}\left(\ln \frac{y_D}{1 - y_D}\right)_s$$

$$= \frac{e_\zeta}{I_s \ln S}.$$

Substituting this into (13) yields a short-cut formula for the linearized value of τ_c (note that e_ζ drops out):

$$\tau_{sc} = \tau_{scI} + \tau_{scD} + \tau_{scD} = \frac{M_I}{I_s \ln S}$$

$$+ \frac{M_D(1 - y_D)y_D}{I_s} + \frac{M_B(1 - x_B)x_B}{I_s}. \quad (17)$$

For the special case of equal purities ($x_B = 1 - y_D$) we get $I_s = Fx_B y_D$ and (17) becomes:

$$\tau_{sc} = \frac{M_I/F}{x_B y_D \ln S} + M_D/F + M_B/F. \qquad (18)$$

Here the term $1/x_B y_D \ln S$ which multiplies the holdup inside the column is:

$x_B = 1 - y_D$: 0.3   0.1   0.01   0.001 10^{-4} 10^{-6},
$(x_B y_D \ln S)^{-1}$: 2.81   2.53   11.0   72.5   543   36191.

This clearly shows that usually the contribution to τ_c from the holdup *inside* the column dominates, especially for separations with *both* products of high purity. Also recall that the contributions to τ_c from the condenser and reboiler holdup are generally overestimated by (17) and (18) because Assumption 2 does not hold.

Values for τ_{sc} found from (17) are compared with τ_c (8) in Table 3. The agreement is of course best for the cases when Assumptions 4 and 5 are likely to hold, i.e. for columns with high reflux (Assumption 4 is valid) and for high-purity columns (Assumption 5 is valid). However, the main value of the analytical formula (17) is the insight it yields into the *nonlinear* dynamic behavior of distillation columns. Consider the contribution from the holdup *inside* the column:

$$\tau_{scI} = \frac{M_I}{I_s \ln S}. \qquad (19)$$

Here $\ln S$ usually does not change very much with operating conditions. The time constant is therefore determined mainly by I_s which again is determined by the composition of the *least pure* product:

$$I_s \approx \begin{cases} D(1 - y_D) \text{ if distillate least pure} \\ \quad [(1 - y_D) \gg x_B], \\ Bx_B \text{ if bottoms least pure} \\ \quad [x_B \gg (1 - y_D)]. \end{cases} \qquad (20)$$

For columns with *both* products of high purity any disturbance or input to the column is likely to take
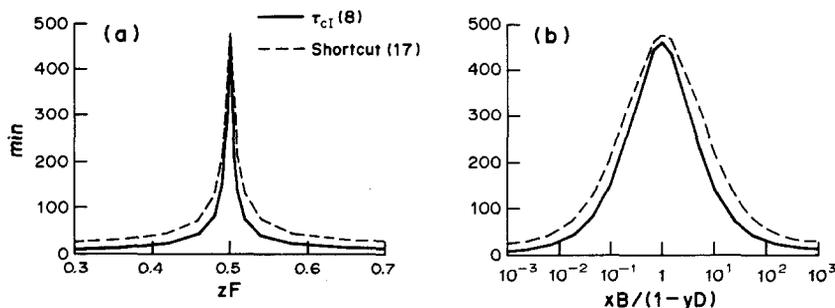
Fig. 3. Column WH. *Linearized* time constant τ_{cl} as a function of z_F with all flows fixed. Each value of z_F corresponds to a new steady-state with a particular y_D and x_B and the right-hand figure is included to show clearer the variation in τ_{cl} with $x_B/1 - y_D$. ($M_i/F = M_D/F = M_B/F = 1$ min).

the column to a new steady-state where *one* of the products is *less pure* and the actual time constant for this change will be smaller than found by linear analysis [which (19) is based on].

It also follows from (19) that τ_{cl} reaches its maximum value approximately when both products have equal purity; by differentiating (19) we find that for $z_F = 0.5$ the maximum value of τ_{scl} when D/B is varied is obtained for $D/B = 1$ corresponding to $1 - y_D = x_B$. Also for other values of z_F the maximum is obtained when $(1 - y_D)/x_B$ is of the order one.

