

DYNAMICS AND CONTROL OF DISTILLATION COLUMNS - A CRITICAL SURVEY

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Abstract

Distillation column dynamics and control has been viewed by many as a very mature or even dead field. However, as is discussed in this paper significant new results have appeared over the last 5-10 years. These results include multiple steady states and instability in simple columns with ideal thermodynamics (which was believed to be impossible), the understanding of the difference between various control configurations and the systematic transformation between these, the feasibility of using the distillate-bottom structure for control (which was believed to be impossible), the importance of flow dynamics for control studies, the fundamental problems in identifying models from open-loops responses, the use of simple regression estimators to estimate composition from temperatures, and an improved general understanding of the dynamic behavior of distillation columns which includes a better understanding of the fundamental difference between internal and external flow, simple formulas for estimating the dominant time constant, and a derivation of the linearizing effect of logarithmic transformations. These issues apply to all columns, even for ideal mixtures and simple columns with only two products. In addition, there have been significant advances for cases with complex thermodynamics and complex column configurations. These include the behavior and control of azeotropic distillation columns, and the possible complex dynamics of nonideal mixtures and of interlinked columns. However, both for the simple and more complex cases there are still a number of areas where further research is needed.

1 Introduction

The objective of this paper is to give a critical survey of the present status within the field of distillation dynamics and control. The paper is mostly a literature review, but a few new ideas are also presented. New papers in this field appear at a rate of at least 50 each year, and no attempt has been made to reference all papers which have appeared in the seven

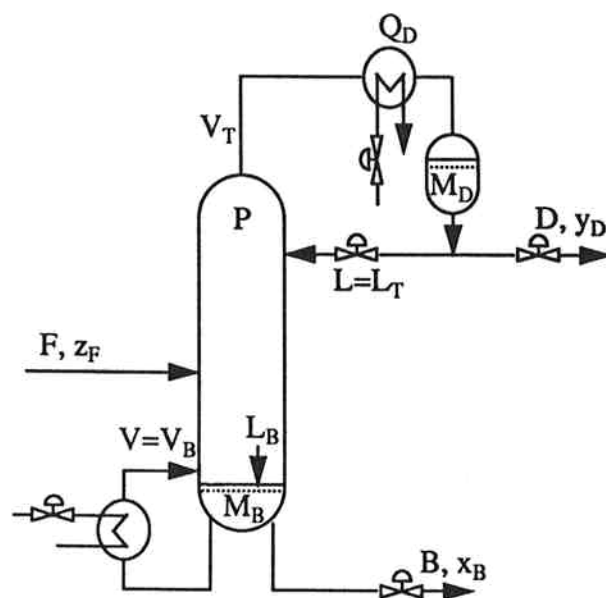


Figure 1: Typical simple distillation column. z_F , y_D and x_B are mole fractions.

years from 1985 to 1991 since the last detailed survey was published (McAvoy and Yang, 1986). Although I have tried to select the papers which I personally find most useful, it is clear that a number of good papers have been left out.

A typical two-product distillation column is shown in Fig.1. The behavior of distillation columns has been extensively studied over the last 70 years, and still remains an active area of research. The early work from the 1920's into the 1950's mainly treated the steady-state behavior using graphical and simple short-cut models. With the introduction of the digital computer in the 1950's the research was shifted towards developing and solving rigorous models for simulating the steady-state and dynamic behavior, and studying the control behavior. Important contributions in the early period (up to about 1965) were made by industrial researchers; notably by Rosenbrock from John Brown in the UK (e.g., Rosenbrock, 1962a-d), and by Rademaker and Rijnsdorp from Shell in the Netherlands. These people did pioneering work on dynamic modeling, dynamic simulation, understanding the dynamic behavior, uniqueness and stability of solutions,

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as well on dual composition control, control configuration selection and the importance of interactions in distillation.

Rosenbrock (1962d) presents a good overview of the early work on distillation dynamics with 173 references. The book by Rademaker et al. (1975) contains about 300 references on dynamics and control covering the period up to 1973. Tolliver and Waggoner (1980) present a comprehensive and critical review of the literature on both dynamics and control covering papers published during the 70's with 195 references. McAvoy and Yang (1986) present a similar study covering the years 1980 to 1984 with 270 references. Waller (1982) gives a thorough review of academic research on composition control with 80 references. In his book on interaction analysis McAvoy (1983) presents a good overview of dual (two-point) composition control with 60 references.

