DYNAMICS AND CONTROL OF DISTILLATION COLUMNS
A tutorial introduction

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The paper summarizes some of the important aspects of the steady-state operation, dynamics and control of continuous distillation columns. The treatment is mainly limited to two-product distillation columns separating relatively ideal binary mixtures.

Keywords. Separation factor, logarithmic compositions, external flows, internal flows, initial response, dominant time constant, configuration selection, linearization, mass flows, disturbances, one-point control, two-point control, controllability analysis, RGA, CLDG, multivariable control, design changes.

1 Introduction

Distillation is the most common unit operation in the chemical industry and understanding its behavior has been a defining characteristic of a good chemical engineer. Yet, distillation research has repeatedly been proclaimed to be a dead area, and some universities have even considered to stop teaching the basics of McCabe-Thiele diagrams. However, there has been renewed interest the last years, especially since distillation columns has become a favorite subject in the process systems engineering field, including the areas of process synthesis, process dynamics and process control. The reason is that distillation columns are themselves a system; a distillation columns may be viewed as a set of integrated, mostly cascaded, flash tanks. However, this integration gives rise to a complex and non-intuitive behavior, and it is difficult to understand the system (the column) based on the knowledge about the behavior of the individual pieces (the flash tanks).

In this paper I want to present, in a simple manner, some of the important issues for understanding the dynamics, operation and control of distillation columns, including some useful tools for controllability analysis in the frequency domain. The goal is to develop insight and intuition. It is hoped that, when the reader has understood the essentials, then the details can easily be obtained from the literature.

Five years ago, I wrote a quite detailed literature survey on distillation dynamics and control (Skogestad, 1992), concentrating on the the period 1985-1991, and I had the ambition to update that survey, but I have not had the capacity to keep up with my ambition. In any case, the 1992 survey paper was in 1997 reprinted in the Norwegian journal *Modeling, Identification and Control*, so it should be easily available. The reader should consult it for more detailed and appropriate references.

However, I would like to mention at least a few of the important books. In terms of design and steady-state behavior there are many books, but let me here only mention King (1971) which gives a comprehensive and insightful treatment. In terms of distillation dynamics and control, the book by Rademaker et al. (1975) contains a lot of excellent material, but the exposition is rather lengthy and hard to follow. Furthermore, since most of the work was completed around 1959, the book is somewhat outdated. It includes a good treatment of the detailed material and energy balances for each tray, including the flow dynamics, but discusses only briefly the overall response of the column. The discussion on control configuration selection is interesting, but somewhat outdated. The books by Shinskey (1977, 1984) on distillation control contain many excellent practical recommendations which reflect the authors vast experience in the field. There is a detailed treatment on the issue of composition control and various configuration alternatives. However, the explanations are often lacking or difficult to follow. Buckley et al. (1985) give a detailed discussion of the design of level and pressure control systems, but the issue of composition control (configuration selection) is only briefly discussed. There is a lot of good material in the book based on the extensive experience of Page Buckley, but it could be argued that the book was published about 20 years too late. The book by

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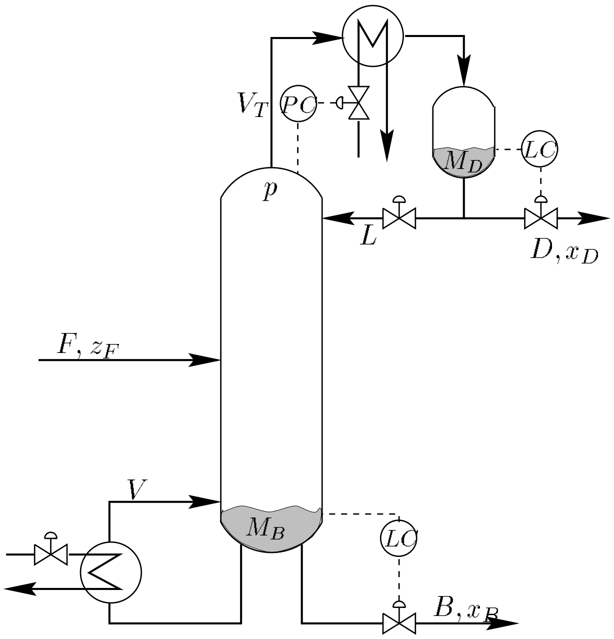

Figure 1: Typical simple distillation column controlled with LV-configuration.

Kister (1990) concentrates on distillation operation, and has a wealth of practical recommendations. The book has a good discussion on one-point composition control, level- and pressure control, and on location of temperature sensors. Finally, Luyben (1992) has edited a book with many good contributions from the most well-known authors in the field of distillation dynamics and control. However, being a collection of stand-alone papers, it is not really suitable as an introductory text.

Table 1: Notation

F - Feed rate [kmol/min]
z_F - feed composition [mole fraction]
q_F - fraction of liquid in feed (1 in all examples shown)
D and B - distillate (top) and bottoms product flowrate [kmol/min]
x_D and x_B - distillate and bottom product composition (usually of light component) [mole fraction]
$L = L_T = L_{N_{tot}}$ - reflux flow [kmol/min]
$V = V_B = V_1$ - boilup flow [kmol/min]
N - no. of theoretical stages including reboiler
$N_{tot} = N + 1$ - total number of stages (including total condenser)
i - stage no. (1=bottom. N_F - feed stage)
L_i and V_i - liquid and vapor flow from stage i [kmol/min]
x_i and y_i - liquid and vapor composition on stage i (usually of light component) [mole fraction]
M_i - liquid holdup on stage i [kmol] (M_B - reboiler, M_D - condenser holdup)
M_I - total liquid holdup on inside column [kmol]
α - relative volatility between light and heavy component
τ_L - time constant for liquid flow dynamics on each stage [min]
$\theta_L = (N-1)\tau_L$ - time “delay” for change in reflux to reach reboiler [min]
λ - constant for effect of vapor flow on liquid flow (”K2-effect”)

A typical two-product distillation column is shown in Figure 1. The most important notation is summarized in Table 1 and the column data for the examples are given in Table 2. We use index i to denote the stage number, and we number the stages from the bottom ($i = 1$) to the top ($i = N_{tot}$) of the column. Index B denotes bottom product and D distillate product. We use index j to denote the components; $j = L$ refers to the light component, and $j = H$ to the heavy component. Often there is no component index, then this usually refers to the light component.

Table 2: Column Data*

	N	N_{tot}	N_F	F	z_F	q_F	α	D	L	V	x_D	x_B	M_i	τ_L
Column A	40	41	21	1	0.5	1	1.5	0.5	2.706	3.206	0.99	0.01	0.5	0.063
3-stage column	2	3	2	1	0.5	1	10	0.5	3.05	3.55	0.9	0.1	1.0	0

* For both columns $\lambda = 0$. The nominal liquid holdup M_i on all N_{tot} stages is assumed to be the same (including the reboiler and condenser); in practice the reboiler and condenser holdups, M_D and M_B, are usually much larger.

2 Fundamentals of steady-state behavior

The basis for understanding the dynamic and control properties of distillation columns, is to have a good appreciation of its steady-state behavior.

It is established that the steady-state behavior of most real distillation columns, both trayed and packed columns, can be modeled well using a staged equilibrium model. [2] The critical factor is usually to obtain a good description of the vapor-liquid equilibrium. For an existing column, one usually adjusts the number of theoretical stages in each section to match the observed product purities and temperature profile. Tray efficiencies are sometimes used, especially if the number of theoretical stages is small, and we cannot achieve good agreement with an integer number.

To describe the degree of separation between two components in a column or in a column section, we introduce the separation factor

$$S = \frac{(x_L/x_H)_{top}}{(x_L/x_H)_{btm}} \tag{1}$$

where here L denotes light component, H heavy component, top denotes the top of the section, and btm the bottom. We will present short-cut formulas for estimating S below.

In this paper, we want to develop insight into the typical behavior of distillation columns. For this reasons we will make two simplifying assumptions.

1. *Constant relative volatility.* In this case the vapor-liquid equilibrium between any two components is given by

   $$\alpha = \frac{y_L/x_L}{y_H/x_H} = \frac{y_L/y_H}{x_L/x_H} \tag{2}$$

   where α is independent of composition (and usually also of pressure). This assumption holds well for the separation of similar components, for example, for alcohols or for hydrocarbons. Obviously, this assumption does not hold for non-ideal mixtures such as azeotropes. For a *binary mixture* (2) yields

   $$\alpha = \frac{y/(1-y)}{x/(1-x)} \quad \Rightarrow \quad y = \frac{\alpha x}{1+(\alpha-1)x} \tag{3}$$

2. *Constant molar flows.* In this case the molar flows of liquid and vapor along the column do not change from one stage to the next, that is, if there is no feed or product removal between stages i and $i+1$, then at steady-state

   $$L_i = L_{i+1}; \quad V_i = V_{i+1} \tag{4}$$

   Again, this assumption usually holds well for similar components if their heats of vaporization do not differ too much.

We will also assume in most cases that the feed mixture is binary, although many of the expressions apply to multicomponent mixtures if we consider a pseudo-binary mixture between the two key components to be separated.

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[2] There are exceptions, especially if chemical reactions taking place; for more details see e.g. the work of Taylor et al. (1992, 1994) on nonequilibrium models.

Estimating the relative volatility. For an ideal mixture where Raoults law applies, we can estimate the relative volatility from the boiling point difference. We have [3]

$$\ln \alpha \approx \frac{\Delta H^{vap}}{RT_B} \frac{\Delta T_B}{T_B} \tag{5}$$

where $\Delta T_B = T_{BH} - T_{BL}$ is boiling point difference, $T_B = \sqrt{T_{BL} T_{BH}}$ is the geometric average boiling temperature, and ΔH^{vap} is the heat of vaporization which is assumed constant. The factor $\frac{\Delta H^{vap}}{RT_B}$ is typically about 13.

For example, for methanol (L) - n-propanol (H), we have $T_{BL} = 337.8$ K, $T_{BH} = 370.4$ K, and the heats of vaporization at their boilings points are 35.3 kJ/mol and 41.8 kJ/mol, respectively. We use $\Delta H^{vap} = \sqrt{35.3 \cdot 41.8} = 38.4$ kJ/mol, $T_B = \sqrt{337.8 \cdot 370.4} = 353.7$ K and $\Delta T_B = 32.6$ K. This gives $\frac{\Delta H^{vap}}{RT_B} = 13.1$ and we find $\alpha \approx 3.33$, which is a bit lower than the experimental value because the mixture is not quite ideal.

As an another example, consider a mixture with α =1.5 and $T_B = 350K$. Then (5), with $\frac{\Delta H^{vap}}{RT_B} \approx 13$, gives $\Delta T_B \approx 10.7$ K, which will be the temperature difference across the column if we separate a binary mixture into its pure components (neglecting the pressure drop).

2.1 Column design

To increase the separation (factor) we can either increase the number of stages in the column or we can increase the energy usage (i.e. the reflux). To quantify this trade-off, we usually consider the two extreme cases of (i) infinite reflux, which gives the minimum number of stages (N_{min}), and (ii) infinite number of stages, which gives the minimum energy usage ($Q_{min} = V_{min} \cdot \Delta H^{vap}$). Typically, we select the mumber of theoretical stages N in the column as $N = 2N_{min}$, which gives a corresponding boilup rate V of about $1.2V_{min}$. From the expressions for N_{min} and V_{min}, given in equations (8) and (11)-(12), we see that the most important parameter is the relative volatility α. For example, as α is decreased from 2 to 1.1, we find that the required number of stages N increases by a factor of about 7, and the energy usage (i.e. V) increases by a factor of about 10. In practice, distillation becomes uneconomical for mixtures with α less than about 1.1, corresponding to a boiling point difference of less than about 2 K.

2.1.1 Minimum number of stages (infinite reflux)

With infinite internal flows, L_i and V_i, a material balance across any part of the column gives $V_i = L_{i+1}$, and similarly a material balance for any component gives $V_i y_i = L_{i+1} x_{i+1}$. Thus, $y_i = x_{i+1}$, and with constant relative volatility we have

$$\alpha = \frac{y_{L,i}/y_{H,i}}{x_{L,i}/x_{H,i}} = \frac{x_{L,i+1}/x_{H,i+1}}{x_{L,i}/x_{H,i}} \tag{6}$$

For a column or column section with N stages, repeated use of (6) gives Fenske's formula for the overall separation factor

$$S = \frac{(x_L/x_H)_{top}}{(x_L/x_H)_{btm}} = \alpha^N \tag{7}$$

For a column with a given separation, this yields Fenske's formula for the minimum number of stages

$$N_{min} = \ln S / \ln \alpha \tag{8}$$

Note that a high-purity separation (S is large) requires a large number of stages, although the increase is only proportional to the logarithm of separation factor. Expressions (7) and (8) do not assume constant molar flows and apply to the separation between any two components with constant relative volatility.

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[3] Raoults law gives $y_j/x_j = p_j^{sat}/p$ and we have $\alpha = \frac{y_L/x_L}{y_H/x_H} = p_L^{sat}/p_H^{sat}$ where $p_L^{sat}(T)$ and $/p_H^{sat}(T)$ are evaluated at the same temperature T. From The Clausius-Claperyon equation we have that $p_L^{sat}(T_{BH}) = p_L^{sat}(T_{BL}) \exp\left(-\frac{\Delta H^{vap}}{R}(\frac{1}{T_{BH}} - \frac{1}{T_{BL}}\right)$. Then $\alpha = p_L^{sat}(T_{BH})/p_H^{sat}(T_{BH})$ and using $p_L^{sat}(T_{BL}) = p_H^{sat}(T_{BH}) = 1$ atm, we derive (5).

2.1.2 Minimum energy usage (infinite no. of stages)

With an infinite number of stages, we can reduce the reflux (i.e. the energy consumption) until a pinch zone occurs somewhere inside the column. For a binary separation this will usually occur at the feed stage (where the material balance line and the equilibrium line will meet), and we can easily derive an expression for the minimum reflux. For saturated *liquid feed* (e.g. King, 1971, p. 447):

$$L_{min} = \frac{\phi_L^D - \phi_H^D \alpha}{\alpha - 1} F \tag{9}$$

where $\phi_L^D = D x_{D,L} / F z_{F,L}$ is the recovery fraction of light component, and ϕ_H^D of heavy component, both in the distillate. The result depends relatively weakly on the product purity, and for sharp separations ($\phi_L^D = 1, \phi_H^D = 0$) we get $L_{min} = F/(\alpha - 1)$. Actually, (9) applies without stipulating constant molar flows or constant α, but then L_{min} is the liquid flow entering the feed stage from above, and α is the relative volatility at feed conditions. A similar expression, but in terms of V_{min} entering the feed stage from below, applies for a saturated *vapor feed* (King, 1971):

$$V_{min} = \frac{\phi_H^B - \phi_L^B \alpha}{\alpha - 1} F \tag{10}$$

where ϕ^B is the recovery in the bottom product. For sharp separations with $\phi_H^B = 1$ and $\phi_L^B = 0$ we get $V_{min} = F/(\alpha - 1)$. In summary, for a binary mixture with constant molar flows and constant relative volatility, the minimum boilup V_{min} for *sharp separations* is:

$$\text{Feed liquid}: \quad V_{min} = \frac{1}{\alpha - 1} F + D \tag{11}$$

$$\text{Feed vapor}: \quad V_{min} = \frac{1}{\alpha - 1} F \tag{12}$$

Note that V_{min} is independent of the product purity for sharp separations. From this we establish one of the key properties of distillation: *We can achieve any product purity* (even "infinite separation factor") *with finite energy* (as long as the boilup V is higher than V_{min}) *by increasing the number of stages*.[4]

The expressions in (9)-(12) also apply to multicomponent mixtures if the non-key components lie between the key components (L and H) in boiling point, and distribute to both products in the "preferred" way with respect to minimum boilup. The reason is that the pinch then occurs at the feed stage. In general, the values computed by the above equations give a (conservative) *upper bound* when applied directly to multicomponent mixtures (King, 1971, p. 452).