Example 5. Column WH. Consider the high-purity column ($1 - y_D = x_B = 0.005$) presented by Wahl and Harriot[4]. In Fig. 3 the linearized time constant τ_{cl} is shown as a function of z_F with all flows fixed. Each value of z_F corresponds to a specific steady-state with a given ratio $x_B/(1 - y_D)$ and we have also plotted τ_{cl} against this ratio. We see that τ_{cl} has a very high peak at the nominal operating point $z_F = 0.5$ which corresponds to $x_B/(1 - y_D) = 1$. This illustrates that Fig. 7 in Wahl and Harriot[4] for estimating the linearized time constant is highly misleading; it is based on the assumption $1 - y_D = x_B$. Also note from Fig. 3 that very similar values for τ_c are obtained from (8) and the short-cut formula (17).

Example 6. Column B. A similar example for column B is shown in Fig. 4. In this case $z_F = 0.1$ and $L/F = 2.329$ are fixed, and different steady states are obtained by varying D/F. The nominal operating points has $D/F = 0.0918$ corresponding to $(1 - y_D)/x_B = 1$ which yields $\tau_{cl} = 501$ min. The peak

value of the linearized time constant τ_{cl} is 656 min which is obtained for $D/F = 0.0952$ corresponding to $(1 - y_D)/x_B = 2.8$.

4. DISCUSSION AND CONCLUSION

The dynamics of most distillation columns are dominated by one large time constant (τ_c), which is nearly the same, regardless of where a disturbance is introduced or where composition is measured. Physically, this dominant time constant reflects the change in component holdup inside the column. The dominant time constant can be estimated using the inventory time concept introduced by Moczek *et al.*[3]. Based on this concept we have derived a simple analytic formula for estimating its linearized value for binary separations:

$$\tau_{cl} \approx \tau_{scl} = \frac{M_I}{I_s \ln S}. \tag{19}$$

(In addition there are contributions to τ_c from the reboiler and condenser holdup; these are usually of less importance.) The formula (19) gives reasonable agreement with observed values, but its main value is the simple analytical form which provides insight into the *nonlinear* behavior of distillation columns. In particular, the value of τ_{cl} is determined mainly by the purity of the least pure product [equation (20)] and it will be large when both products have high purity (I_s is small).
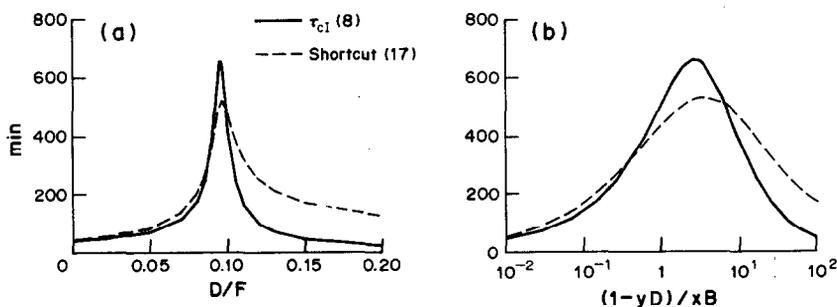

Fig. 4. Column B. *Linearized* time constant τ_{cl} as a function of D/F (with $z_F = 0.1$ and $L/F = 2.329$ fixed). Each value of D/F corresponds to a particular $1 - y_D/x_B$. ($M_i/F = M_D/F = M_B/F = 1$ min).
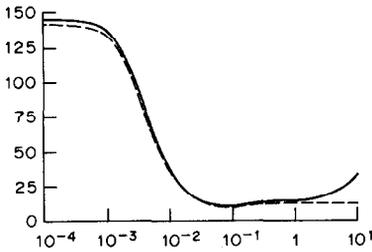
Fig. 5. Column A. Condition number $\gamma(G) = \bar{\sigma}(G)/\underline{\sigma}(G)$ and $\| \text{RGA} \|_1 = \Sigma |\lambda_{ij}|$ (dotted line) as a function of frequency. $(M_i/F = M_D/F = M_B/F = 1 \text{ min})$.

Numerical results[3,9] have shown that the inventory time concept gives best agreement with actual simulated responses for columns with both products of high purity. This observation may be justified with (19): Assumption 2, which is the basis of the inventory time concept, is most likely to hold for columns with $\tau_M \ll \tau_c$. Using $\tau_M = M_I/L$ and τ_c from (19) we find that this is satisfied if:

$$L/D \gg \frac{\dfrac{B}{D}x_B + (1 - y_D)}{\ln S}$$

This inequality holds for columns with large reflux (left hand side is large) and columns with both products of high purity (right hand side is small). The inventory time concept may *not* yield accurate estimates if this inequality is not satisfied. For example, this may be the case for low-purity separations (e.g. column I in Weigand *et al.*,[9]) and for cases when a large forcing function makes one of the products unpure (e.g. $V/F = 0.20$ discussed in Example 1).