There are several books published on 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 book by Desphande (1985) is, in spite of its title, more of an undergraduate textbook on dynamics and control, than a book on distillation dynamics and control.

A few books concentrate on distillation control. Shinsky (1984) contains 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. The book by Buckley et al. (1985) gives a detailed discussion of the design of level and pressure control systems, but the issue of composition control (configuration selection) is only briefly discussed. Most of the material in the book by Nisenfeld and Seeman (1981) is covered by Shinsky (1984), but there is a good section on the use of temperatures to infer compositions. The book by 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. Most of the 444 references are from the industrial literature. A new book by Luyben (1992) with contributions from numerous authors was not available at the time of this review.

Example column. All simulations presented in this paper are for a high purity column with product compositions $x_B = 1 - y_D = 0.01$ (Column A of Skogestad and Morari, 1988a). It has $N=40$ theoretical trays plus a total condenser. Thermodynamic data:

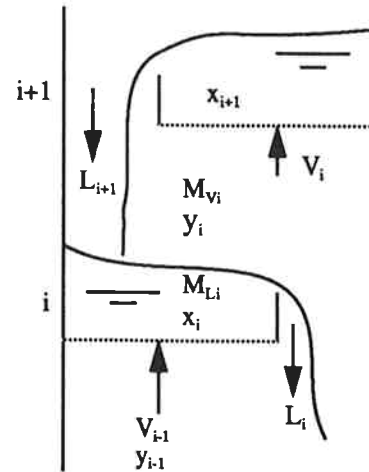


Figure 2: Stage in distillation column.

Constant molar flows and constant relative volatility $\alpha = 1.5$ between the two components. Vapor holdup neglected, constant pressure. Other column data: $z_F = 0.5$, $N_F = 21$, $D/F = 0.5$, $L/F = 2.706$, $V/F = 3.206$. Nominal liquid holdups: $M_i/F = 0.5$ min on all 41 stages, except for Fig.8 where condenser holdup $M_D/F = 32.1$ min. Liquid flow dynamics: For $i = 2, 40$: $\Delta L_i = \Delta M_i/\tau_L$ where $\tau_L = 0.063$ min (i.e., $\theta_L = N\tau_L = 2.46$ min). This yields a nonlinear model with 82 states. All data are on a molar basis. Assume perfect control of reboiler and condenser level, except for Fig.8 where $\Delta L = K\Delta M_D$.

2 Dynamic modeling and simulation

2.1 Rigorous models

The term "rigorous" model of a distillation column usually refers to a staged model which includes mass- and energy balances on each stage, includes a model of the liquid flow dynamics (changes in liquid holdup), and includes a model of the pressure dynamics. The model may also include a detailed model of the reboiler and condenser. However, even in this "rigorous" model a number of model simplifications are included. These typically include perfect mixing in both phases on all stages, thermal and thermodynamic equilibrium between the phases, (i.e., 100% tray efficiency or possibly some simple Murphee relationship for the efficiency of each component), and neglecting the effect of column internals on the energy balance.

Consider a stage i that is not a feed stage, and which does not have any product streams or heat input/output (see Fig.2). On each such stage differential equations may be formulated for,

(i) component material balances (composition dy-

namics) for components $j = 1, n_c - 1$

$$\frac{dN_{ij}}{dt} = L_{i+1}x_{i+1,j} + V_{i-1}y_{i-1,j} - L_i x_{i,j} - V_i y_{i,j} \quad (1)$$

$$\text{where : } N_{ij} = M_{L_i}x_{ij} + M_{V_i}y_{ij}$$

(ii) overall material balance (flow dynamics)

$$\frac{d}{dt}M_i = \frac{d}{dt}(M_{iL} + M_{iV}) = L_{i+1} + V_{i-1} - L_i - V_i \quad (2)$$

and (iii) energy balance

$$\frac{dU_i}{dt} = L_{i+1}h_{L,i+1} + V_{i-1}h_{V,i-1} - L_i h_{L_i} - V_i h_{V_i} \quad (3)$$

$$\text{where : } U_i = M_{L_i}u_{L_i} + M_{V_i}u_{V_i}$$

Here i is the index for stages, j the index for components and n_c is the number of components. There are only $n_c - 1$ independent component balances since $\sum_j N_{ij} = M_i$. In addition, there are algebraic relations for the tray hydraulics and pressure drop

$$L_i = f_1(M_{L_i}, V_i, \Delta p_i); \quad V_i = f_2(M_{L_i}, \Delta p_i) \quad (4)$$

and algebraic thermodynamic equations for the assumed vapor-liquid equilibrium (VLE) between the phases on each stage. Details on the hydraulic and pressure drop equations are given for example by Gani et al. (1986), Ruiz and Gani (1986), and Lockett (1986).