2.1.3 Finite number of stages and finite reflux

Fenske's formula $S = \alpha^N$ applies to infinite reflux. At an earlier *Distillation and Absorbtion symposium* in Brighton in 1987, we proposed a nice generalization to the case with finite reflux (Skogestad and Morari, 1987a) [5]

$$S = \alpha^N \frac{(L/V)_T^{N_T}}{(L/V)_B^{N_B}} \tag{13}$$

Here N_T is the number of stages in the top section and N_B in the bottom section, and

$$L_B = L_T + q_F F; \quad V_T = V_B + (1 - q_F) F \tag{14}$$

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[4] Obviously, this statement does not apply to azeotropic mixtures (for which $\alpha = 1$ for some composition), but we can get arbitrary close to the azeotropic composition, and useful results may be obtained in some cases by treating the azeotrope as a pseudo-component and using α for this pseudo-separation.

[5] The paper with the derivation and discussion of (13) appeared in my Ph.D. thesis in 1987, but was otherwise unpublished, but it is now available as an internal report over the internet (Skogestad and Morari, 1987b). A simple way to derive (13) is by repeated use of (68) and (69).

where q_F is the fraction of liquid in the feed. The main assumptions behind (13) is that we have constant relative volatility, constant molar flows, that there is no pinch zone around the feed, and that the feed is optimally located. It should be stressed that even when these assumptions hold, (13) is only an approximation. The shortcut formula (13) is somewhat misleading since it suggests that the separation may always be improved by transferring stages from the bottom to the top section if $(L/V)_T > (V/L)_B$. This is not generally true and also violates the assumption of having the feed is optimally located, so to avoid this problem we may follow Jafarey et al. (1979) and choose $N_T \approx N_B \approx N/2$, to derive

$$S = \alpha^N \left[\frac{(L/V)_T}{(L/V)_B} \right]^{N/2} \tag{15}$$

The shortcut formulas in (13) and (15) are very similar to expressions given by Jafarey et al. (1979) which have been adopted by Shinskey (1984). They give similar results, but (13) and (15) are esthetically much nicer and easier to remember.

Formulas (13) and (15) give the correct limiting value $S = \alpha^N$, for infinite reflux, but at finite reflux they usually overestimate the value of S (at least for cases where the feed stage is optimal). For example, (15) says that the minimum reflux (corresponding to $N = \infty$) is obtained with $\alpha^2 \frac{(L/V)_T}{(L/V)_B} = 1$, and for a liquid feed we derive $L_{min} = F/(\alpha^2 - 1)$, which is smaller than the correct value of $L_{min} = F/(\alpha - 1)$ in (9) for a sharp separation. The fact that (13) and (15) are poor close to minimum reflux is not surprising, since we then have a pinch zone around the feed stage.

The short-cut formula (15) has proven itself useful for estimating the number of stages for use in column design, and also for estimating the effect of changes in internal flows in column operation (Skogestad and Morari, 1987ab). However, for us the main value of (15) is the insight it provides. First we see, as already stated, that the best way to increase S is to increase the number of stages. Second, during operation where N is fixed, (15) provides us with the important insight that the separation factor S is increased by increasing the *internal flows* (L and V), thereby making L/V closer to 1.

The separation factor also depends on the external flows (D and B), but in practice only small variations in these flows are allowed (since we must keep D/F close to z_F to achieve high purity; see below) and thus we can, for most practical purposes, assume that S remains constant when we change the external flows. Shinskey (1967, 1977, 1984) has used this insight to derive several useful results.

2.2 Logarithmic compositions

Distillation columns are known to be strongly nonlinear, that is, the effect of changes depends strongly on the magnitude of the change and on the operating point. The primary reason for this is the nonlinear VLE, e.g. see (3).

However, it turns out that the behavior, both at steady-state and especially dynamically, is much less dependent on operating point if we instead consider the logarithmic composition *defined* as the logarithm between the ratio of the key components,

$$X = \ln(x_L/x_H) \tag{16}$$

Similarly, if we have a temperature measurement T, we may use the logarithmic temperature defined as (Mejdell and Skogestad, 1991)

$$T^{log} = \ln \frac{T_{H,\mathrm{ref}} - T}{T - T_{L,\mathrm{ref}}} \tag{17}$$

where $T_{L,\mathrm{ref}}$ is the boiling point of light component (or some reference temperature near the top), and $T_{H,\mathrm{ref}}$ is the boiling point of the heavy component (or some reference temperature near the bottom). Usually we have $X \approx T^{log}$.

Note that Fenske's formula (7) for total reflux in a column or column section, becomes in terms of logarithmic compositions

$$X_{top} - X_{btm} = N \ln \alpha \tag{18}$$

That is, the logarithmic composition increases approximately linearly with the number of stages.[6] This is illustrated in Figure 2, which shows composition profiles for column A. We note that the profile in terms of logarithmic compositions (right plot) is close to linear, especially near the column ends.

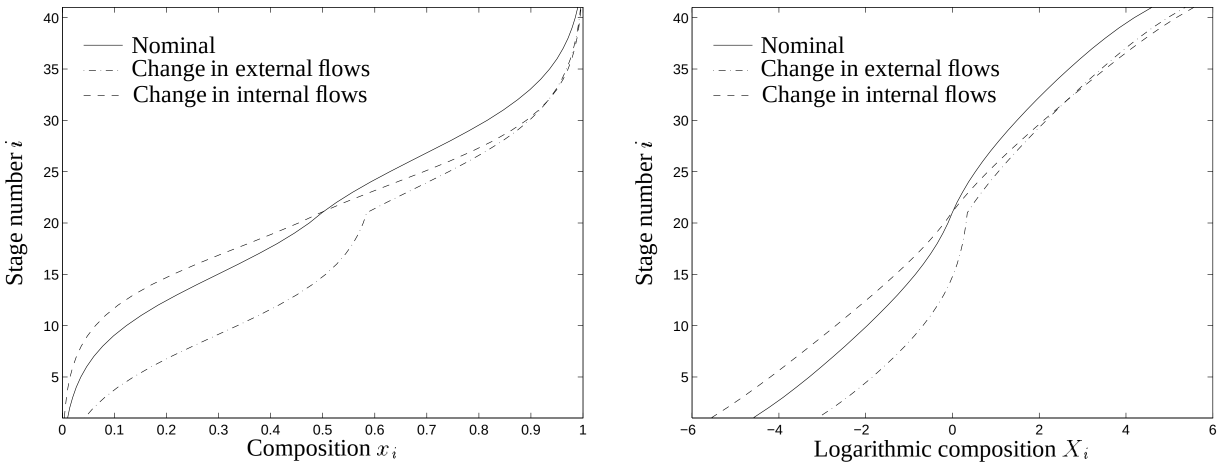

Figure 2: Composition profiles for column A. Right: Logarithmic compositions.
(Change in external flows: $\Delta L = -\Delta D = 0.02$ with $\Delta V = 0$; Change in internal flows: $\Delta L = \Delta V = 1$)

Another reason for using logarithmic composition is that it approximately gives the change divided by the impurity concentration (the "relative" change), which usually is more reasonable to consider from a practical point of view. To see this, note that, if the sum of key components is constant i.e. $dx_L = -dx_H$ (e.g. for a binary mixture), then a differentiation of (16) gives

$$dX = \frac{x_L + x_H}{x_L x_H} dx_L \tag{19}$$

Thus, for sharp separations of a binary mixture, we get for the logarithmic product compositions

$$dX_D \approx \frac{dx_{D,L}}{x_{D,H}}; \quad dX_B \approx \frac{dx_{B,L}}{x_{B,L}} \tag{20}$$

2.3 Internal and external flows

We are now ready to discuss one of the key aspects of distillation operation and control; namely the difference between internal and external flows.

Consider first the following simple example, which illustrates that changes in external flows (D/F and B/F) usually have large effects on the compositions.

Example. *Consider a column with z_F=0.5, $x_D = 0.99$, $x_B = 0.01$ (all these refer to the mole fraction of light component) and $D/F = B/F = 0.5$. To simplify the discussion set $F = 1$ [kmol/min]. Now consider a 20% increase in the distillate D from 0.50 to 0.6 [kmol/min]. This will have a drastic effect on composition. Since the total amount of light component available in the feed is $z_F F = 0.5$ [kmol/min], at least 0.1 [kmol/min] of the distillate must now be heavy component, so the amount mole faction of light component is now at best 0.5/0.6 = 0.833. In other words, the amount of heavy component in the distillate will increase at least by a factor of 16.7 (from 1% to 16.7%).*

Thus, we generally have that a change in *external flows* (D/F and B/F) has a large effect on composition, at least for sharp splits, because any significant deviation in D/F from z_F implies large changes in composition.

On the other hand, the effect of changes in the *internal flows* are much smaller. For example, for column A the steady-state effect on product compositions, x_D and x_B, of a small increase in external flows (e.g. $\Delta L = -\Delta D = 0.001$) is about 100 times larger than the effect of corresponding change in the the internal

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[6] Actually, a plot of X_i as a function of the stage location i is frequently used in design to pinpoint a poorly located feed for multicomponent separations; we want this plot to be as straight as possible, also around the feed point.

flows (e.g. $\Delta L = \Delta V = 0.001$ with D constant). In general, the ratio between the effect of small changes in the external and internal flows is large if the "impurity sum" $I_s = Bx_B(1-x_B)+Dx_D(1-x_D)$ is small (see (92) in Appendix), and such columns then have a large condition number for the gain matrix (they are "ill-conditioned").

To further illustrate the difference between changes in external and internal flows, consider the composition stage profiles in Figure 2, where the solid line is for the nominal operating point. The result of a 4% decrease in the distillate flow ($\Delta L = -\Delta D = 0.02$ with V constant) is shown by the dashed-dot curve. We see that the effect of this change in external flows is to move the entire stage composition profile, so that the column now contains a lot more light component. This results in a less pure bottom product (with more light component) and a purer top product (with more light component). On the other hand, a 50 times larger increase in the internal flows ($\Delta L = \Delta V = 1$ with D constant; the dashed line) has a smaller effect. It changes the slope of the curve and makes both products purer. In this case, light component is shifted internally from the bottom to the top part of the column, but the overall amount of light component inside the column remains almost unchanged.

In any case, the conclusion is that changes in external flows have large effects on the compositions, and makes one product purer and the other less pure. The opposite is true for changes in the internal flows. There are also fundamental differences between external and internal flow changes when it comes to the dynamic response; the external flow changes are associated with the "slow" dominant time constant of the column, whereas the dynamic effect of internal flow changes may be significantly faster. This may be explained by the fact that we need to change the overall holdups of each component in the column when we make changes in the external flows, and this takes time.

2.4 Configurations and the gain matrix

From a control point of view, a two-product distillation column with a given feed, has five degrees of freedom (five flows which can be adjusted; L, V, V_T, D and B). At steady state, the assumption of constant pressure and perfect level control in the condenser and reboiler, reduces the number of degrees of freedom to two. These two degrees of freedom can then be used to control the two product compositions, x_D and x_B (or some other indicator of the composition, like the tray temperature).

The effect of small changes in the two remaining degrees of freedom can be obtained by linearizing the model. For example, with the "LV-configuration" we have L and V as the degrees of freedom (independent variables), and we can write at steady-state[7]

$$dx_D = g_{11}dL + g_{12}dV \tag{21}$$

$$dx_B = g_{21}dL + g_{22}dV \tag{22}$$

where $g_{11} = (\partial x_D/\partial L)_V$ represents the effect (the steady-state gain) of a small change in L on x_D with V constant, etc. In matrix form we write

$$\begin{pmatrix} dx_D \\ dx_B \end{pmatrix} = G^{LV}\begin{pmatrix} dL \\ dV \end{pmatrix}; \quad G^{LV} = \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} \tag{23}$$

Similarly, for the DV-configuration, with D and V as independent variables (in operation, we would need to change the condenser level control in Figure 1 from using D to using L), we have

$$\begin{pmatrix} dx_D \\ dx_B \end{pmatrix} = G^{DV}\begin{pmatrix} dD \\ dV \end{pmatrix} \tag{24}$$

In fact, there are infinitely many combinations of the five "original" flows which could be used as independent variables, and in particular, ratios are frequently used. In particular, the double ratio configuration with L/D and V/B as independent variables,

$$\begin{pmatrix} dx_D \\ dx_B \end{pmatrix} = G^{(L/D)(V/B)}\begin{pmatrix} dL/D \\ dV/B \end{pmatrix} \tag{25}$$

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[7] This model is on differential form, i.e. in terms of deviation variables. To simplify notation we often replace dx_D by simply x_D, etc., and write (21) as $x_D = g_{11}L + g_{12}V$, etc.

has many attractive features. As mentioned, the steady-state gains in any of these models can be easily obtained by linearizing a model of the column, for example, we can use the simplified separation factor model in (15), see e.g. the gain expressions in (88) - (90). However, usually we prefer to linearize the equations of the exact nonlinear model, as this also gives easily a dynamic model; see sections 3 and 4.

The control properties of the various configurations may be drastically different, and this is exemplified by studying the the steady-state two-way interactions, as expressed by the relative gain array (RGA). The relative gain λ_{ij} expresses how the gain g_{ij} changes as we close the other loop(s). For example, consider the effect of a change in L on x_D with the LV-configuration. With no control V is constant ($dV = 0$), and the effect is $dx_D = g_{11}dL$; see (21). Now assume that we introduce feedback control in the other loop, i.e. we adjust V to keep x_B constant. From (22) with $dx_B = 0$ this is achieved with $dV = -(g_{21}/g_{22})dL$. This change in V also affects x_D, so substitute it into (21) to get $d\hat{x}_D = (g_{11} - g_{12}(g_{21}/g_{22}))dL$. Thus, the corresponding relative gain is

$$\lambda_{11} = \frac{dx_D}{d\hat{x}_D} = \frac{g_{11}}{g_{11} - g_{12}(g_{21}/g_{22})} \tag{26}$$

Similar expression apply to the other relative gains. In fact, the rows and the columns in the RGA always sum to 1, so we have that the RGA-matrix is

$$\Lambda = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} = \begin{pmatrix} \lambda_{11} & 1-\lambda_{11} \\ 1-\lambda_{11} & \lambda_{11} \end{pmatrix} \tag{27}$$

Generally, we prefer to "pair on" RGA-elements close to 1. For example, if we intend to use L to control x_D, then we would like that the effect of L on x_D does not depend on the control of x_B, that is, we would like λ_{11} close to 1. Large RGA-elements (say, larger than 10) generally imply serious control problems.[8]

Approximate steady-state gains for any configurations can be obtained from the simplified separation factor model in (15). In fact, we can derive the following useful approximations for the steady-state RGA for the three configurations mentioned above (set F=1 and assume feed liquid):

$$\begin{aligned} \lambda_{11}(G^{LV}) &\approx \frac{(2/N)L(L+1)}{Bx_B + D(1-x_D)} && (28) \\ \lambda_{11}(G^{DV}) &\approx 1/\left(1 + \frac{D(1-x_D)}{Bx_B}\right) \quad \text{(Shinskey, 1967)} && (29) \\ \lambda_{11}(G^{(L/D)(V/B)}) &\approx \lambda_{11}(G^{LV})/\left(1 + \frac{L}{D} + \frac{V}{B}\right) && (30) \end{aligned}$$

We find that the RGA-elements for the LV-configuration[9] are always large for sharp separations where *both* products are pure. On the other hand, for the DV-configuration the RGA-elements are always between 0 and 1; we see from (29) that λ_{11} is close to 1 for columns with a pure bottom product and close to 0 for a column with a pure top product. For the (L/D)(V/B)-configuration the RGA is reduced relative to the LV-configuration when the internal flows are large, which is typically the case for close-boiling mixtures with α close to 1.

Example. Column A. The exact steady-state gain matrices and corresponding RGA for the three configurations mentioned above are[10]:

$$\begin{aligned} G^{LV} &= \begin{pmatrix} 0.8754 & -0.8618 \\ 1.0846 & -1.0982 \end{pmatrix} \qquad \lambda_{11} = 35.94 && (31) \\ G^{DV} &= \begin{pmatrix} -0.8754 & 0.01365 \\ -1.0846 & -0.01365 \end{pmatrix} \qquad \lambda_{11} = 0.45 && (32) \\ G^{(L/D)(V/B)} &= \begin{pmatrix} 0.03754 & -0.03072 \\ 0.03887 & -0.04570 \end{pmatrix} \qquad \lambda_{11} = 3.29 && (33) \end{aligned}$$

---

[8] Note, we are here considering the RGA at steady-state, whereas it is really the RGA-value at the frequency corresponding to the closed-loop response time which is important for control.

[9] The estimate of the RGA for the LV-configuration in (28) is half of the estimate of the condition number γ given in (92).