From the derivation of τ_c it is clear that this dominant time constant only applies if there is a change in the *external* material balance. The time constant τ_2 for changes in the *internal* flows is often much smaller. As an example consider Fig. 5 which shows the condition number as a function of frequency for column A. If a *single* time constant τ_c were used for all transfer function elements, corresponding to the model $G(s) = G(0)/1 + \tau_c s$, then the condition number would be the same at all frequencies. This is

clearly not the case as seen from Fig. 5 and the lower value at high frequencies is caused by τ_2 being significantly smaller than τ_c. This is discussed in detail in another paper[13] where we propose a model in terms of τ_c and τ_2 which is consistent with the behavior in Fig. 5.

From the derivation of (5) we know that if Assumptions 1 and 2 hold then the composition response should be first order, even for large deviations from steady-state. The simulations indicate that the first order approximation is indeed valid for small perturbations. However, recall Fig. 2 which shows that the response in y_D to a small decrease in z_F is first order (Fig. 2a), but that it is approximately second-order for a large decrease (Fig. 2b). In the last case y_D decreases from 0.995 to 0.958, that is, the amount of heavy impurity increases from 0.005 to 0.042. Although the initial response in terms of absolute compositions is sluggish (second order), there is initially a large *relative* change in the amount of impurity. This suggests that a lower-order response may be obtained if logarithmic compositions are used:

$$Y_D = \ln(1 - y_D) \quad \text{and} \quad X_B = \ln x_B. \quad (21)$$

Fig. 6 shows the same responses as in Fig. 2, but using logarithmic compositions. The time constants of the first- and second-order approximations of the observed responses are summarized below:

	$\Delta z_F = -0.0001$:	$\Delta z_F = -0.05$:
y_D	$\tau_1 = 388$	$\tau_1 = \tau_2 = 400$
Y_D	$\tau_1 = 388$	$\tau_1 = 563$
x_B	$\tau_1 = 341$	$\tau_1 = 217$
X_B	$\tau_1 = 341$	$\tau_1 = 320$

The responses are much less dependent on the magnitude of the disturbance when logarithmic compositions are used and the observed second-order response for y_D almost "disappears" (becomes first-order) when Y_D is used. This confirms the results by Skogestad and Morari[13] who suggest using logarithmic compositions *as a means of reducing the effect of nonlinearity*. Note that for *small* deviations from steady-state the use of logarithmic compositions merely corresponds to a rescaling of the outputs and
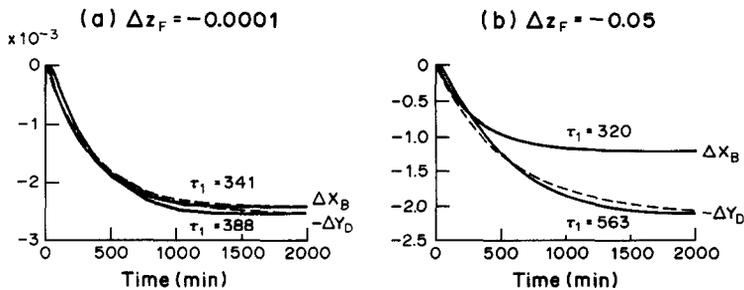

Fig. 6. Column D. Nonlinear open-loop responses to small (a) and large (b) change in z_F. Logarithmic compositions $Y_D = \ln(1 - y_D)$ and $X_B = \ln \chi_B$ are used. Dotted line: approximation with first-order response $k/(\tau_1 s + 1)$. The responses should be compared to the ones in terms of y_D and x_B in Fig. 2.

the time constants in terms of Y_D and X_B are the same as for y_D and x_B. This of course means that the *linearized* time constants derived in this paper [equations (8) and (17)] also apply to Y_D and X_B.

However, as shown above, for *large* deviations from steady-state the responses are different and it seems that the response in terms of logarithmic compositions, Y_D and X_B, is closer to first-order than when y_D and x_B are used. We can not explain this from (5), which was derived in terms of absolute compositions and our only justification is that the linear response at each operating point is approximately first-order [from (5)] and that the use of logarithmic compositions makes the linear response only weakly dependent on operating conditions[13].