Solution procedure. This set of equations has $N \times (n_c + 1)$ independent state variables where N is the number of stages. As state variables we typically select the n_c component holdups N_{ij} and the internal energy U_i . Solution (integration): 1) The values of the states are known at each time step. 2) With given N_{ij} , U_i and total tray volume, perform a UV-flash for each stage. This yields the phase split (M_{L_i}, M_{V_i}), phase compositions (x_i, y_i), temperature (T_i), pressure (p_i) and specific energies (h_{L_i}, h_{V_i}). 3) L_i and V_i are computed from the algebraic expressions for tray hydraulics and pressure drop. 4) All the variables on the right hand side of Equations 1-3 above are now known and the derivatives of the state variables may be computed and the integration may proceed. Kinoshita (1986) presents an alternative procedure with x_{ij} as state variables, but which involves differentiation of the thermodynamic relationships.

2.2 Model simplifications

No references were found on dynamic distillation programs which solve the equations in this rigorous fashion. Some of the most common model simplifications are presented below.

2.2.1 Simplifications to the vapor dynamics

Case V1. Neglecting vapor holdup.

Usually the holdup in the vapor phase is neglected, that is, $M_{iV} = 0$. This assumption is valid when the vapor phase component holdup can be neglected

compared to that in the liquid phase. Thus, the assumption may be poor for volatile components, for columns with high pressure and for cryogenic separations where the liquid density often is low (Kinoshita, 1986). Choe and Luyben (1987) recommend including the vapor holdup if it is higher than 20% of the liquid holdup. Typically, the vapor volume is about 10 times the liquid volume, and the vapor holdup may be neglected for columns operating at less than 10 bar (Choe and Luyben, 1987). Neglecting the vapor holdup implies that a change in vapor flow at the bottom of the column *immediately* will change the vapor flow at the top. This is of course somewhat unrealistic. The solution procedure is similar to that outlined above, except that the often time-consuming UV-flash is replaced by a bubble point flash with given x_{ij} and h_i (eg., Gani et al., 1986, and eq. 8-10 in Choe and Luyben, 1987).

Case V2. Fixed pressure and neglecting vapor holdup.

This is a very common assumption. The assumption of constant pressure is often justified because pressure is tightly controlled. Since pressure is known we get one state less on each tray (the total number of independent states is $N \times n_c$), but the number of differential equations remains the same – this signals an “index” problem (see Gritsis et al, 1988). The solution (integration) of the equations may proceed as follows: 1) Known at each stage: The n_c state variables N_{ij} (or equivalently x_{ij} and M_{L_i}), and the pressure p_i . 2) Perform a bubble point flash with given x_i and p_i to compute y_i , T_i and the specific energies $h_{L_i} = u_{L_i}$. 3) Compute L_i from the algebraic expression for the tray hydraulics. 4) Use the energy balance (3) to compute V_i : Since h_{L_i} and thereby dh_{L_i}/dt is “known” this may be done by transforming (3) into an algebraic expression. This gives rise to an index problem that may give numerical problems. It may be circumvented (a) by estimating dh_{L_i}/dt numerically using previous time steps (Doukas and Luyben, 1978), or (b) for cases with simple thermodynamic equations by evaluating dh_{L_i}/dt analytically using expressions for $(\partial h_{L_i}/\partial x_{ij})_p$, etc. (Howard, 1970, Stathaki et al., 1985). 5) If we want to consider a case with fixed top pressure and variable pressure drop, we may, since V_i is now known, compute p_i along the column from the pressure drop equation and use it for the next integration step.

Case V3. Fixed pressure, but with vapor holdup included.

This corresponds closely to assuming constant vapor holdup, M_{V_i} . One makes use of the known total tray volume, but otherwise the procedure is similar to case V2 (see eq. 4-6 in Choe and Luyben, 1987).