[10] The outputs are in mole fractions units. Note that no scalings have been applied as one would normally do for a control analysis.

These RGA-values compare well with the approximations in (28), (29) and (30), which give RGA-values of 50.1, 0.5 and 3.62, respectively.

The gain matrices given above are clearly related. For example, for the case of constant molar flows we have at steady-state that $dD = -dL + dV$, and it follows that

$$G^{DV} = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} G^{LV} \tag{34}$$

However, if we do not assume constant molar flows and for the dynamic case, transformations such as (34) get rather complicated. Therefore, instead of using transformations, it is recommended to start from an "uncontrolled" dynamic model (5×5), and then close the appropriate level and pressure loops to derive the model for the configuration under consideration.

Dynamics. We have here discussed the steady-state behavior, which is not by itself too important for control. One good illustration is the DB-configuration,

$$\begin{pmatrix} dx_D \\ dx_B \end{pmatrix} = G^{DB}(s) \begin{pmatrix} dD \\ dB \end{pmatrix} \tag{35}$$

with D and B as independent variables for composition control. At steady-state (at $s = 0$) we have $D + B = F$, so D and B cannot be adjusted independently. This originally led most distillation experts to label the DB-configuration as "impossible". An analysis shows that at steady-state all elements in $G^{DB}(0)$ are infinite and also its RGA-elements are infinite. Again, this indicates that control with the DB-configuration is impossible. However, by considering the dynamics, one finds that control is in fact possible, because D and B can be adjusted independently dynamically. Furthermore, the RGA approaches unity at relatively low frequencies, especially for columns with large internal flows (Skogestad et al., 1990). This is discussed in more detail later, e.g. see Figure 11.

3 A simple example (3-stage column)

Some important aspects of modeling, and in particular of the energy balance, are considered in the survey paper by Skogestad (1992). Here, we want to illustrate, by way of a simple column with only three stages, the fundamentals of dynamic modeling, simulation and linearization.

We assume binary separation, constant pressure and negligible vapor holdup, perfect control of levels using D and B (LV-configuration), constant molar flows (which replaces the energy balance), vapor-liquid equilibrium on all stages, constant relative volatility for the VLE, and constant liquid holdup (i.e. neglect flow dynamics). With these assumptions the only states are the mole fraction x_i of light component on each stage.

The column data are summarized in Table 2. The column separates a binary mixture with a relative volatility $\alpha = 10$, and has two theoretical stages ($N = 2$) plus a total condenser. Stage 3 is the total condenser, the liquid feed enters on stage 2, and stage 1 is the reboiler. With these data the steady-state column profile becomes

Stage	i	L_i	V_i	x_i	y_i
Condenser	3	3.05		0.9000	
Feedstage	2	4.05	3.55	0.4737	0.9000
Reboiler	1		3.55	0.1000	0.5263

We now want to:

1. Formulate the dynamic equations for the composition response with L and V as independent variables (LV-configuration).

2. Linearize the equations and write them on the form $dx/dt = A\Delta x + B\Delta u + E\Delta d$ where $\Delta x, \Delta u$ and Δd represent small deviations from the steady-state.

3. Obtain from the linearized model the steady-state gains.
4. Simulate the dynamic response and compare with the eigenvalues computed from the linear model.

1) The material balances for the light component on each stage are:

$$M_3 \frac{dx_3}{dt} = V_2 y_2 - L_3 x_3 - D x_3 \quad \text{(condenser)} \tag{36}$$

$$M_2 \frac{dx_2}{dt} = F z_F + V_1 y_1 + L_3 x_3 - V_2 y_2 - L_2 x_2 \quad \text{(feed stage)} \tag{37}$$

$$M_1 \frac{dx_1}{dt} = L_2 x_2 - V_1 y_1 - B x_1 \quad \text{(reboiler)} \tag{38}$$

where by definition $V = V_1$ and $L = L_3$. With the assumptions above the flow responses are decoupled from the composition dynamics and we have at any given time:

$$V_2 = V, \quad L_2 = L + F, \quad D = V - L, \quad B = L + F - V \tag{39}$$

(the last two equations follow because D and B are used for perfect level control).

2) Linearizing the material balance for the condenser (stage 3) yields after a little work

$$M_3 \frac{dx_3}{dt} = V(\Delta y_2 - \Delta x_3) + (y_2 - x_3)\Delta V \tag{40}$$

Here the last term is zero because $y_2 = x_3$ at steady-state for a total condenser. By linearizing the VLE on each stage we have $\Delta y_i / \Delta x_i = K_i'$, where for the case of constant relative volatility $K_i' = \alpha/(1 + (\alpha - 1)x_i)^2$. The component balances for the other stages may be linearized in similar manner, and we obtain the linear model

$$M_i \frac{dx}{dt} = A\Delta x + B\Delta u + E\Delta f \tag{41}$$

$$x = \begin{pmatrix} x_3 \\ x_2 \\ x_1 \end{pmatrix}; \quad u = \begin{pmatrix} L \\ V \end{pmatrix}; \quad d = \begin{pmatrix} F \\ z_F \end{pmatrix} \tag{42}$$

where

$$A = \begin{pmatrix} -V & VK_2' & 0 \\ L & -(L + F + VK_2') & VK_1' \\ 0 & L + F & -(B_V K_1') \end{pmatrix} = \begin{pmatrix} -3.550 & 1.282 & 0 \\ 3.050 & -5.332 & 9.834 \\ 0 & 4.050 & -10.334 \end{pmatrix}$$

$$B = \begin{pmatrix} 0 & 0 \\ x_3 - x_2 & y_1 - y_2 \\ x_2 - x_1 & -(y_1 - x_1) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0.4263 & -0.3737 \\ 0.3737 & -0.4263 \end{pmatrix}$$

$$E = \begin{pmatrix} 0 & 0 \\ z_F - x_2 & F \\ x_2 - x_1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0.0263 & 1 \\ 0.3737 & 0 \end{pmatrix}$$

The overall dynamic transfer matrix $G(s)$ which gives the effect of L, V, F, z_F on x_3, x_2, x_1 is given by

$$G(s) = (sI - A)^{-1}[B \quad E] \tag{43}$$

The eigenvalues of the state matrix A are -0.22, -4.26 and -14.7 [min^{-1}]. Note that the inverse of the smallest eigenvalue magnitude is $1/0.22 = 4.5$ min.

Note that all the elements in the first row of B and E are all zero. This implies the changes in L, V, F or z_F have no *immediate* effect on top composition. The reason is of course that $x_3 = y_2$ at steady-state because of the total condenser. However, as shown next, this does not mean that the *steady-state* effect is zero, because there are interactions with the other stages.

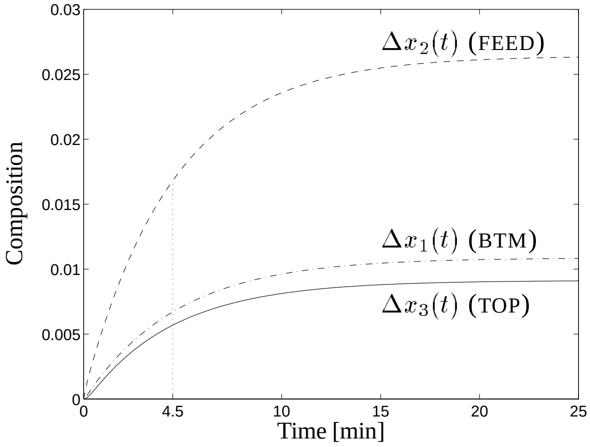

Figure 3: Composition response for 3-stage column to change in feed composition

MATLAB call for 3-stage column:

```
x0 = [0.9; 0.4737; 0.1];
[t, x]= ode45(‘dist‘, 0, 25, x0, 1e-6, 1);
```

dist.m (MATLAB subroutine):

```
function yprime=dist(t,x);

a=10;
y(3)=x(3);
y(2)=a*x(2)/(1+(a-1)*x(2));
y(1)=a*x(1)/(1+(a-1)*x(1));

l3 = 3.05;
l2 = 4.05;
v2 = 3.55;
v1 = 3.55;
b = 0.5;
d = 0.5;
f=1;
zf=0.51; % Step in zF from 0.5 to 0.51

dx3dt = v2*y(2)-l3*x(3)-d*x(3);
dx2dt = f*zf+v1*y(1)+l3*x(3)-v2*y(2)-l2*x(2);
dx1dt = l2*x(2)-v1*y(1)-b*x(1);

yprime=[dx3dt;dx2dt;dx1dt];
```

3) *Steady-state gains.* The overall steady-state gain matrix ($s = 0$) for the effect of all independent variables on all compositions (states) is

$$G = -A^{-1}[B \quad E] = \begin{pmatrix} 0.750 & -0.748 & 0.366 & 0.959 \\ 2.08 & -2.07 & 1.01 & 2.65 \\ 0.850 & -0.853 & 0.433 & 1.04 \end{pmatrix} \tag{44}$$

Usually, we are only interested in the product compositions and we write

$$\begin{pmatrix} dx_D \\ dx_B \end{pmatrix} = G^{LV} \begin{pmatrix} dL \\ dV \end{pmatrix} + G_d^{LV} \begin{pmatrix} dF \\ dz_F \end{pmatrix} \tag{45}$$

$$G^{LV} = \begin{pmatrix} 0.750 & -0.748 \\ 0.850 & -0.853 \end{pmatrix}; \qquad G_d^{LV} = \begin{pmatrix} 0.366 & 0.959 \\ 0.433 & 1.04 \end{pmatrix} \tag{46}$$

The RGA of G^{LV} is 163.5 (which compares well with the value $3.05 \cdot 4.05/0.1 = 123.5$ obtained from the shortcut formula (28)). The column is thus expected to be difficult to control, which is rather surprising for a column with such low purity. However, this is actually an unrealistic design with too few stages in the column. If we increase the number of theoretical stages from 2 to 3, then L drops from 3.05 to 0.095, and the RGA drops from 163.5 to 1.94.

4) *Dynamic response.* A nonlinear simulation of an increase of z_F of 0.01, using the program MATLAB, is shown in Figure 3. We note that the dominant time constant (time it takes for the compositions to reach 63% of their steady-state change) is about 4.5 min as expected from the smallest eigenvalue magnitude of the A-matrix. We also note that the composition change inside the column is significantly larger than at the columns ends. This is typical for a change which upsets the external material balances, and is actually the primary reason for the large time constants which are often observed for distillation columns.

The model in this example did not include liquid flow dynamics, which generally are important if the model is used for control studies. In the next example, we consider a more realistic column example (“column A”) where we also include liquid flow dynamics.

4 A more realistic example (Column A)

In this section we consider ”column A” studied by Skogestad and Morari (1988). Details about the model and all the MATLAB files are available over the internet.

The following assumptions are used: Binary separation, constant pressure and negligible vapor holdup, total condenser, constant molar flows, equilibrium on all stages with constant relative volatility, and linearized liquid flow dynamics. These assumptions may seem restrictive, but they capture the main effects important for dynamics and control (except possibly for the assumption about constant pressure).

4.1 The model

The model is given by the MATLAB code in Table 3. The states are the mole fractions of light component, x_i and the liquid holdup, M_i, - a total of $2N_{tot}$ states.

Note that we do not assume constant holdup on the stages, that is, we include liquid flow dynamics. Specifically, we use the following linearized relationship (we may alternatively use Francis' Weir formula etc.):

$$L_i = L_{0i} + (M_i - M_{0i})/\tau_L + (V_{i-1} - V_{0,i-1})\lambda \tag{47}$$

where L_{0i} [kmol/min] and M_{0i} [kmol] are the nominal values for the liquid flow and holdup on stage i.

This means that it takes some time, about $\theta_L = (N-1)\tau_L = 39 \cdot 0.063 = 2.46$ [min] (see Figure 4), from we change the liquid in the top of the column (L_T) until the liquid flow into the reboiler (L_B) changes. This is good for control as it means that the initial ("high-frequency") response is decoupled. This means that if we have sufficiently fast control, then we can avoid some of the strong interactions that exist at steady-state between the compositions at the top and bottom of the column.

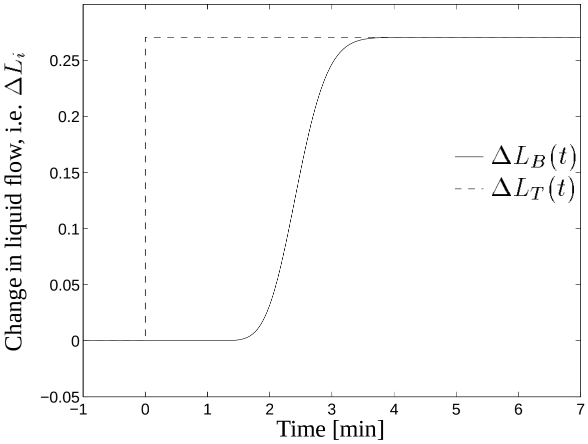

Figure 4: Liquid flow dynamics for column A

The vapor flow into the stage may also effect the liquid holdup as given by the parameter λ (sometimes denoted the "K_2-effect). A positive value of λ may result if an increase in vapor flow gives more bubbles and thus pushes liquid off the stage. For $\lambda > 1$ we get an inverse response in the reboiler holdup M_B in response to an increase in boilup V, and we also get an inverse response in the bottom composition. This makes it difficult to use V for single-loop control. For tray columns, λ may also be negative if the increased pressure drop caused by larger V results in a larger holdup in the downcomers. In general, it is difficult to estimate λ for tray columns. For packed columns λ is usually close to zero. In all examples in this paper we use $\lambda = 0$.

4.2 Steady-state operating point

The steady-state data for column A are summarized in Table 2, and composition stage profiles are shown in Figure 2. The steady-state gain matrices for the LV-, DV- and $(L/D)(V/B)$-configurations were given in (31)-(33).

Table 3: Part of MATLAB code of dynamic distillation model

```
% Vapor-liquid equilibria
i=1:NT-1;    y(i)=alpha*x(i)./(1+(alpha-1)*x(i));

% Vapor Flows assuming constant molar flows
i=1:NT-1;    V(i)=VB*ones(1,NT-1);
i=NF:NT-1;   V(i)=V(i) + (1-qF)*F;

% Liquid flows assuming linearized tray hydraulics with time constant taul
% Also includes coefficient lambda for effect of vapor flow ("K2-effect").
i=2:NF;      L(i) = L0b + (M(i)-M0(i))./taul + lambda.*(V(i-1)-V0);
i=NF+1:NT-1; L(i) = L0  + (M(i)-M0(i))./taul + lambda.*(V(i-1)-V0t);
L(NT)=LT;

% Time derivatives from  material balances for
% 1) total holdup and 2) component holdup

% Column
i=2:NT-1;
dMdt(i) = L(i+1)         - L(i)       + V(i-1)         - V(i);
dMxdt(i)= L(i+1).*x(i+1) - L(i).*x(i) + V(i-1).*y(i-1) - V(i).*y(i);

% Correction for feed at the feed stage
% The feed is assumed to be mixed into the feed stage
dMdt(NF) = dMdt(NF)  + F;
dMxdt(NF)= dMxdt(NF) + F*zF;

% Reboiler (assumed to be an equilibrium stage)
dMdt(1) = L(2)      - V(1)      - B;
dMxdt(1)= L(2)*x(2) - V(1)*y(1) - B*x(1);

% Total condenser (no equilibrium stage)
dMdt(NT) = V(NT-1)         - LT       - D;
dMxdt(NT)= V(NT-1)*y(NT-1) - LT*x(NT) - D*x(NT);

% Compute the derivative for the mole fractions from d(Mx) = x dM + M dx
i=1:NT;
dxdt(i) = (dMxdt(i) - x(i).*dMdt(i) )./M(i);

% Output
xprime=[dxdt';dMdt'];
```

4.3 Dynamic responses

We first consider the dynamic response using the LV-configuration, that is, with reflux L and boilup V as independent variables for composition control, and with D and B adjusted to obtain tight level control, see Figure 1. The responses are very similar to those of the uncontrolled "4×4 model", which may be generated using the MATLAB files available over the internet.