NOMENCLATURE

B = Bottom product rate (kmol min^{-1})
D = Distillate (top product) rate (kmol min^{-1})
F = Feed rate (kmol min^{-1})
$I_s = Dy_D(1 - y_D) + Bx_B(1 - x_B)$—"impurity sum"
L = Reflux flow rate (kmol min^{-1})
M_B = Holdup in reboiler (kmol)
M_D = Holdup in condenser (kmol)
M_i = Holdup on tray i (kmol)
$M_I = \sum_{i=2}^{N} M_i$ = total holdup of liquid inside column (kmol)

N = Total number of theoretical trays (including reboiler)
N_F = Feed tray location from bottom (feed enters above this tray)
$S = \dfrac{y_D(1 - x_B)}{(1 - y_D)x_B}$ = separation factor

V = Boilup from reboiler (kmol min^{-1})
x_B = Mol fraction of component in bottom product
x_i = Liquid mol fraction of component on stage i
$\bar{x}_I = \sum_{i=2}^{N} x_i M_i/M_I$ = average liquid mol fraction inside column

$y_D = x_D$ = mol fraction of component in distillate (top product)
y_i = vapor mol fraction of component on stage i
z_F = mol fraction of component in feed
$\alpha = \dfrac{y_i/x_i}{(1 - y_i)/(1 - x_i)}$ = relative volatility (binary mixture)

τ_c = Dominant time constant for change in holdup (min)
τ_{sc} = Shortcut estimate of τ_c
$\tau_{je} = 1/\lambda_j(A)$ = time constant corresponding to the jth smallest eigenvalue of matrix A in equation (10) (min)
$\tau_M = M_I/L$ = mixing time for column (min)

Subscripts
   B = Bottom product
   D = Distillate product
   F = Feed

I = Inside column
f = Final steady-state
0 = Initial steady-state
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)

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APPENDIX

Formula for $\bar{x}_I$ for Binary Mixtures

The expression (12) for $\bar{x}_I$ is derived by assuming:

(i) all trays have the same holdup (Assumption 3),
(ii) constant relative volatility α,
(iii) the shape of the composition profile is the same as that derived from Fenske's exact equation for total reflux:

$$\frac{y_i/1 - y_i}{x_B/1 - x_B} = \alpha^i, \quad .$$

(iv) this composition profile may be approximated by straight lines:

$$x_B \leqslant x_i \leqslant w: \bar{x} \approx 0 \ (i \leqslant N_w)$$
$$w < x_i < 1 - w: \bar{x} \approx 0.5$$
$$1 - w \leqslant x_i \leqslant y_D: \bar{x} \approx 1 \ (i \geqslant N_{1-w})$$

(N_w and N_{1-w} are defined by the above equations, w is a fixed number).

The average composition in the column from (iii):

$$\bar{x}_I = \frac{1}{N_{\min} - 1} \int_{i=1}^{N_{\min}} x_i \, di.$$

Here $N_{\min}$ is the number of trays needed with total reflux. Using (iv):

$$\bar{x}_I \approx \frac{1}{N_{\min} - 1} [0.5(N_{1-w} - N_w) + 1.0(N_{\min} - N_{1-w})]. \quad (A1)$$

Here $N_{\min}$, N_w and N_{1-w} are found using (iii):

$$N_{\min} = \frac{\ln S}{\ln \alpha}, \quad N_w = \frac{\ln \dfrac{w}{1-w} \dfrac{1-x_B}{x_B}}{\ln \alpha} + 1,$$

$$N_{1-w} = \frac{\ln \dfrac{1-w}{w} \dfrac{1-x_B}{x_B}}{\ln \alpha} + 1.$$

This gives:

$$0.5(N_{1-w} - N_w) = \frac{\ln \dfrac{1-w}{w}}{\ln \alpha},$$

$$(N_{\min} - N_{1-w}) = \frac{\ln \dfrac{y_D}{1-y_D} - \ln \dfrac{1-w}{w} - 1}{\ln \alpha}.$$

Note that w drops out when this is substituted into (A1) and we get:

$$\bar{x}_I = \frac{\ln \dfrac{y_D}{1-y_D} - \ln \alpha}{\ln S - \ln \alpha} \approx \frac{\ln \dfrac{y_D}{1-y_D}}{\ln S} = \left[1 + \frac{\ln \dfrac{1-x_B}{x_B}}{\ln \dfrac{y_D}{1-y_D}} \right]^{-1}.$$