2.2.2 Simplifications to the energy balance

In the following we shall neglect the vapor holdup, $M_{V_i} = 0$, and use the approximation $h_{L_i} \approx u_{L_i}$ which holds for liquids. The left hand side of the energy

balance (3) then becomes

$$dU_i/dt = d(M_i h_{Li})/dt = M_i dh_{Li}/dt + h_{Li} dM_i/dt \quad (5)$$

Case E1. Neglect changes in energy holdup

This corresponds to neglecting (5) and is quite commonly used because one directly gets an algebraic energy balance. However, except for cases when h_{Li} or dM_i/dt are identically zero, this assumption is fundamentally wrong and should *not* be used. As seen from (5) one may for nonzero dM_i/dt get very (arbitrary) large errors in the energy balance if the reference state for energy is chosen such that h_{Li} is large. Therefore, one should at least use the expression for dM_i/dt from the material balance (2) to rewrite the energy balance (3) as

$$M_i dh_{Li}/dt = L_{i+1}(h_{L,i+1} - h_{Li}) + V_{i-1}(h_{V,i-1} - h_{Li}) - V_i(h_{Vi} - h_{Li}) \quad (6)$$

Case E2. Neglect changes in liquid enthalpy

As seen from (6) one gets an algebraic energy balance by making the often reasonable assumption $dh_{Li}/dt \approx 0$ as used, for example, by Berber and Karadurmus (1989). However, the validity depends on the assumed reference state for energy, and we shall use the following:

- Reference state: pure components as saturated liquids at a given reference *pressure* (usually the column pressure).

Note that this means that the individual components have different reference temperatures. In this case the assumption $dh_{Li}/dt \approx 0$ is usually good, except for cases with very different molar heat capacities, for nonideal mixtures with large heats of mixing, or for large changes in column pressure (see Appendix 1). Fuentes and Luyben (1982) conclude from a simulation study for a methanol-water column that one should not neglect dh_{Li}/dt . However, they used as reference state the pure components as liquids at a given *temperature* (0° C), and in this case the approximation $dh_{Li}/dt \approx 0$ is not valid unless the temperature difference along the column is small.

Case E3. Equal vapor flows up the column ("constant molar flows").

With the above reference state for energy and constant column pressure the energy balance may be further simplified by assuming $h_{Li} = h_L = 0$ on all stages (see Appendix 1). The energy balance becomes

$$0 = V_{i-1}(h_{V,i-1} - h_L) - V_i(h_{Vi} - h_L) \quad (7)$$

The very commonly used "constant molar flows" or "equimolar overflow" assumption is derived if we in addition assume that the pure components at column pressure have the same heat of vaporization h^{vap} (see Appendix 1). Then $h_{Vi} = h^{vap}$ and the energy and overall material balances become

$$V_i = V_{i-1}; \quad dM_{Li}/dt = L_{i+1} - L_i \quad (8)$$

That is, the vapor flow up the column is equal on all trays (except at locations where there is a vapor feed stream or a vapor product). At steady state $L_i = L_{i+1}$, but dynamically these are not equal because the liquid holdup M_{Li} varies.

2.2.3 Simplifications for the liquid flow dynamics

Case M1. Neglecting liquid dynamics.

This corresponds to assuming constant liquid holdups and setting $dM_i/dt = 0$ in (2). This very common assumption is partly justified by the fact that the dominant composition dynamics are much slower than the flow dynamics and nearly unaffected by the flow dynamics (eg., Levy et al., 1969), and it may be used to obtain good estimates of the dominant response (see Section 2.5). However, for control purposes the initial response is generally important and this assumption should *not* be used.

Case M2. Linearized liquid dynamics.

This simplification is generally acceptable for a model that is used for feedback control purposes, and if prediction of flooding etc. is not needed in the model. We get in terms of deviation variables (Rademaker et al., 1975)

$$\Delta L_i = \lambda \Delta V_{i-1} + \frac{1}{\tau_L} \Delta M_i \quad (9)$$

λ represents the initial effect of a change in vapor flow on liquid flow, and τ_L is the hydraulic time constant. If we also assume constant molar flows then (8) is valid and the liquid flow dynamics become completely decoupled from the composition dynamics. Repeated combination of (9) and (8) assuming the same values for τ_L and λ on all N_T trays then yields the transfer functions (Rademaker et al., 1975, p.102)

$$\Delta L_B = g_L(s) \Delta L_T + \lambda(1 - g_L(s)) \Delta V_B \quad (10)$$

where

$$g_L(s) = 1 / \left(1 + \frac{\theta_L}{N_T} s \right)^{N_T} \quad (11)$$

Here $\theta_L = N_T \tau_L$ is the apparent delay for an increase in reflux to reach the reboiler.