External flows

Small changes in the external flows have large effects on the product compositions. This is illustrated in Figure 5 (upper curves) where we have increased the reflux L by 0.0027 (about 0.1%) with constant V, i.e., we have decreased D from 0.5 to 0.4973. At steady-state, x_D increases from 0.99 to about 0.992 and x_B increases from 0.01 to about 0.0135. The response is rather sluggish with a time constant of about 194 minutes. Similarly, if we increase the boilup V by the the same amount, but now with constant L, i.e. we increase D from 0.5 to 0.5027, then the effect on composition is almost the same, but in opposite direction (see the lower part of the plot in Figure 5).

In fact, the same dynamic response with a long time constant of about 194 min, is observed for any small change which upsets the the external material balances, including changes in F and z_F.

Internal flows

Next, consider a change in the internal flows. More specifically, in Figure 6 we simultaneously increase L and V by 0.27 (about 10%), such that D and B are kept constant (at least at steady-state). From the simulation of the individual changes in Figure 5, we expect that the changes in L and V will counteract each other, and this is confirmed by the the simulations in Figure 6. We observe from the plots that the

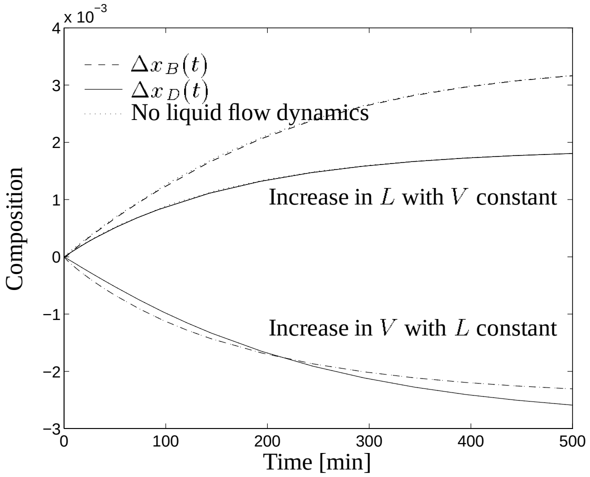

Figure 5: External flows changes: 0.1% individual increases in L and V

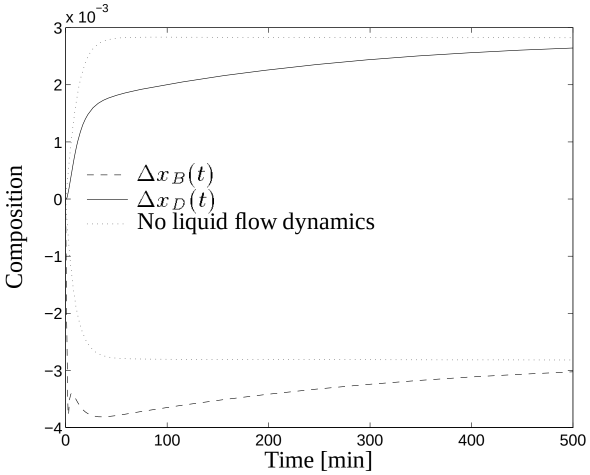

Figure 6: Internal flows change: 10% simultaneous increase in L and V with D constant.

effect on product compositions of a given change in L is now about 100 times smaller. This also agrees with the steady-state gains given in (31). However, there are also two other differences: First, *both* products get purer in this case, and, second, the dynamics are much faster.

To understand better the dynamic response to changes in internal flows, let us consider the case, admittedly unrealistic, where we neglect the liquid flow dynamics. The corresponding response is given by the dotted lines in Figure 6, and we see that it is close to first-order with a time constant of about 15 min. Note that, in this case, the change in reflux flow L_T immediately results in a corresponding change in liquid flow entering the reboiler L_B. Next, consider the actual response with liquid flow dynamics included (solid and dashed lines in Figure 6), for which it takes some time (about 2.54 min) for the change in reflux to reach the reboiler. During this time period the bottom part of the column only “feels” the change in boilup, so the bottom composition x_B drops very sharply, as for a change in the external flows. But, then the reflux flow reaches the bottom, and this counteracts the increase in the boilup, and the bottom composition levels off. In the top of the column, we see less of this behavior since we have assumed immediate response for the vapor flow (which is reasonable).

4.4 Linearized model

The model may be linearized as illustrated above for the 3-stage column, but we here we used numerical differentiation. To check the linearized model we compute the eigenvalues of the A-matrix, and we find that the three eigenvalues furthest to the right are -0.00516, -0.0830 and -0.2851, and the corresponding time constants (take the inverse) are 193.9 min, 12.0 min and 3.5 min. The slowest mode, with time constant 194 min, corresponds closely to the time constant observed for changes in external flows, and the second time constant of 12 min corresponds closely to that observed for changes in internal flows when flow dynamics are neglected[11].

The main advantage with a linear model is that it is suitable for analysis (RGA, poles, zeros, CLDG, etc.) and for controller synthesis. The above linear model has 82 states, but using model reduction the order can easily be reduced to about 10 states or less without any noticable difference in the response.

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[11] With constant molar flows, the flow dynamics are unaffected by the composition dynamics. Thus, the part of the A-matrix belonging to the flow dynamics is only one-way coupled with the part belonging to the composition dynamics. It then follows that the *eigenvalues* belonging to the composition dynamics are unaffected by the flow dynamics, and *vica versa*. However, there is one-way coupling, so the composition *response* is affected by the liquid flow dynamics, as seen in Figure 6.

4.5 Nonlinearity

For small changes, the nonlinear and linear models give the same response, but for large changes the difference is very large. One simple reason is that x_i must always lie between 0 and 1, so, for example, when we increase L the top composition x_D can at most increase by 0.01 (from 0.99 to 1.0).

Consider the response in top composition x_D to increases in L, with V constant. In Figure 7 we compare the linear response (dashed line) to the nonlinear responses for changes in L of 0.01%, 0.1%, 10% and 50% (solid lines). To compare the responses on a equal basis we divide the change in the composition by the magnitude of the change in L, i.e., the plot shows $\Delta x_D(t)/\Delta L$. We show the responses for a simulation time of 30 minutes, because this is about the interesting time scale for control. As expected, the response is very nonlinear, and we observe that $\Delta x_D(t)/\Delta L$ is much smaller for large changes in the reflux.

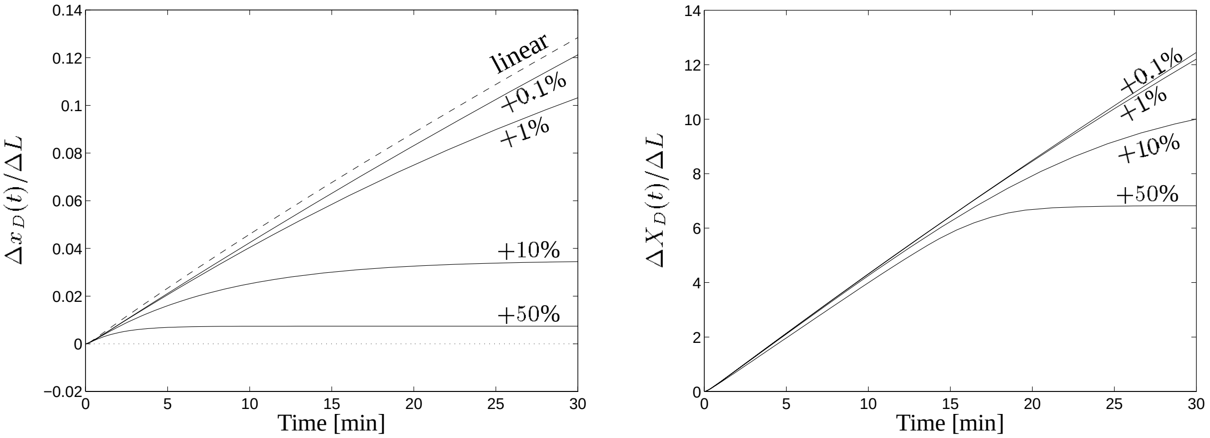

Figure 7: Nonlinear response in distillate composition for changes in L of 0.1%, 1%, 10% and 50%. Right plot: Logarithmic composition

Next, consider the corresponding responses (right plot) in terms of logarithmic compositions, i.e., consider $\Delta X_D(t)/\Delta L$ where $X_D(t) = \ln(x_D(t)/(1 - x_D(t))$. This is seen to have an amazing linearizing effect on the initial response, as the responses for the first 10 minutes for changes in L from 0% to 50% are almost indistinguishable. Obviously, this is an important advantage if a linear controller is to be used.

4.6 Effect of mass flows on response

Throughout this paper we make the implicit assumption that all flows, L, V, D, B etc., and all holdups are on a molar basis, and this assumptions is implicit in most of the distillation literature. This is the most natural choice from a modeling point of view. However, in a real column one can, at least for liquid streams, usually only adjust the mass or volumetric flows. Therefore, the responses on a real column will differ from those observed from simulations where molar flows are fixed. The reason is that a constant mass flow will result in a change in the corresponding molar flow when the composition changes. Specifically, we consider here the mass reflux L_w [kg/min]. We have

$$L_w = LM; \quad M = 35x_D + 40(1 - x_D)$$

where M [kg/kmol] is the mole weight of the distillate, and we have assumed that the mole weight of the light component is 35, whereas that of the heavy component is 40. From Figure 8 we see that the responses to a decrease in z_F from 0.50 to 0.495 are very different for the case with fixed molar reflux, L [kmol/min] (solid lines), and with fixed mass reflux, $L_w[\mathrm{kg/min}]$ (dashed lines). In both cases the molar boilup V [kmol/min] is kept constant.

The importance of using mass flows when studying real columns seems to have been appreciated only recently (Jacobsen and Skogestad, 1991). In fact, the use of mass flows may even introduce multiple steady-states and instability for columns with ideal VLE and constant molar flows. Jacobsen and Skogestad (1991)

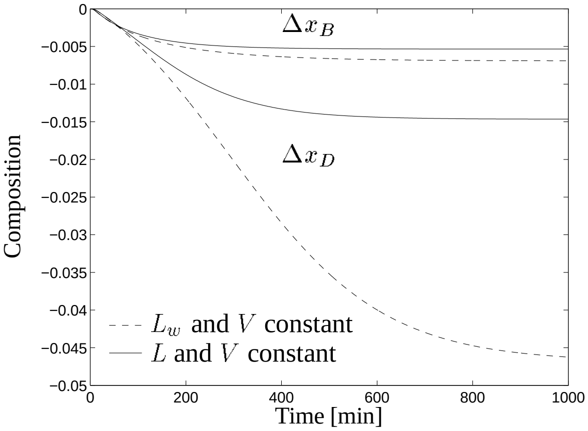

Figure 8: The use of mass reflux L_w may strongly affect the open-loop response. The plot shows the response when z_F is decreased from 0.5 to 0.495.

have derived exact conditions for local instability, and, for our example, they find that local instability would occur if the mole weight of light component was reduced from 35 to 28.1 kg/kmol[12].

However, note that these effect are caused by composition changes, and therefore affect only the long-term response. Therefore, the implications for practical control may not necessarily be too important.

4.7 Comparison of various control configurations

In this section we want to give some insights in the difference between various control configurations, more specifically the LV, DV, LB, DB and $(L/D)(V/B)$-configurations. We will do this by considering the effect of a feed flow disturbance, by discussing the effect of level control, and finally by plotting the dynamic RGA.

4.7.1 Effect of change in feed rate

In Figure 9 we show the response in product composition to a 1% increase in feed rate F from 1 to 1.01 [kmol/min]. The solid line (“ no level control”) show the response for the *uncontrolled column* with all four flows (L, V, D and B) constant. We compare this response to that with the four configurations assuming tight (perfect) level control. However, no composition control is used, so for the LV-configuration we keep L and V constant (in addition to constant M_D and M_B), for the $(L/D)(V/B)$-configuration we keep L/D and V/B constant, etc..

LV-configuration. An increased feed rate goes down to the bottom of the column, and this results, thorough the action of the bottom level controller, in a corresponding increase in the bottoms flow. As expected, this upset in the external material balance a large effect on the product composition, and in particular the bottom composition drifts quite far away (from 0.010 to about 0.017).

The LV-configuration (dotted lines) gives almost the same response as with no level control. This is reasonable, since with no level control, the increase in F will simply accumulate in the reboiler, and this by itself does not have a large effect on the compositions (at least not for x_D, but we can notice that the change in x_B is *slightly* smaller when there is no level control). In general, the column composition response is rather insensitive to actual holdups in the reboiler and condenser holdups, as long as L and V are adjusted in the same manner. The implication is that the LV-configuration is rather insensitive to the tuning of the level loops, which is one of the main advantages with the LV-configuration.

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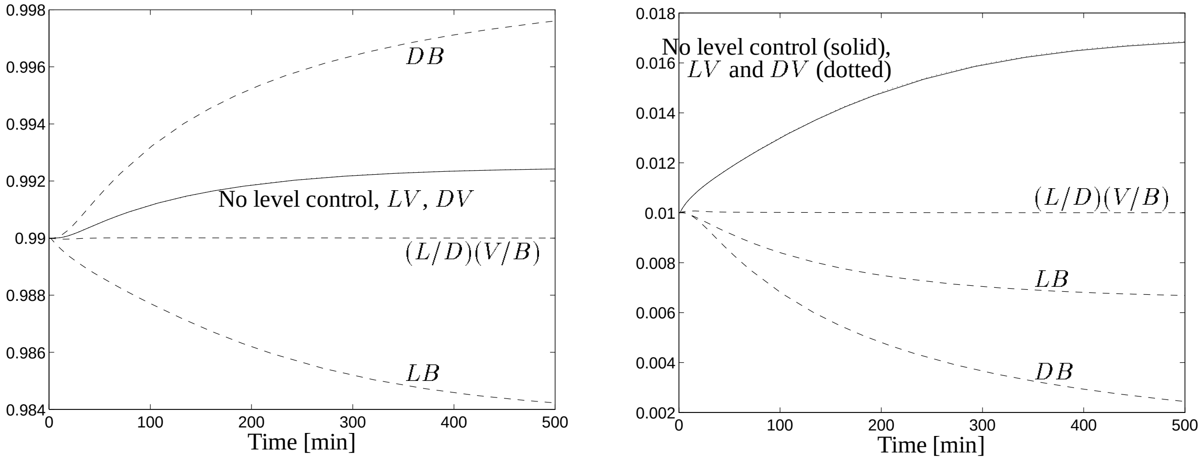
[12] The exact condition for local instability with the $L_W V$ configuration given in Jacobsen and Skogestad (1991) is that $x_D + L(\partial x_D/\partial L)_V > M_H/(M_H - M_L)$. In our case $x_D = 0.99$, $L = 2.706$, $(\partial x_D/\partial L)_V = 0.8754$ and $M_H = 40$, and we find that instability occurs for $M_L < 28.1$ kg/kmol. However, if we are in an operating point (or move towards one) where the bottom product is much purer than the top product, then $(\partial x_D/\partial L)_V$ approaches $x_D/D \approx 2$, see (88), and instability may occur for values of M_L around 33 kg/kmol.



(a) Change in top composition, $\Delta x_D(t)$

(b) Change in bottom composition, $\Delta x_B(t)$

Figure 9: Responses to a 1% increase in F for various configurations

DV-configuration. Also in this case, an increase in feed rate results in a corresponding increase in the bottoms flow, and the response is therefore identical to that with the LV-configuration.

However, in general, the two configurations behave entirely different. For example, if we instead had increased the *vapor* flow in the feed, then this would for the DV-configuration again result in a corresponding increase in B (since D is kept constant), whereas it for the LV-configuration would results in an increase in D. The resulting composition responses would be almost the opposites.

LB-configuration. In this case the increased feed rate results in an increase in D (after being send back up the column by the action of the bottom level controller since B is constant), so, as expected, the response is in the opposite direction of that for the LV-configuration.

DB-configuration. In this case D and B are constant, so the increased feed rate results in a ramp-like increase in the internal liquid holdup and in the internal flows L and V (at $t = 500$ min V has increased from 3.2 to about 5.1 kmol/min). The result is that both products get purer, as expected for an increase in internal flows. Obviously, the DB-configuration cannot be left without adjusting D and B on a long-term basis, because otherwise we would fill up or empty the column, but we see that it does not behave completely unreasonable on a short-term basis. This is why it actually is a viable alternative if we use D and B for composition feedback control.

$(L/D)(V/B)$-configuration. In this case the increased feed rate results in a proportional increase in all streams in the column. This obviously the right thing to do (assuming that the efficiency, i.e. the number of theoretical stages N, remains constant), so we find, as expected, that the product compositions remain almost unchanged.

However, even though the $(L/D)(V/B)$-configuration has a “build-in” mechanism to handle a feed rate increase, it may not behave particularly well for some other disturbances, such as for a disturbance in the feed composition z_F.

4.7.2 Effect of level control

The LV-configuration is almost independent of the level control tuning, but for the other configurations the level control tuning is very important. This can be easily understood, since when the level control is sufficiently slow, all configurations behave initially as the uncontrolled column with no level control (solid line in the simulations), and then eventually, they will behave as shown in the plots where we have assumed fast level control. Thus, if the response for a given configuration differs significantly from that with no level control, then the response will be sensitive to the tuning of the level loop(s). In general, this will be the case for all configurations, except for the LV configuration. [13]

Effect of level control for DV-configuration. We here illustrate that the DV-configuration is sensitive to the tuning of the level loops. As an example, consider the effect on product compositions of an increase in boilup V by 1%. With fast condenser level control, the increase in boilup goes up the column, but is then returned back as reflux through the action of the condenser level controller (since D is constant), and we have an increase in internal flows only. However, with a slow condenser level controller, there is no immediate increase in reflux, so the initial response is almost as if we had send the boilup out the top of the column, as for the LV-configuration. Thus, we expect a strong sensitivity to the level tuning. These predictions are indeed confirmed by the simulations in Figure 10. Note in particular that with a slow condenser level controller, x_D has an inverse response when we change V. This may not be too serious as we probably do not intend to use V to control x_D, but we also note that x_B has a large overshoot, which may make control difficult.

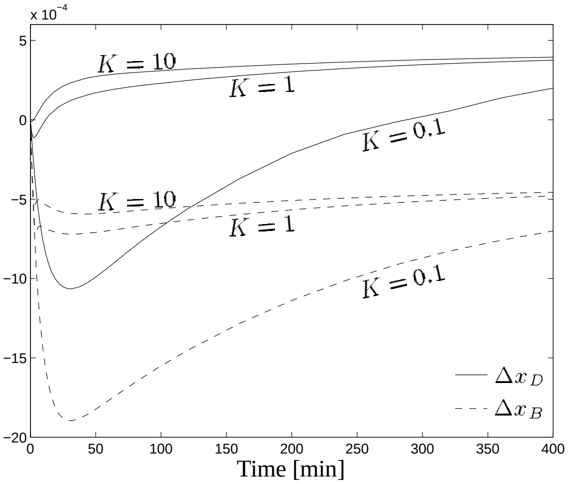


Figure 10: Tuning of the condenser level controller has a strong effect on the "open-loop" response for the DV-configuration. (Responses are for a 1% increase in V with condenser level controller $\Delta L = K \Delta M_D$)

4.7.3 Frequency-dependent RGA

The frequency-response is easily evaluated from a linearized model, $G(s) = C(sI - A)^{-1}B + D$ with $s = j\omega$, and from this we can compute the RGA for various configuration as a function of frequency.

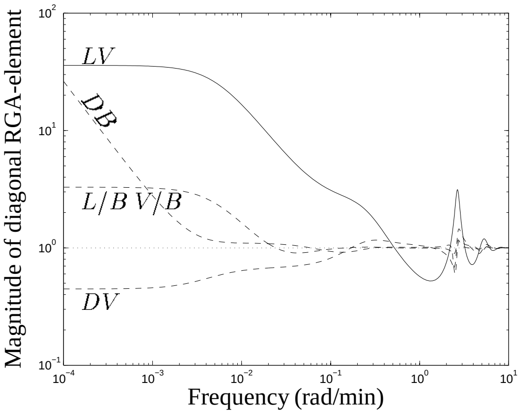


Figure 11: RGA as a function of frequency for four configurations

In Figure 11 the magnitude of the diagonal RGA-element is shown for four configurations. Note that

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[13] Actually, we need not require that the level control itself is fast, but rather that L and V change as if the level control was fast.

the values at steady-state are consistent with those given in (28)-(30). In general, we want to RGA-elements on which we pair on, to about 1 at frequencies corresponding to the closed-loop time constant, and we find that the liquid flow dynamics cause the RGA to approach 1 at high frequencies for all configurations. Interestingly, the DB-configuration, which has infinite RGA-elements at steady-state ($\omega = 0$), approaches 1 at the lowest frequency of the four configurations. This is generally the case when both products are high-purity (Skogestad et al., 1990). For the LV-configuration the RGA approaches 1 at frequencies above $1/\theta_L = 1/2.46 = 0.41$ [rad/min].

5 Understanding the dynamic behavior

The two examples (3-stage column and column A) have provided us with important insight into the dynamic behavior of distillation columns. Here, we derive analytic expressions which quantify these observations regarding the dominant time constant (τ_1) the internal flow time constant (τ_2) and the initial response.

5.1 Dominant time constant (external flows)

For the 3-stage column we observed a dominant time constant of about 4.5 min in response to a change in feed composition z_F. Similarly, for column A we observed a dominant time constant of about 194 minutes for changes in feed rate F, feed composition z_F, and to individual changes in relux L and boilup V.

We here derive an analytic expression for the dominant time constant, denoted τ_1. The approach is to consider the *total* holdup of each component in the column and assume that all stages have the same response. As we show below, this directly leads to a first order model, and the dominant time constant can be estimated very accurately. According to Rademaker et al. (1975, p.280) this idea dates back to the beginning of the century (Lord Raleigh) and seems to get rediscovered every few years.

Consider a column which initially ($t \leq 0$) 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 kown 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 (simultaneous changes in L and V keeping product rates constant).

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

The assumption is reasonable when considering the composition dynamics, provided the flow response is much faster than the composition response. Using Assumption 1 the *overall* material balance for any component for $t > 0$ becomes:

$$\frac{d}{dt}[\sum_{i=1}^{N+1} M_{if} x_i(t)] = F_f z_{Ff} - D_f x_D(t) - B_f x_B(t) \tag{48}$$

Subtracting the final steady state

$$0 = F_f z_{Ff} - D_f x_{Df} - B_f x_{Bf} \tag{49}$$

yields

$$\sum_{i=1}^{N+1} M_{if} \frac{d\Delta x_i(t)}{dt} = -D_f \Delta x_D(t) - B_f \Delta x_B(t) \tag{50}$$

where Δ represents the deviation from the final steady-state, eg., $\Delta x_D(t) = x_D(t) - x_{Df}$, etc..

Assumption 2. *All stages have the same dynamic responses, that is:* $\Delta x_i(t) = \Delta x_i k(t), \; \Delta x_D(t) = \Delta x_D k(t), \; \Delta x_B(t) = \Delta x_B k(t)$. *(Here* $k(0) = 1$ *and* $\Delta x_i = \Delta x_i(0), \Delta x_D = \Delta x_D(0)$ *and* $\Delta x_B = \Delta x_B(0)$ *denote the difference between the initial and final steady state.)*

This assumption is reasonable if the time constant for the internal mixing in the column, τ_{xM}, is much shorter than the dominant time constant. Here

$$\tau_{xM} = \frac{M_I}{L+V}, \quad M_I = \sum_{i=2}^{N} M_i \tag{51}$$

where M_I is the total liquid holdup *inside* the column. τ_{xM} is approximately the time it takes for a composition change to travel from the top to bottom of the column. Assumption 2 and Eq.(50) yield

$$(\sum_{i=1}^{N+1} M_{if}\Delta x_i)\frac{dk(t)}{dt} = (-D_f \Delta x_D - B_f \Delta x_B)k(t) \tag{52}$$

Solving (52) gives a *linear first-order response*

$$k(t) = e^{-t/\tau_1} \tag{53}$$

where the time constant τ_1 is:

$$\tau_1 = \frac{\sum_{i=1}^{N+1} M_{if}\Delta x_i}{\Delta S_i} \tag{54}$$

ΔS_i is the supply imbalance

$$\Delta S_i = D_f \Delta x_D + B_f \Delta x_B = \Delta(F z_f) - x_{D0}\Delta D - x_{B0}\Delta B \tag{55}$$

A simple interpretation of (54) is

$$\tau_1 = \frac{\text{"change in holdup of one component" (kmol)}}{\text{"imbalance in supply of this component" (kmol/min)}}$$

Comments on (54):

1. The column model was <u>not</u> linearized, and (54) applies to any finite change provided Assumptions 1 and 2 hold.

2. The time constant depends on the *magnitude* and *"direction"* (negative or positive change) of the step change introduced. In general, we find that the time constant is long if the column approaches high purity (with Δx_D and Δx_B small), and short if it approaches low purity. This implies that the dynamic response may show and asymmetric behavior, where the dynamic response is different for positive and negative changes.

3. The expression for τ_1 applies to any component in a multicomponent mixture.

4. Eq. (54) applies to any change which changes the <u>external</u> material balance,i.e., which has $\Delta S_i \neq 0$. Eq. (54) does <u>not</u> apply for changes in the internal flows (changing L and V while keeping D and B constant) because the denominator ΔS_i is zero in this case (see (55)).

5. To compute τ_1 according to (54) only a *steady-state* model of the column is needed, plus information about the stage holdups..

6. One disadvantage of (54) is that the compositions on all stages are needed to compute τ_1. However, Skogestad and Morari (1987c) have derived an analytical shortcut (sc) approximation, valid for high-purity binary separations and *small* perturbations to the column, which requires much less data:

$$\tau_{1sc} = \frac{M_I}{\ln S \cdot I_s} + \frac{M_D x_D(1-x_D)}{I_s} + \frac{M_B x_B(1-x_B)}{I_s} \tag{56}$$

where

$$S = \frac{x_D(1-x_B)}{(1-x_D)x_B}; \quad I_s = Bx_B(1-x_B) + Dx_D(1-x_D) \tag{57}$$

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 (56), which represents the contribution from changing the component holdup *inside* the column, dominates for columns with both products of high purity. Note that I_s may be very small in such cases resulting in very large values of τ_{1sc}.

Example 3-stage Column (continued). To illustrate the usefulness of the above methods consider the simple three stage column studied before. The following steady-state profile is obtained when z_F is increased from 0.50 to 0.51 with all flows constant:

Stage	i	L_i	V_i	x_i	y_i
Condenser	3	3.05		0.9091	
Feedstage	2	4.05	3.55	0.5001	0.9091
Reboiler	1		3.55	0.1109	0.5549

From the difference between this "final" steady-state profile and the nominal profile given in Section 3 we get using (54):

$$\tau_1 = \frac{\sum_{i=1}^{N+1} M_{if} \Delta x_i}{\Delta(F z_F) - x_D \Delta D - x_B \Delta B} = \frac{1 \cdot 0.0091 + 1 \cdot 0.0264 + 1 \cdot 0.0109}{0.01 - 0 - 0} = 4.64 \text{ min} \tag{58}$$

As a comparison the shortcut formula (56) with $x_B = 1 - x_D$ and data from Table 2 yields:

$$\tau_{1,sc} = \frac{M_I/F}{x_B x_D \ln S} + \frac{M_D}{F} + \frac{M_B}{F} = \frac{1}{0.1 \cdot 0.9 \cdot 4.39} + 1 + 1 = 4.53 \text{ min} \tag{59}$$

There is an excellent agreement between these estimates of τ_1 and the values obtained from the nonlinear simulations and from the eigenvalues of the state matrix. The main assumption behind the formulas used above for estimating τ_1 is that all stages have the same composition response. This seems reasonable for such a small column with a large reflux ratio, and is also confirmed by considering the time constant for internal mixing, $\tau_{xM} = 1/(3.55 + 3.05) = 0.15$ min, which is much less than 4.5 min, and Assumption 2 is valid.

Example Column A (continued). Similarly, the agreement is excellent for column A. Recall that the time constant corresponding to the smallest eigenvalue was 194 minutes, and approximately this value was also observed in the simulations. As a comparison, for small perturbations in L or V, (54) yields $\tau_1 = 193.5$ min, whereas the shortcut formula (56) with $x_B = 1 - x_D$ and data from Table 2 yields:

$$\tau_{1,sc} = \frac{M_I/F}{x_B x_D \ln S} + \frac{M_D}{F} + \frac{M_B}{F} = \frac{39 \cdot 0.5}{0.01 \cdot 0.99 \cdot 9.19} + 0.5 + 0.5 = 215 \text{ min} \tag{60}$$

which shows good agreement. However, note that, because of nonlinearity, the observed time constant will be much smaller if we consider large changes, e.g. see Skogestad and Morari (1987c). Again, the nonlinear effects can be reduced by use of logarithmic compositions.

5.2 Internal flows time constant

Skogestad and Morari (1988) derived the following estimate for the time constant related to changes in internal flows for a liquid feed

$$\tau_2 \approx \frac{N}{2 \ln S} \frac{M_I}{L_T} \tag{61}$$

where M_I is total liquid holdup *inside* the column. For well-designed columns with α less than about 2 this gives $\tau_2 \approx M_I/F$.

As a comparison, for column A, $M_I/F = 19.5$ min and (61) gives $\tau_2 = 15.7$ min. This compares very well with the "second" eigenvalue of -0.083 and the observed responses in Figure 6.

5.3 Initial response and logarithmic compositions

For control, the "initial" response, corresponding to the desired closed-loop time constant, is of primary importance. We now want to estimate the initial composition response on a stage in response to a change in liquid or vapor flow. For this it is sufficient to consider the "first-order" effect where we neglect the composition chang on neighboring stages. We assume constant molar flows, and, for simplicity, we assume constant liquid holdup, i.e. we neglect the liquid flow dynamics.

The steady-state (indicated by superscript $*$) component material balance on stage i, assuming $L_i = L_{i+1}$ and $V_i = V_{i-1}$, is

$$t \leq 0 : \quad M_i \frac{dx_i^*}{dt} = 0 = (x_{i+1}^* - x_i^*)L_i^* + (y_{i-1}^* - y_i^*)V_i^* \tag{62}$$

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

$$t > 0 : \quad M_i \frac{dx_i}{dt} = (x_{i+1} - x_i)(L_i^* + \Delta L_i) + (y_{i-1} - y_i)(V_i^* + \Delta V_i) \tag{63}$$

Immediately following this change, we may neglect the second-order effects of the change in composition and assume the stage compositions to be unchanged, i.e. $x_i = x_i^*$, etc. Subtracting the steady-state (62) then yields

$$t = 0^+ : \quad M_i \frac{dx_i}{dt} = (x_{i+1}^* - x_i^*)\Delta L_i + (y_{i-1}^* - y_i^*)\Delta V_i \tag{64}$$

Using (62) to eliminate $(y_{i-1}^* - y_i^*)$ then yields the following expression for the initial composition change

$$t = 0^+ : \quad \frac{dx_i}{dt} = \frac{1}{M_i}(x_{i+1}^* - x_i^*)(\Delta L_i - \frac{L_i^*}{V_i^*}\Delta V_i) \tag{65}$$

Because of the term $(x_{i+1}^* - x_i^*)$, the initial response, i.e. the value of dx_i/dt in (65), depends strongly on the stage location and operating point. This follows since the term $x_{i+1}^* - x_i^*$ changes strongly with the stage location (e.g. see the left plot in Figure 2), and also with the operating point.

Now, consider a binary separation and write (65) in terms of the light component (L). Next, divide both sides by $x_{Li}x_{Hi}$ to get the change in logarithmic composition (recall (19) and note that $x_L + x_H = 1$). We omit the superscript * to simplify notation and get

$$t = 0^+ : \quad \frac{dX_i}{dt} = \frac{1}{x_{Li}x_{Hi}}\frac{dx_{Li}}{dt} = \frac{1}{M_i}\frac{1}{x_{Hi}}(\frac{x_{L,i+1}}{x_{L,i}} - 1)(\Delta L_i - \frac{L_i}{V_i}\Delta V_i) \tag{66}$$

$$= \frac{1}{M_i}\frac{1}{x_{Li}}(1 - \frac{x_{H,i+1}}{x_{H,i}})(\Delta L_i - \frac{L_i}{V_i}\Delta V_i) \tag{67}$$

Near the bottom of the column where $x_{Hi} \approx 1$ we have (see proof below)

$$\frac{x_{L,i+1}}{x_{L,i}} \approx \frac{V_B}{L_B}\alpha \tag{68}$$

and it follows from (66) that dX_i/dt at $t = 0^+$ is almost constant (independent of the stage location), and its value depends only weakly on the operating point (due to the factor V_B/L_B). Similarly, near the top of the column where $x_{Li} \approx 1$ we have [14]

$$\frac{x_{H,i+1}}{x_{H,i}} \approx \frac{V_T}{L_T}\frac{1}{\alpha} \tag{69}$$

and it follows again that dX_i/dt at $t = 0^+$ is almost constant. *Proof of (68).* Consider the bottom section at the column, where the the equilibrium line is approximately linear, $y_{L_i} \approx \alpha x_{L,i}$. Combining this with the material balance, $L_i x_{i+1} = V_i y_i + B x_B$, yields

$$\frac{x_{L,i+1}}{x_{L,i}} = \frac{V_B}{L_B}\alpha + \frac{B}{L_B}\frac{x_{LB}}{x_{Li}} \tag{70}$$

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[14] Actually, the repeated use of (68) and (69) may be used to derive the short-cut formula for S in (13)

The second term is negligible as we go up the column, and is also small near the bottom for columns with $(V/L)_B >> 1$, and (68) follows. (69) is derived in an analogous manner since $y_{Hi} \approx x_{Hi}/\alpha$ near the top.