2.2.4 Summary of simplifications

In the literature three different "full-order" models are commonly used. These are sometimes denoted EMC, MC and C (eg., Levy et al., 1969). The EMC model is a rigorous model with the energy balance included (equations 1-3 above), although the assumption of negligible vapor holdup or constant pressure is often used. The MC model usually denotes a model with negligible vapor holdup, constant pressure and constant molar flows (case E3 above) such that the energy balance (3) is not needed. The C model corresponds to a model where one in addition assumes constant liquid holdup (case M1 above) such that the overall material balance (2) is not needed. As noted

above model C should *not* be used for control purposes, while model MC may be good for relatively ideal mixtures.

There are of course a lot of combinations and simplifications possible in addition to the ones above. For example, for models MC and C it is common to also simplify the VLE by assuming constant relative volatility α_j between the components. One should also note that there are simplifications also in the "rigorous" models which may not always hold. For example, McGreavy and Tan (1986) found that in some cases the effect of the tray metal heat capacity can be considerable.

2.3 Dynamic simulation

It is generally agreed that the staged models outlined above describe real trayed columns very well. The number of theoretical stages, N , and the parameters for the flow dynamics are often obtained by matching plant data. The numerical solution of the differential equations is relatively straightforward, although computer times may be excessive when there are many stages or components. Concurrent (parallel) computing has also been proposed (Cera, 1989, Skjellum, 1990) as a means to speed up computations. The equations may be stiff and an integration routine for stiff systems is usually recommended. Lagar et al. (1987) discusses the stiffness and gives expressions for estimation the largest eigenvalue, λ_{max} which is important for determining the step size. A typical recent simulation study of a 20 tray C3-C4 splitter is given by Stathaki et al. (1985). This paper illustrates nicely the nonlinearity with asymmetric dynamics, and the very large open-loop time constant, τ_1 , which are observed for high-purity columns. Gani and Cameron (1989) report use of a dynamic simulator to solve difficult steady state distillation columns. In particular, it may be advantageous for difficult problems, for example, azeotropic and reactive distillation.

2.4 Packed versus trayed columns

A packed bed distillation column is most naturally modeled using partial differential equations (PDE's) (eg., Rosenbrock, 1962d). One may also approximate the staged model, eq.1-3, using difference approximations or PDE's, but as noted by Rosenbrock (1962d) the resulting structure of the PDE's is different.

However, most commonly packed columns are modeled using staged models with N estimated from correlations or observations of the the real column. Staged models are used for numerical reasons and because it is difficult to obtain mass transfer data, etc. for a packed column. The approach is further justified since the general agreement is that there is no marked difference in the behavior between packed and trayed columns (eg., Rosenbrock, 1962d). However, there are also opposing views as Edwards and Guilandoust (1986) claim that the difference in the PDE structure

resulting from staged and packed model give different dynamic characteristics. A detailed recent study of dynamic modeling using PDE's is given by Karlström (1991), but he gives no comparison with staged models.

The dynamic behavior of PDE models has been studied by several authors, eg., Marquardt (1986, 1991) and Hwang (1991). They show that one get asymmetric behavior etc. similar to that observed for the staged model. One may also observe "traveling waves" or "fronts" as is discussed for staged models by Gilles and coworkers (eg., Gilles and Retzbach, 1980).

At present there does not seem to be any clear advantages in using PDE models for distillation, and I recommend that staged models be used.

2.4.1 Typical data for liquid flow dynamics for tray and packed columns

Details on the liquid flow dynamics for trayed columns are presented by Rademaker et al. (1975) and Mizsey et al. (1987). There are some differences between packed and trayed columns, mainly related to the liquid holdup. The following discussion is mainly from Skogestad and Morari (1988a). Let the overall liquid holdup be $M_I = NM_i$. A typical value for trayed columns is that M_I is about 5-10% of the total column volume, or that M_i/F is about 0.5 min (this may vary considerably), while the holdup for packed columns is typically smaller by a factor of two or more. This means that the composition column dynamics will be considerably faster for a packed column. This may be a disadvantage from a control point of view since one cannot allow as long measurement delays. Also, the reboiler and condenser dynamics will be more important for packed columns. For both packed and trayed columns the overall liquid lag may be estimated from

$$\theta_L = nM_I/L \quad (12)$$

where typically $n = 0.6$ for packed columns and $n = 0.67f$ for trayed columns. Here f is the fraction of liquid holdup above the weir and thus active for liquid flow dynamics; typically f is about 0.5, but it may be much smaller for small diameter columns. Because of the generally larger value of n , the liquid lag is more important relative to the composition dynamics for packed columns. This is an advantage from a control point of view, since the liquid lag decouples the column response. Also note that for trayed columns $\theta_L = N_T\tau_L$ where N_T is the number of trays and τ_L is typically about 5 seconds. The parameter λ which represents the initial effect of an increase in vapor flow on liquid flow also varies considerably. For most trayed columns λ is positive (eg., vapor pushes liquid off the tray), but it may also be negative (eg., buildup of liquid in downcomer or buildup of liquid on tray if there is no downcomer). For $\lambda > 0.5$ one may observe undesirable inverse response characteristics in level and composition for an increase in boilup