In summary, we have shown that the initial response in terms of logarithmic compositions is almost independent of the operating point. Furthermore, since neighboring stages have the same composition response, the neglected second-order composition changes tend to cancel out, and this "prolongs" the initial response. The practical implication is that the dynamic behavior is much less nonlinear if we use logarithmic compositions, and this was also confirmed in the simulations in Figure 7. This is important for control as it implies that linear control methods may be used if we consider logarithmic compositions.

6 Control

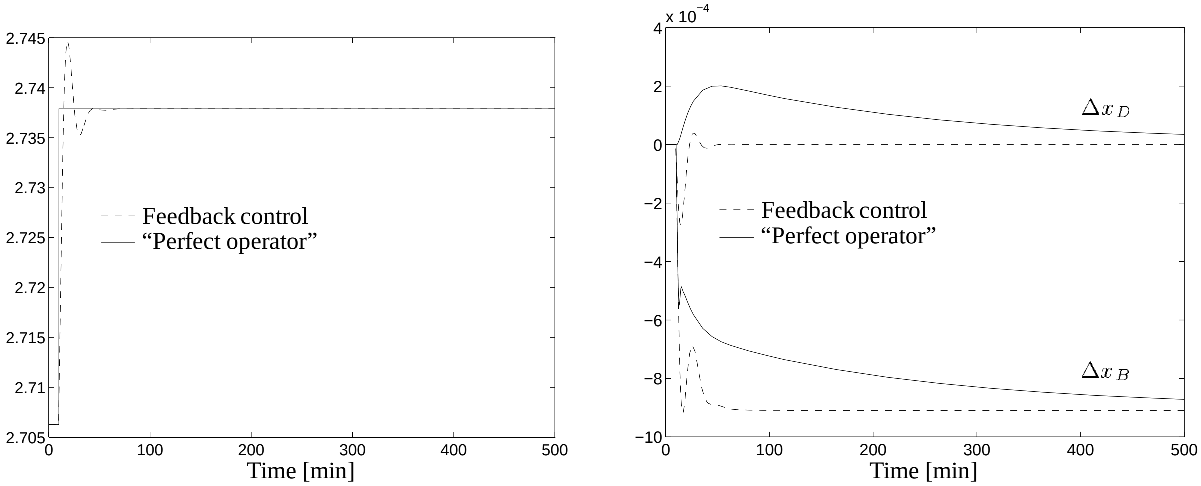
Distillation is probably the most studied unit operation in terms of control. However, most papers use distillation as an example to study their control algorithm, and do not really consider the best way to control a given distillation column. For example, there has been almost countless control studies using the linear Wood and Berry (1973) column model, but these studies probably have not benefited distillation control very much. Also, there has been a large number of control studies based on unrealistic column models, with no flow dynamics, with no measurement and valve dynamics/delays, and using multivariable controllers (e.g. decouplers) assuming the model is perfect (e.g. with no input gain uncertainty). Similarly, distillation columns have become a popular example to test nonlinear control algorithms. However, these studies almost never compare their performance with that which could be obtained using linear controllers with logarithmic transforms to counteract nonlinearity.

All the examples in this section are for column A.

6.1 Myths about slow response

There are some myths about distillation control. One is based on the observation of the very large open-loop time constants, τ_1, observed for high-purity columns. This has led people to believe incorrectly that distillation columns are inherently slow and thus hard to control. However, the use of feedback changes the dynamics (moves the poles) and the closed-loop response time may be much shorter.

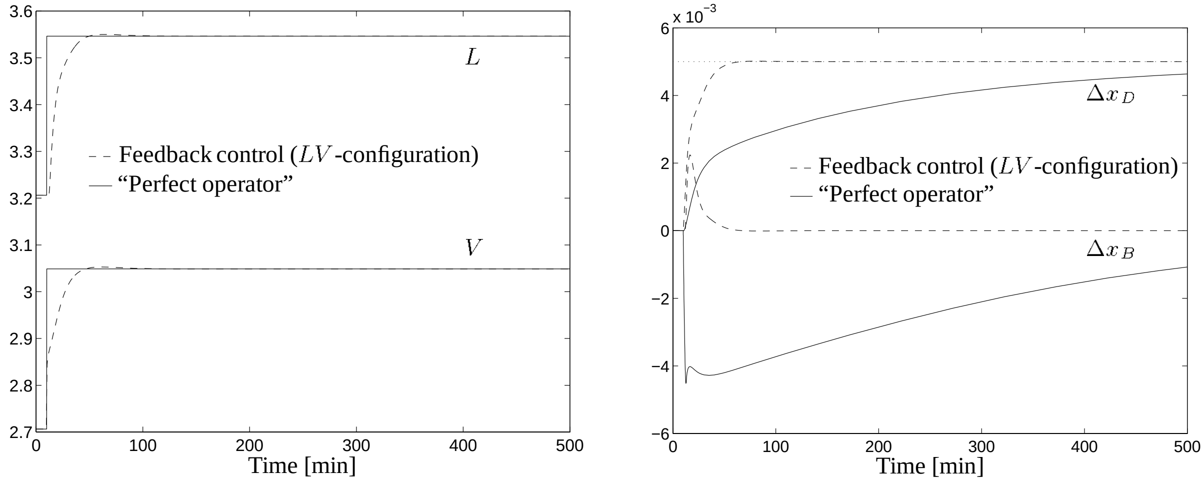
A convincing example is shown in Figure 12. Here we are concerned with keeping the top composition x_D constant by adjusting the reflux L. The bottom composition is not important in this case. Consider a step increase (disturbance) in boilup V, e.g. due to a change in the steam pressure. First consider the "perfect



(a) Reflux L

(b) Compositions, $\Delta x_D(t)$ and $\Delta x_B(t)$

Figure 12: One-point control of x_D: Response to a 1% step increase (disturbance) in V. Solid line: Simultaneous step increase in L ("perfect operator"). Dashed line: Feedback where L is used to control x_D (PI-settings: $k = 60$, $\tau_I = 3.6$ min)



(a) Reflux L and boilup V

(b) Compositions, $\Delta x_D(t)$ and $\Delta x_B(t)$

Figure 13: Two-point control: Setpoint change in x_D from 0.99 to 0.995 with x_B constant. Solid line: Simultaneous step increase in L and V to their new steady-state values ("perfect operator"). Dashed line: Feedback control using the LV-configuration with PI-settings in (82).

operator", who notices the change in V, and is able to directly set L to its new desired value in an open-loop (feedforward) fashion. As expected this yields a rather slow settling towards the steady-state (solid line), with a time constant of about about 194 min (τ_1). Next, consider the use of feedback where L is used to control x_D (one-point control; dashed line). This yields a much faster response, with a closed-loop time constant of less than 10 minutes. The rather large difference in composition response is surprising since we see from Figure 12(a) that there is only a minor difference in L.

A similar example, but with two-point control, where we want to make a setpoint change in the top composition, is shown in Figure 13. Again, the perfect operator is able to directly set the reflux and boilup to their desired values in a feed-forward fashion, and again this results in a sluggish response. However, with feedback control (here shown using two PI controllers) we can change the dynamics, and achieve a much faster settling towards the new steady-state.

The closed-loop simulations in Figures 12 and 13 are without measurement delay, but similar results are obtained with a 1 minute measurement delay for x_D and x_B. This illustrates that the closed-loop simulations are realistic from a practical point of view.

6.2 The control problem

Let us here give a more clear description of the overall control problem. Consider the distillation column in Figure 1 with a given feed.[15] which has 5 manipulated inputs,

$$u = (\,L \quad V \quad D \quad B \quad V_T\,)^T$$

(these are all flows), and 5 controlled outputs,

$$y = (\,x_D \quad x_B \quad M_D \quad M_B \quad p\,)^T$$

(these are compositions and inventories: top composition x_D, bottom composition x_B, condenser holdup M_D, reboiler holdup M_B, pressure p). The process has poles in or close to the origin and needs to be stabilized. In addition, especially for for high-purity separations, the system is often strongly interactive as indicated by large elements in the 5×5 RGA-matrix. Another complication is that composition measurements are often expensive, unreliable and with time delays.

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[15] Throughout this paper we assume that the feed is given, i.e. it is a disturbance in terms of control. However, sometimes one of the product flows, D or B, is given instead. In this case F takes the role of a manipulated input, whereas D or B is a disturbance.

Control configurations

In almost all cases, the distillation column is first stabilized by closing three decentralized (SISO) loops for level and pressure, involving the outputs

$$y_2 = (\, M_D \quad M_B \quad p \,)^T$$

The remaining outputs are then the product compositions

$$y_1 = (\, x_D \quad x_B \,)^T$$

The linear model of this partially controlled system (after closing the level and pressure loops involving u_2 and y_2) may then be written

$$y_1 = P_u(s)u_1 + P_d(s)d + P_r(s)y_2 \tag{71}$$

The three SISO loops for controlling y_2 usually interact weakly and may be tuned independently of each other. However, since each level (tank) has an inlet and two outlet flows, there exists many possible choices for u_2 (and thus for u_1). By convention, each choice ("configuration") is named by the inputs u_1 left for composition control. For example, the "LV-configuration" refers to a partially controlled system with

$$u_1 = (\, L \quad V \,)^T, \quad u_2 = (\, D \quad B \quad V_T \,)^T$$

and we have in this case

$$P_u(s) = G^{LV}(s)$$

As mentioned, the LV-configuration is good from the point of view that the effect of u_1 on y_1 is nearly independent of the tuning of the level and pressure controllers (involving y_2 and u_2). However, we found that the problem of controlling y_1 by u_1 is often strongly interactive with large steady-state RGA-elements in G^{LV}.

Another common configuration is the DV-configuration with

$$u_1 = (\, D \quad V \,)^T, \quad u_2 = (\, L \quad B \quad V_T \,)^T$$

In this case, the steady-state interactions from u_1 to y_1 are generally much less, and $P_u = G^{DV}$ has small RGA-elements. But, as discussed earlier, $G^{DV}(s)$ depends strongly on the tuning of the level loops, and a slow level loop for M_D may introduce unfavorable dynamics for the response from u_1 to y_1.

There are also many other possible configurations (choices for the two inputs in u_1); with five inputs there are 10 alternative configurations. Furthermore, one often allows for the possibility of using ratios between flows, e.g. L/D, as possible degrees of freedom in u_1, and this sharply increases the number of alternatives. For more details the reader is referred to e.g. Shinskey (1984) and Skogestad and Morari (1987d).

Control issues

It is clear that we need to control the levels and pressure (y_2) in order to stabilize the system. It also seems reasonable that we should control both the product compositions (y_1), or at least some related quality variables, because, after all, the reason for having the distillation column in the first place is to split the feed stream into two products with different composition. However, in practice, this is often not the case. Therefore, we need for *composition control* to consider three different cases:

1. Open-loop[16]: No composition control; the operators manully adjust the two remaining flows (u_1).
2. One-point control: One composition loop is closed.
3. Two-point control: Both composition loops are closed.

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[16] The term "open-loop", which here refers to the composition control problem, is not quite correct since we assume there is already a level and pressure control system in place involving u_2 and y_2.

The case with no control ("open-loop") has been common in industrial practice. This is somewhat surprising, since we have shown that without composition control, the distillation almost behaves as a large mixing tank (with a long time constant τ_1), and if we leave the compositions uncontrolled, the columns will tend to drift away and be "filled up" of light or heavy component. In conclusion, from a practical point of view, the composition profile behaves almost like an "unstable" system. Thus, the composition profile needs to be continuously monitored to maintain stable operation, and this puts a heavy burden on the operators.

To "stabilize" the composition profile, it is therefore recommended to close at least one composition loop (one-point control, e.g. involving V and x_B). In this case the remaining degree of freedom (e.g. L) is adjusted manually.[17]

From an economic point of view, disregarding the control and measurement problems, two-point control is the best. This follows since the optimal operating point generally corresponds to a given purity specification. With one-point control, the operator usually "overpurifies" the uncontrolled composition. While this makes control relatively simple, it requires extra energy usage and reduces the capacity. However, there is an important case where one-point control often is optimal – this is when the column is operated at maximum capacity, e.g. maximum vapor load, and there effectively is only one degree of freedom left for composition control.

To select a good distillation control configuration, one should first consider the problem of controlling levels and pressure (y_2), and then consider the 2×2 composition control problem (y_1). Another important issue is that one often does not want large variations in the flows (L, V, V_T, D, B) because these changes usually cause disturbances in other parts of the plant. In particular, we often want to avoid large variations in D and B because these often are feed streams to downstream units.

6.3 What is the best control configuration?

The main problem when selecting the "best" configuration for distillation control is that there are so many issues to consider.

First, there is the level control problem. Clearly, if there is a large flow entering a tank, and this large flows varies, then it is almost impossible to use a small flow for level control. In practice, this means that we cannot use D and B for level control for columns with very large internal flows, that is, for separation of close-boiling mixtures with α close to 1.[18] This effectively rules out the LV-configuration for close-boiling mixtures, and makes the DB-configuration attractive (because then the large flows L and V are used for level control).

Next, there are the three different cases for the composition control problem; open-loop, one-point and two-point. And, to make things more difficult, the ranking is very different for the three cases. We will illustrate this below.

It then becomes clear that there is not a single "best" configuration, and this explains why there sometimes seem to be conflicting rankings given in the literature; one expert focuses on level control; another on the feasibility for using no composition control; another on one-point control; and finally some people (e.g. Shinskey, 1984) mostly consider two-point control. Nevertheless, good tools have been developed to analyze the various choices, so if you know want to want, then one can probably find a good configuration to fit your needs.

Below we introduce some useful frequency-dependent tools for analyzing the alternative configurations. One important advantage with these tools, is that they are controller-independent, and the use of time-consuming closed-loop time simulations is minimized.

6.4 Disturbance rejection using various configurations: controllability analysis

We here consider, using column A as an example, the disturbance rejection properties of four configurations, for the three different cases for the composition control problem; open-loop, one-point and two-point.

---

[17] The DB-configuration has a pole at $s = 0$ (an integrator) in addition to the slow pole corresponding to the time constant τ_1. With onle one loop closed, we will have D and B constant and the composition profile will "drift away". Therefore, we need to close both composition loops to "stabilize" the system with the DB-configuration.

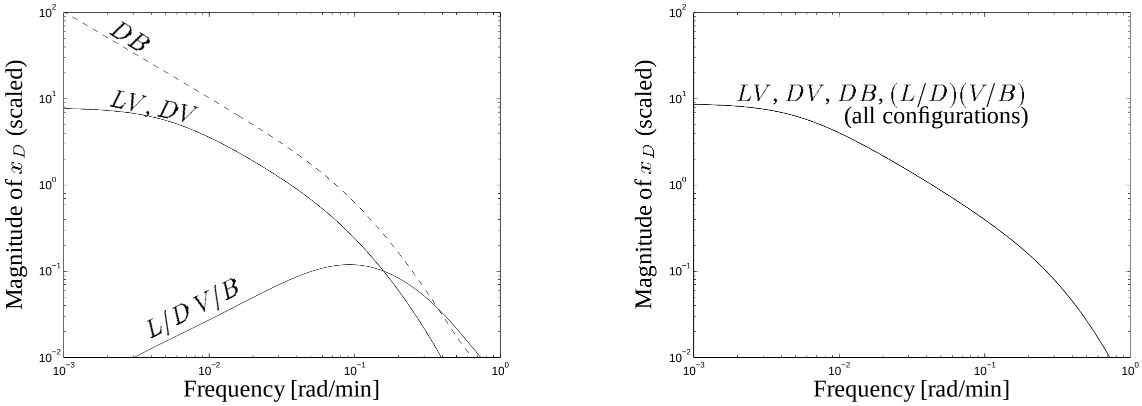
[18] This follows since for a liquid feed, we have $L_{min} \approx F/(\alpha - 1)$, see (9).