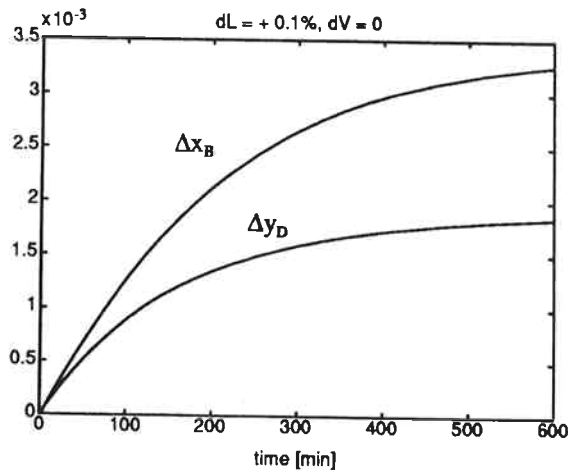


Figure 3: Typical response to a small change in external flows. One can observe the dominant time constant, τ_1 , of about 194 min.

(Rademaker et al., 1975). For packed columns λ is typically close to zero, except at high vapor rates close to flooding where liquid entrainment becomes important and $\lambda < 0$. Patwardhan and Edgar (1991) observed for a packed column that the composition became worse in response to an increase in internal flows, and they attribute this to mass transfer effects.

2.5 Understanding the dynamic composition response

Although simulation of most distillation columns is relatively straightforward, it yields limited insight into understanding the dynamic behavior. The material in this section is mainly based on the paper by Skogestad and Morari (1988a) (denoted SM88 in the following).

2.5.1 Dominant composition response

If we assume constant molar flows (model MC) then one finds that the modes (eigenvalues) for the composition dynamics are independent of the flow dynamics, and thus are equal to those of model C where the flow dynamics are neglected (Levy et al., 1969). In the following we therefore consider model C only. It has been known for a long time that the open-loop composition response is essentially first-order and dominated by one large "inventory" time constant, τ_1 (see Fig.3). τ_1 which may be estimated by assuming that all the stages have the same dominant response and thus behave almost as a single large mixing tank (e.g., Davidson, 1956), and one may obtain good estimates for τ_1 from data of the initial and final steady-state. For small perturbations to the column $\tau_1 = -1/\lambda_{min}$ where λ_{min} is the smallest eigenvalue of the state matrix. Skogestad and Morari (1987a) have derived a simple analytical formula for τ_1 which applies for binary separations and small per-

turbations to the column

$$\tau_1 = \frac{M_I / \ln S + M_D y_D (1 - y_D) + M_B x_B (1 - x_B)}{B x_B (1 - x_B) + D y_D (1 - y_D)} \quad (13)$$

Here $S = \frac{y_D (1 - x_B)}{(1 - y_D) x_B}$ is the separation factor. $\ln S$ is typically about 10 and is relatively constant for a given column (Shinsky, 1984). We therefore see from this expression that the time constant can be very large if *both* products are pure. The reason for the large time constant in this case is that composition inside the column may change considerably even though the compositions at the column ends are nearly constant. One can also explain the observed asymmetric dynamic responses from this expression: the response will be slow when the column approaches a steady-state where both products are pure, and will be fast if one product is non-pure. In some columns there is a pinch region around the feed which stops interactions between the column sections. In this case the column end with the pure product will have a much faster response than given by τ_1 (Weigand et al., 1972). Kapoor et al. (1986) present an alternative explanation for the observed long time constants in terms of positive feedback caused by the recycle (reflux).

2.5.2 Effect of internal flows

One of the main features of high-purity distillation columns is that the steady state behavior is "ill-conditioned" or has strong "directionality" (SM88). In short, it is easy (large gain) to make one product more pure and the other less pure by making changes in the external flows D and B, see Fig.3. On the other hand, it is difficult (low gain) to make both products purer at the same time which corresponds to increasing the internal flows with D/B constant (Rosenbrock, 1962b), see Fig. 4. It is for the changes in external flows one observes the slow time constant, τ_1 , while the internal flows often have a much shorter time constant (SM88, Andersen et al., 1989a), τ_2 , which is close to M_I/F in magnitude (SM88). For columns with relatively low purity the time constant τ_1 and τ_2 may be close in magnitude. The internal flows time constant, τ_2 is very easy to observe from simulations when the liquid flow dynamics are neglected (model C). However, this is of course an unrealistic model, and we see from Fig.4 that the response when the liquid flow dynamics are included is quite different, and the importance of τ_2 is less clear.

2.5.3 Nonlinearity and logarithmic transformations

Another main feature of high-purity distillation columns is the strong nonlinearity stemming from the nonlinear VLE. The resulting asymmetric dynamics were mentioned above, and also the steady-state gains are strongly nonlinear. However, it has been

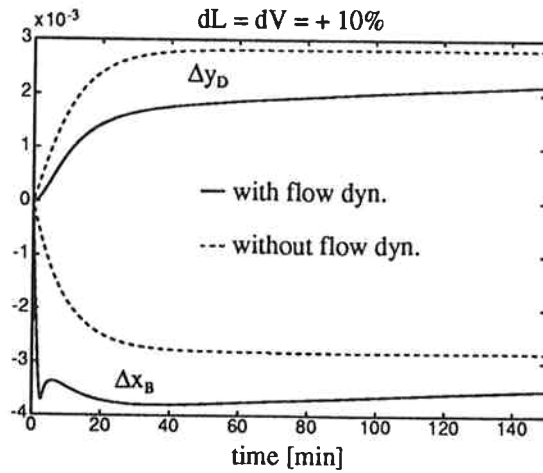


Figure 4: Response to an increase in internal flows (D and B constant). For the case without flow dynamics one can observe the internal flows time constant, τ_2 , of about 15 minutes.

known for sometime that logarithmic compositions make the response of distillation columns more linear (eg., Joseph and Brosilow, 1976, Shinskey, 1977, p. 259). This transformation may also be derived from the model equations as shown by SM88. For example, from (1) the *initial response* to an increase in reflux is given by

$$\frac{dx_i}{dt} = k\Delta L; \quad k = \frac{x_{i+1} - x_i}{M_{Li}} \quad (14)$$

The “gain” k depends strongly on operating conditions. However, since the ratio x_{i+1}/x_i is only weakly dependent on operation conditions in the bottom part of the column (SM88), we may introduce the logarithmic composition and get for the initial response

$$\frac{1}{x_i} \frac{dx_i}{dt} = \frac{d \ln x_i}{dt} = k' \Delta L; \quad k' = \frac{(x_{i+1}/x_i) - 1}{M_{Li}} \quad (15)$$

where k' is almost constant in the bottom part of the column. Similar expressions apply to the top part of the column, and we may introduce the following transformation which linearizes the response for the entire column

$$X_i = \ln \frac{x_{Li}}{x_{Hi}} \quad (16)$$

where subscripts L and H denote light and heavy key component. This transformation also linearize the steady-state response, but to a lesser extent. Note that this transformation in addition to linearizing the dynamic response (X_i as a function of time is nearly independent of operating point), also linearizes the column profile (X_i as a function of stage no. i is nearly a straight line) (Mejdell and Skogestad, 1991a). For binary mixtures and pure products such that $y_D \approx 1$ and $x_B \approx 0$ (16) becomes

$$Y_D = -\ln(1 - y_D); \quad X_B = \ln x_B \quad (17)$$

These transformations are sometimes denoted “relative” or “scaled” compositions. A linearizing transformation in terms of temperatures is derived by

Mejdell and Skogestad (1991a):

$$T_i^{log} = \ln \left(\frac{T_H - T_i}{T_i - T_L} \right) \approx X_i \quad (18)$$

For binary mixtures T_L and T_H represent the boiling points of the pure components or the column end temperatures, and for multicomponent mixtures they represent some reference temperatures in the column.

2.5.4 Effect of flow dynamics on response

The vapor flow lag is usually negligible (eg., McGreevy and Tan, 1986), so this discussion mainly has to do with the liquid flow dynamics. Although the liquid flow dynamics as mentioned above may only weakly affect the dominant composition response, they are crucial for the initial part of the response and, in spite of what is sometimes claimed in the literature (eg., Yang et al., 1990), they should *always* be included in models used for control purposes (Skogestad and Lundström, 1990). Häggblom (1991) also comes to the same conclusion. For example, the flow dynamics decouple the initial response, and the DB-configuration discussed later only works when flow dynamics are included. Also, as shown in Fig.4 the flow dynamics strongly affect the response to changes in internal flows.