As disturbances we consider a 20% change in feed flow ($F = 1 \pm 0.2$ [kmol/min]) and a 20% change in feed composition ($z_F = 0.5 \pm 0.1$). We assume that these disturbances are sinusoids with frequency ω [rad/min], and we want to consider the effect of varying ω. Thus, a frequency-analysis is needed. We will consider the effect of these disturbances on the top composition, x_D.

Scaling. To make it easier to interpret the plots we need to scale the variables. We scale the disturbances by their maximum changes of ±20%, and we scale x_D such that a value of 1 (in the scaled variables) corresponds to an actual change in x_D of ± 0.01 [mole fraction units], which we here regard as the largest acceptable variation in composition. In summary, this means: If, at a given frequency ω, the effect of F on x_D is 1 (in scaled variables), then a sinusoidal variation in F of 1 ± 0.2 [kmol/min] will results in a sinusoidal variation in x_D of 0.99 ± 0.01 [mole fraction units], which is on the borderline of what we accept. Thus, in terms of scaled variables, we want the effect of the two disturbances (F and z_F) on x_D to be less than 1 (approximately). Note that we use a linear analysis based on the linearized model.

1. No composition control ("open-loop")

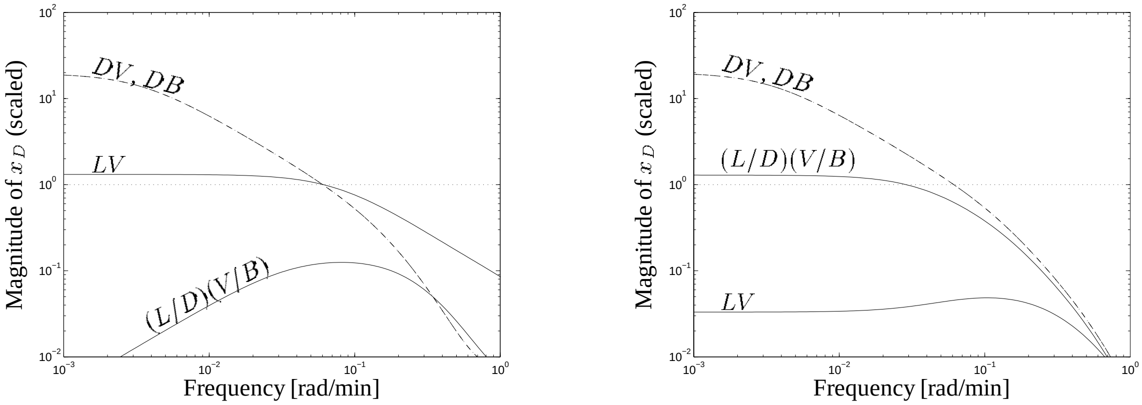
In Figure 14 is shown the "open-loop" effect of the two disturbances on x_D (more precisely, we plot $|g_{d1}|$ in (72) as a function of frequency for $d = z_F$ and $d = F$). The plot on the left shows the effect of a $\pm 20\%$ disturbance in F on the scaled x_D, and the plot on the right shows the effect of a $\pm 20\%$ disturbance in z_F. Plots are shown for the LV, DV, DB and $(L/D)(V/B)$ configurations.



(a) Effect of feed flow F on x_D

(b) Effect of feed composition z_F on x_D

Figure 14: Open-loop: Effect of disturbances on top composition x_D



(a) Effect of feed flow F on x_D

(b) Effect of feed composition z_F on x_D

Figure 15: One-point control of x_B: Effect of disturbances on top composition x_D

The frequency plot for the feed rate disturbance in Figure 14a confirms our findings from the simulations in Figure 9; there is no steady-state effect for the $(L/D)(V/B)$ configuration, the LV- and DV-configurations are identical and yield a quite large effect, and the DB-configuration is somewhat worse. The curve for the $(L/D)(V/B)$ configuration increases with frequency, but only reaches 0.1 (well below 1), so we conclude that the $(L/D)(V/B)$ configuration is "self-regulating" (i.e. needs no control) with respect to disturbances in F. The LV- and DV- configurations are not self-regulating for disturbances in F, except at frequencies above 0.04 rad/min where the column dynamics "average out" the effect of high-frequency variations. In other words, we need control at frequencies up to 0.04 rad/min, and, if we close a feedback loop involving x_D (one-point control, e.g. using the reflux L), then we need a closed-loop time constant better than (i.e. less than) 1/0.04 = 25 min (approximately). This should be easy to achieve in practice.

For the feed composition disturbance, see Figure 14b, there is no difference between the four configurations. The reason is that we have assumed constant molar flows, so the change in z_F does not affect the flows, and is thus not detected by the level controllers. Obviously, if the assumption of constant molar flows does not hold, then the configurations will differ. In any case, in our example, the curves for z_F are close to 10 at steady-state and cross 1 at about frequency 0.045 rad/min, that is, with one-point control of x_D we need a closed-loop response time better than 1/0.045 = 22 min (approx) to achieve satisfactory control when there are disturbances in z_F.

In conclusion, some composition control is needed to achieve acceptable disturbances rejection for this column (as we will find for most distillation columns).

2. One-point control (perfect control of x_B)

Consider the case when the second manipulated input (e.g. V for the LV-configuration) is used to control x_B. But x_D is left uncontrolled, and we want to evaluate the effect (denoted p_{d1}) of the two disturbances on x_D in this case. As an example, consider the effect of a disturbance d using the LV-configuration. The linear model in terms of deviation variables is[19]

$$x_D = g_{11}L + g_{12}V + g_{d1}d \tag{72}$$

$$x_B = g_{21}L + g_{22}V + g_{d2}d \tag{73}$$

For simplicity (to avoid the effect of the tuning) we assume that x_D is perfectly controlled using V. Thus, set $x_B = 0$ in (73) and solve for V, and substitute the results into (72) to get

$$x_D = \underbrace{\left(g_{11} - g_{12}g_{22}^{-1}g_{21}\right)}_{p_{u1}} L + \underbrace{\left(g_{d1} - g_{12}g_{22}^{-1}g_{d2}\right)}_{p_{d1}} d \tag{74}$$

Thus, by controlling x_B, the effect of a disturbance d on x_D has changed from g_{d1} to $p_{d1} = g_{d1} - g_{12}g_{22}^{-1}g_{d2}$.

In Figure 15 we show the effect of the two disturbances on x_D with one-point control (more precisely, we plot $|p_{d1}|$ as a function of frequency for the four configurations). The results are quite interesting. Let us take the least interesting first; with the DV- and DB-configurations, we are now keeping D constant, so, as expected, the disturbances still have a large effect on x_D, especially at low frequencies. Thus, we need to close also the loop involving x_D and D to achieve acceptable control for these configurations.

Next, consider the LV-configuration. We see that with x_B controlled, the effect of both disturbances are drastically reduced, and especially the effect of z_F. The reason is that the two product compositions are strongly coupled, so by controlling one of them, we effectively control the other. In fact, the effect of z_F ob x_D is less than 1 at all frequencies, so we have "self-regulation". The effect of F is slightly above 1 at low frequencies. However, if we measure F and implement a "feed-forward controller" by using the ratio L/F, then we should also achieve "self-regulation" for F. In summary, for this example we may achieve acceptable control of *both* products, by using one-point control of x_B and keeping L/F constant.

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[19] In (72) x_D is really dx_D etc., but we have omitted the differential symbol to simplify notation

For the $(L/D)(V/B)$ configuration, we still have "self-regulation" with respect to F, and the effect the disturbance in z_F is significantly reduced. Nevertheless, it remains above 1 at low frequencies, and since a feed-forward controller based on measuring z_F may be rather costly and difficult to implement, we need to use feedback control also of x_D.

In conclusion, for one-point control the LV-configuration is the probably the best choice. It is also very simple to implement, and this explains the popularity of this scheme in industry for one-point control.

3. Two-point control (CLDG)

With two-point control both compositions are controlled, so the effect of disturbances will be small at low frequencies. However, the often severe interactions (caused by nonzero values of g_{12} and g_{21}), may make two-point control difficult and thus result in poor dynamic performance. Let us assume that two single-loop (decentralized) controllers are to be used to control the compositions, e.g. with the LV-configuration we typically use one PI-controller to control x_D using L, and another PI-controller to control x_B using V. The question is: How fast must these controllers be tuned to achieve acceptable control? This can be answered by plotting the closed-loop disturbance gain (CLDG) which gives the effective disturbance effect caused by interactions.

To derive the expression for the CLDG, we need a little control theory. Let G denote the 2×2 plant for the effect of the inputs u (e.g. L and V) on the product compositions y (x_D and x_B), and let G_d denote the effect of the disturbances d (F and z_F). In terms of deviation variables we then have the transfer function model

$$y = Gu + G_d d \tag{75}$$

Now, let $\tilde{G}$ denote the diagonal elements in G, and let

$$E = (G - \tilde{G})\tilde{G}^{-1} \tag{76}$$

represent the relative interactions (which we obviously want small). The closed-loop response with the two-composition loops closed is given by

$$y = SG_d; \quad S = (I + GK)^{-1} \tag{77}$$

where K is the *diagonal* composition controller (it is diagonal since we assume decentralized control) and S is the sensitivity function (it is not diagonal). The corresponding closed-loop response if we neglected interactions in G would be

$$\tilde{y} = \tilde{S}G_d; \quad \tilde{S} = (I + \tilde{G}K)^{-1} \tag{78}$$

Actually, $\tilde{S}$ (which is diagonal) is the closed-loop response of the loops when considered one-by-one. It is relatively easy to show that the following relationship between S and $\tilde{S}$ holds (e.g. Skogestad and Postlethwaite, 1997)

$$S = \tilde{S}\left(I + E(I - \tilde{S})\right)^{-1} \tag{79}$$

Now, assume that $g_{11} \neq 0$ and $g_{22} \neq 0$, and that the controllers have integral action, and consider the low frequencies where we have tight control and thus $\tilde{S} \approx 0$. At these frequencies we then get

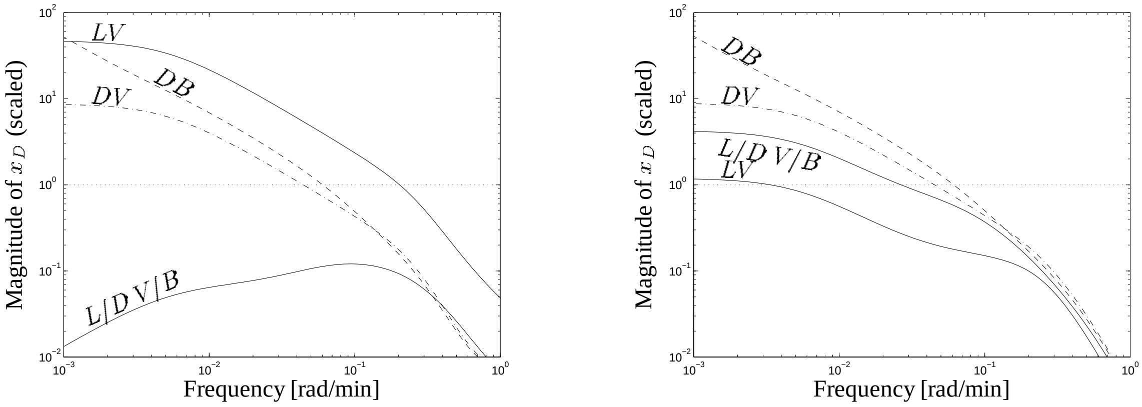
$$S \approx \tilde{S}\,(I + E)^{-1} = \tilde{S}\tilde{G}G^{-1} \tag{80}$$

where $\Gamma = \tilde{G}G^{-1}$ is the performance RGA (PRGA) which has elements γ_{ij}. The PRGA has the same diagonal elements as the RGA, but different off-diagonal elements. *The PRGA gives the effect of interactions on closed-loop performance with decentralized control.* Combining (77) and (80) then gives the closed-loop disturbance response at lower frequencies

$$y \approx \tilde{S}\tilde{G}_d d, \quad \tilde{G}_d = \tilde{G}G^{-1}G_d \tag{81}$$

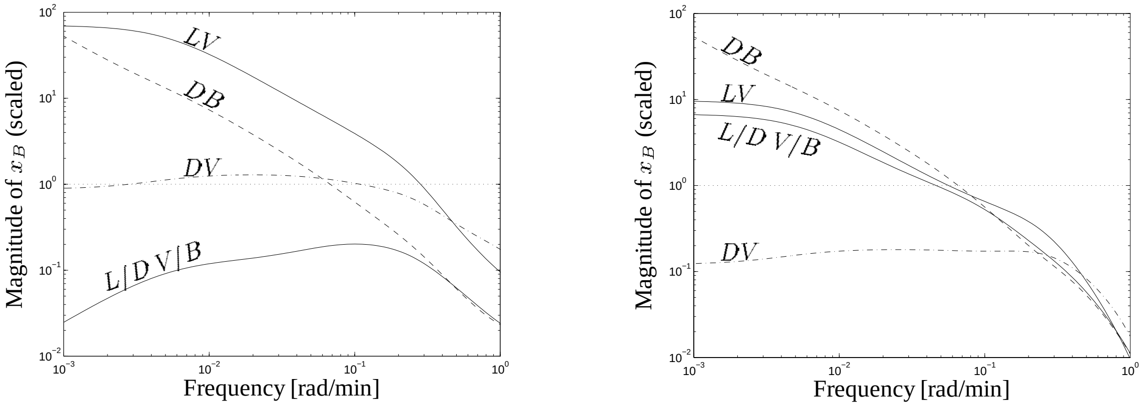
where $\tilde{G}_d$ is the matrix of closed-loop disturbance gains (CLDG). By comparing (78) and (81), we see that G_d gives the effect of the disturbances when the interactions are neglected, whereas *the CLDG ($\tilde{G}_d$) gives* *the effect of the disturbances for decentralized control when interactions are taken into account.* More precisely, from (81) we need $1/|\tilde{s}_i| = |1 + L_i|$ to be larger than $|\tilde{g}_d|$ to achieve acceptable performance, i.e. $|y_i| \leq 1$. Here $L_i = g_{ii}k_i$ is the loop gain in loop i. At lower frequencies where $|L_i|$ is large, we must then require $|L_i| > |\tilde{g}_d|$. Similarly, for setpoints changes of unit magnitude, we want $|L_i|$ to be larger than the the PRGA's $|\gamma_{ij}|$ (at least at frequencies where we want to track the setpoints).

We can therefore, from frequency-dependent plots of $\tilde{G}_d$ (CLDG) and Γ (PRGA) for each output, tell how fast the controller in this loop (involving the output in question) must be to achieve acceptable closed-loop performance. (This ends the control theory part.)



(a) Effect of feed flow F on x_D

(b) Effect of feed composition z_F on x_D



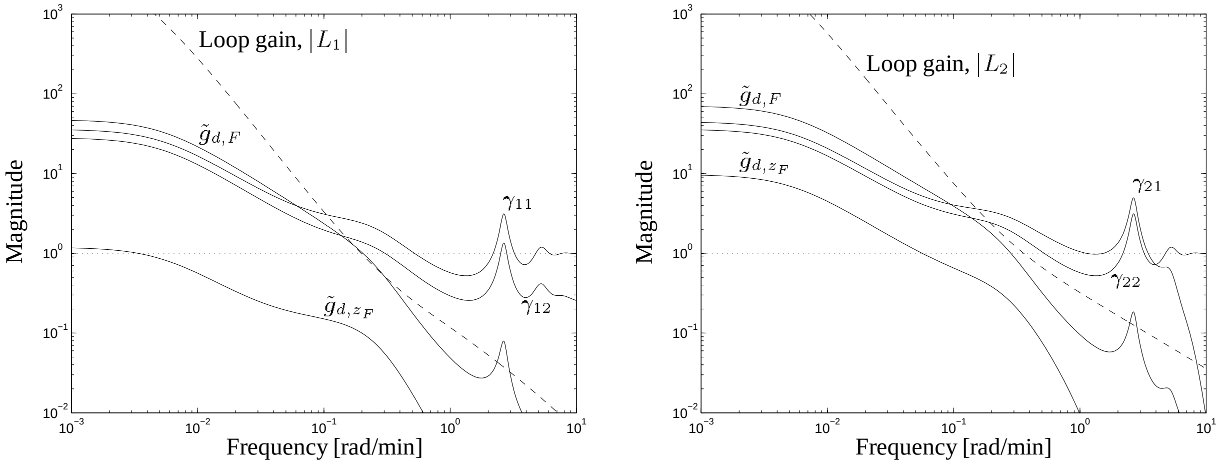
(c) Effect of feed flow F on x_B

(d) Effect of feed composition z_F on x_B

Figure 16: Two-point decentralized control (CLDG): Effect of disturbances on product compositions

Now, consider Figures 16a-b which show the effects on x_D of disturbances in F and z_F, with decentralized control (more precisely, the plot shows the CLDG, $|\tilde{g}_{d1}|$, as a function of frequency).

For the *LV-configuration* the interactions strongly amplify the effect of F whereas they reduce the effect of z_F (compare Figure 16 with Figure 14). For the disturbance in F, we see from the curve LV in Figure 16a, that its effect, $|\tilde{g}_{d1}|$, is larger than 1 up to about 0.2 [rad/min]. This means that, to achieve acceptable control, we need the top composition loop (when evaluated alone) to be effective up to about 0.2 [rad/min], i.e., we need the closed-loop response time for the loop involving L and x_D to be better than $1/0.2 = 5$ min (approximately). A similar analysis, based on the CLDG for x_B (Figure 16c-d) shows that we need the closed-loop response time for the bottom composition loop to better than $1/0.3 = 3.3$ min (approximately). In summary, it is possible to achieve acceptable two-point control with the LV-configuration, but it requires fast control in both composition loops in order to reject disturbances in F.



(a) Top loop: $x_D - L$

(b) Bottom loop: $x_B - V$

Figure 17: Loop gains $L_i = g_{ii}k_i$, CLDG's $\tilde{g}_d$, and PRGA's γ_{ij} for LV-configuration.

To check the validity of this conclusion for the LV-configuration we use two single-loop PI controllers:

$$k_1(s) = 26.1\frac{1+3.76s}{3.76s}\ (x_D - L \text{ loop}); \quad k_2(s) = -37.5\frac{1+3.31s}{3.31s}\ (x_B - V \text{ loop}) \tag{82}$$

The loop gains, $|L_i| = |g_{ii}k_i|$, with these controllers are larger than the closed-loop disturbance gains, $|\tilde{g}_d|$, at frequencies up to crossover, see Figure 17 (note that the gain is slightly higher for the bottom composition controller as required by the CLDG-analysis). Closed-loop simulations with these controllers are shown in Figure 18.[20] The simulations confirm that the disturbance in F is more easily rejected than the disturbance in z_F. They also confirm that z_F has a smaller effect on x_D then on x_B. In general, we find an excellent agreement between a CLDG-analysis which requires no controller tuning, and the simulated closed-loop performance with decentralized control.

The CLDG-plot for the other configurations in Figure 16 show that we do not need as fast control to get acceptable performance as for the LV-configuration. In particular, the $(L/D)(V/B)$-configuration performs well. However, recall that this assumes that the levels are tightly controlled.

6.5 Conclusion configurations

The following conclusion is from Skogestad et al. (1990b). The arguments mainly refer to composition control, although comments on level control are included. For “simple” control problems, with $\lambda_{11}^{LV}(0)$ less than about 5, the LV-configuration is usually recommended.

Thus, the arguments below regarding two-point control refer to columns which are “difficult ” to control with the conventional LV-configuration, that is, with $\lambda_{11}^{LV}(0) > 10$ (approximately).

LV-configuration. A good choice for one-point control. It is usually not recommended for two-point control for cases where $\lambda_{11}^{LV}(0) > 10$ because of sensitivity to disturbances and strong interactions between control loops. In particular, the LV-configuration performs poorly with large dead-times. However, if it possible to achieve fast control, e.g. by controlling instead two temperatures inside the column, then the LV-configuration may still be a viable option.

DV-configuration. One-point control: D must be used for automatic control (not in manual). May be better than LV for columns with large reflux because top level control is simpler. Two-point control: Works relatively poor when bottom product is not purer than top, but is better when bottom product is pure. Disadvantages: 1) Performance may change depending on operating conditions , 2) Poor performance if failure leeds to D constant (for example, if the top measurement fails).

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[20] We did not use logarithmic compositions as controller inputs in these simulations, although this is generally recommended. This is especially the case if we want to make large setpoint changes, say between 99% and 99.9% which would change the initial process gain by a factor 10 unless we used logarithmic compositions, recall (66).

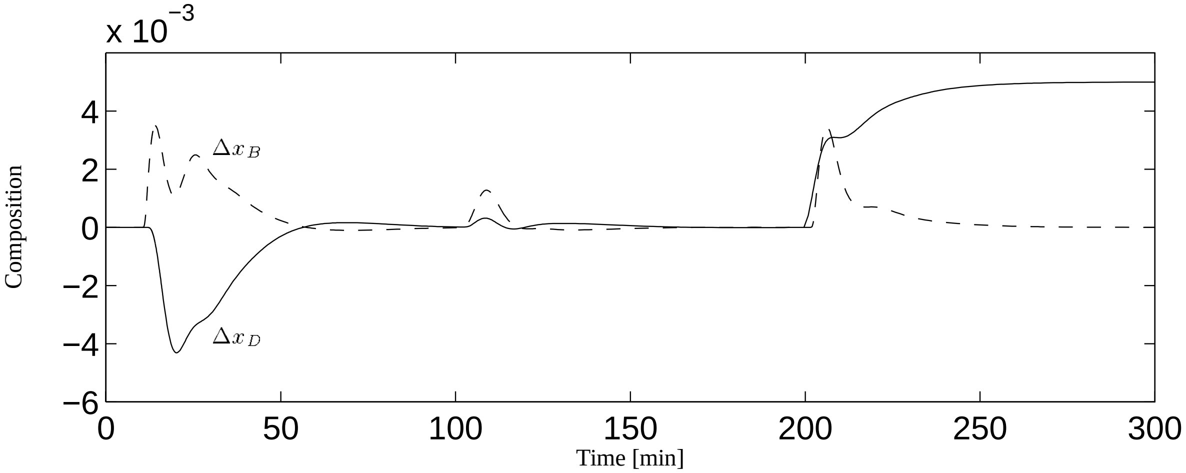

Figure 18: Closed-loop simulations with LV-configuration using PI-tunings from (82). Includes 1 min measurement delay for x_D and x_B. $t = 10$: F increases from 1 to 1.2; $t = 100$: z_F increases from 0.5 to 0.6; $t = 200$: Setpoint in x_D increases from 0.99 to 0.995.

DB-*configuration.* Unacceptable performance if used for one-point control. Two-point control: Good control quality, in particular for columns with high purity and/or large reflux. Simple to implement. Level control also favors this configuration for columns with large reflux. The main disadvantage is that it lacks integrity; performance is very poor if failure gives D or B constant. In particular, one can not put one of the loops in manual.

$(L/D)(V/B)$-*configuration.* This is a good overall choice for all modes of operation. The main disadvantage is the need for measurements of all flows L, D, B and V which makes it more failure sensitive and more difficult to implement, and the need for tight level control.

$(L/D)V$-*configuration.* Behaves somewhere between LV and $(L/D)(V/B)$.

In summary, two-point distillation control is probably not as difficult as many people believe. After all, the liquid flow dynamics decouple the two column ends at high frequency, so if sufficient effort is put into making the quality loops fast (e.g. by using temperature measurements with an outer composition cascade), then it should be possible to achieve good control in most cases. Finally, logarithmic compositions (or the similar logarithmic transformations on the temperatures, see (17)), should be used to counteract the effect of nonlinearity.

6.6 5×5 control

From a theoretical point of view it is clear that the “optimal” controller should use *all* available information (measurements of outputs and disturbances, plant model, expected model uncertainty, expected disturbances, known future reference changes, given constraints, etc.) to manipulate all 5 inputs (but avoiding large changes) to keep all 5 outputs close to their desired setpoints. Something close to this “optimal 5×5 controller” can be realized using model predictive control (MPC). In addition to achieving better control performance, one then avoids the issue of selecting a control configuration, and the need to design special systems to handle input saturation (constraints) etc.

In fact, Lundström and Skogestad (1995) found in a simulation study that very good control, even when model uncertainty taken into account, could be achieved using MPC. However, so far no industrial implementations of 5×5 or even 4×4 MPC have been reported. The reason is the cost of obtaining the dynamic 5×5 model and tuning the controller, which must be traded off against the improvements in control performance. Also, most of the industrial implementations of MPC today use a model based on on-line identification, whereas it probably is better, due to the strong interactions in the distillation models which may be difficult to identify, to use a first-principle model.

7 Effect on control of column design

How should the column be designed to make feedback control easier?[21] In terms of composition control, the best is probably to add extra stages. This has two potential advantages:

1. It makes it possible to overpurify the products with only a minor penalty in terms of energy cost; recall the expression for V_{min} in (12) which is independent of the purity. The control will then be less sensitive to disturbances.

2. If we do not overpurify the products, then with "too many" stages a pinch zone will develop around the feed stage. This pinch zone will effectively stop composition changes to spread between the top and bottom part of the column, and will therefore lead to a decoupling of the two column ends, which is good for control.

In may columns, the disturbances have a fast effect, and we need fast control to counteract them. It is recommended to install at least three temperature sensors in each column section. This makes it possible to correct for pressure changes and to use cascade control based on fast temperature measurements or to use the temperatures for estimating the product compositions. Furthermore, the reflux system and reboiler should be designed such that t is possible to make fast changes in the reflux L and boilup V.

What about trayed versus packed columns? A packed column usually has a factor of two or smaller liquid holdup. This is in itself a disadvantage since disturbances will have a faster effect, and we can tolerate less delays in the measurements and in the manipulated inputs (valves). On the other hand, in a packed column the decoupling effect of the liquid flow dynamics is more significant, because there is no "dead volume" below the weir as in a tray column, and this will be an advantage with two-point control. Furthermore, in a packed column, the parameter λ, representing the initial effect of an increase in vapor flow on liquid flows, is close to zero. This is an advantage compared to a trayed column where we may have $\lambda > 1$, resulting in an undesirable inverse response behavior.

8 Conclusion

In this paper, we have presented some important topics for the dynamics and control of distillation columns, including a treatment of the steady-state operation. The issues covered include the separation factor, logarithmic compositions, external flows, internal flows, initial composition response, dominant time constant, gain matrix for various configurations, linearization, mass flows, disturbances, myths about slow control, one-point and two-point control, controllability analysis using the RGA and CLDG, selection of control configurations, and 5×5 control. The treatment has been mainly through examples, and it is hoped that the reader can develop insight and intuition, which is needed for applying the results in practice and for reading the literature in more detail.

Appendix. State-state gain expressions

It has been mentioned that the separation factor can be assumed constant when considering the effect of changes in external flows. Here we consider this in more detail, and derive simplified gain expressions for small changes in external and internal flows.

The separation factor and the steady-state material balance written in terms of the light component for a binary separation is

$$S = \frac{(x_L/x_H)_{top}}{(x_L/x_H)_{btm}} = \frac{x_D(1-x_B)}{(1-x_D)x_B} \tag{83}$$

$$Dx_D + (F-D)x_B = Fz_F \tag{84}$$

With a given feed (Fz_F given) and with S and D given, this gives a second order equation for x_D and x_B (Shinskey, 1984).

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[21] We are not here considering the steady-state operability which, for example, involves the ability to run the column at smaller or higher loads.

Example. Column A. Consider a column with z_F=0.5, $x_D = 0.99$, $x_B = 0.01$ (all these refer to the mole fraction of light component) and $D = B = 0.5$ [kmol/min]. We have $S = (0.99 \cdot 0.99)/(0.01 \cdot 0.01) = 9801$. Now consider a 20% increase in the distillate D from 0.50 to 0.6 [kmol/min]. With D=0.6 and $Fz_F = 0.5$, (83) and (84) can be solved to obtain

$$x_D = 0.8330 \text{ and } x_B = 0.00051$$

To check the estimate obtained by assuming S constant, we can compute the exact composition for column A. With $D = 0.5$ we find that $x_D = 0.99$ and $x_B = 0.01$ are obtained with $L = 2.706$. We then keep L fixed and increase D to 0.6. This gives

$$x_D = 0.8324 \text{ and } x_B = 0.00134$$

so S has actually decreased from 9801 to 3687. Thus, the assumption of constant S was not really valid in this case.

A more careful analysis shows that the assumption of S constant for changes in the external flows holds best as long as both products remain relative pure, e.g. see (85). This is confirmed by considering a small (and more realistic) increase in D from 0.5 to 0.505. By assuming S constant we find that x_D changes from 0.99 to 0.98399 and x_B from 0.01 to 0.00623. For "column A" this is almost the same as the exact values of 0.98402 and 0.00612 (i.e., we have a small increase in S from 9801 to 9872).

To analyze the difference between external and internal flows, we differentiate (83) and (84) assuming Fz_F constant. This yields the following exact expressions for the changes in the logarithmic compositions (binary separation)

$$dX_D = \frac{1}{(1-x_D)x_D} dx_D = \frac{-(x_D - x_B)dD + Bx_B(1-x_B)d\ln S}{I_s} \tag{85}$$

$$dX_B = \frac{1}{(1-x_B)x_B} dx_B = \frac{-(x_D - x_B)dD - Dx_D(1-x_D)d\ln S}{I_s} \tag{86}$$

where the "impurity sum" is defined as

$$I_s = Bx_B(1-x_B) + Dx_D(1-x_D) \tag{87}$$

First consider changes in external flows, i.e. changes in D and B, for which the second term on the right hand side in (85) and (86), involving changes in S, usually can be neglected. We get in terms of logarithmic compositions

$$\frac{\partial X_D}{\partial D} \approx \frac{\partial X_B}{\partial D} \approx -\frac{x_D - x_B}{I_s} \tag{88}$$

(These logarithmic gains change with the operating point, but note that the changes are even larger if we do not use logarithmic compositions.) Next consider, changes in internal flows, for which $dD = 0$ so only the second term involving changes in S remains. We get in terms of logarithmic compositions

$$\left(\frac{\partial X_D}{\partial L}\right)_D = \frac{Bx_B(1-x_B)}{I_s}\left(\frac{\partial \ln S}{\partial L}\right)_D \tag{89}$$

$$\left(\frac{\partial X_B}{\partial L}\right)_D = -\frac{Dx_D(1-x_D)}{I_s}\left(\frac{\partial \ln S}{\partial L}\right)_D \tag{90}$$

where from the short-cut model (15) we have

$$\left(\frac{\partial \ln S}{\partial L}\right)_D \approx \frac{N}{2}\frac{1}{L}\frac{q_F F}{L + q_F F} + \frac{N}{2}\frac{1}{V}\frac{(1-q_F F)}{V + (1-q_F)F} \tag{91}$$

To compare the effect of changes in internal and external flows, we consider the effects of a unit flow change in D and L on $|X_D| + |X_B|$, and take the ratio (denoted γ). We get from (88)–(90)

$$\gamma = 2\frac{x_D - x_B}{I_s}\frac{1}{\left(\frac{\partial \ln S}{\partial L}\right)_D} \tag{92}$$

γ also gives an estimate of the condition number of the steady-state gain matrix of the plant (the ratio between the largest and smallest effect of flow changes). For example, for column A we get from (91)

$$x_D - x_B = 0.98, \quad I_s = 0.0099, \quad \left(\frac{\partial \ln S}{\partial L}\right)_D \approx \frac{20}{2.706 \cdot 3.706} = 1.99 \quad \Rightarrow \quad \gamma = 92.27$$

As a comparison, the exact value is $\left(\frac{\partial \ln S}{\partial L}\right)_D = 2.76$ which gives $\gamma = 71.7$.

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Additional information. MATLAB files to generate the figures in this paper are available over the internet; see the www home page of S. Skogestad at `http://www.chembio.ntnu.no/users/skoge`.