2.5.5 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 assumption 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 may be drastically different from those observed from simulations where molar flows are fixed. For example, Fig.5 shows that the responses to a disturbance in Z_F are very different for the case with fixed L [kmol/min] and with fixed L_w [kg/min] = L/M . Here $M = 30y_D + 40(1 - y_D)$ [kg/kmol] is the mole weight of the distillate. The importance of using mass flows when studying real columns seems to have been appreciated only recently (Jacobsen and Skogestad, 1991a). As discussed in Section 5 the use of mass flows may even introduce multiple steady-states and instability for columns with ideal VLE and constant molar flows. In the above example we get instability if the mole weight of light component was reduced to 20 kg/kmol.

2.5.6 Effect of energy balance on response

When we neglect vapor holdup and assume constant molar flows the energy balance reduces to $V_i = V_{i-1}$ and we get model MC. It should be noted that this is an excellent model in many cases, for example, for the methanol-water column of Wood and Berry (1973).

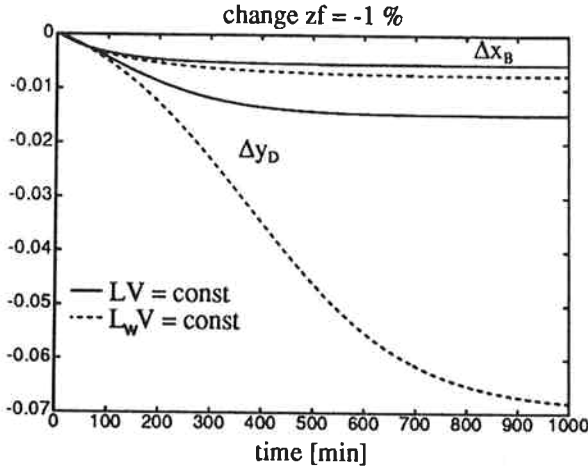


Figure 5: The use of mass flows may strongly affect the open-loop response; here shown for a decrease in feed composition. Solid line: constant L (kmol/min) and V (kmol/min). Dotted line: Constant L_w (kg/min) and V (kmol/min).

The fact that for this column the steady state value of dL_wB/dL_wT with constant boilup is 0.25 rather than 1.0 (Hägglom and Waller, 1988) is therefore because mass flows are used, and not because the assumption of constant molar flows is invalid.

The energy balance must be included when the assumption of constant molar flows does not hold, for example, when the components have different heats of vaporization. In this case the flows affect the compositions through the component material balance, while the compositions affect the flows through the energy balance. The effect of this interaction on the dynamic behavior is still not well understood. Rademaker et al. (1975, p.154-159) claim that the influence is usually negligible. However, this is clearly not correct in all cases as recent results by Jacobsen and Skogestad (1991a) show that even for the relatively ideal methanol-propanol system the effect can be so strong as to give negative values of $(\partial L_B/\partial L_T)_V$ and thus give open loop instability. There is clearly a need for future work towards better understanding the effect of including the energy balance.

2.5.7 Effect of pressure dynamics

The common assumption of constant pressure is often invalid. A number of authors consider the pressure dynamics, and in particular Rademaker et al. (1975) has a detailed discussion. Some work on the interactions between compositions and pressure responses has been done by Kim and McAvoy (1981) for the steady-state and by Shimizu and Matsubara (1984). Wilder and Shah (1989) find that in some cases even small changes in pressure can cause upsets to the column. The open-loop pressure dynamics may be approximated by (note that the overall vapor holdup M_V and pressure p are closely related)

$$\Delta M_V(s) = \frac{k_p}{s + 1/\tau_p} (\Delta V_B - \Delta V_T + \Delta F_V) \quad (19)$$

The initial gain k_p may be significantly less than 1 because an increase in pressure will lead to condensation. The time-constant τ_p may be relatively short if the increase in pressure (and thus in temperature) is counteracted by an increase in cooling or decrease in heating due to self-regulation in the condenser and reboiler. Roffel and Rijnsdorp (1975, p. 176) have derived expressions for k_p for a single tray. Skogestad (1991b) derived expressions for k_p and τ_p by considering the energy balance and the effect of pressure on temperature through the VLE, and found $k=0.12$ and $\tau_p = 1.1 \text{ min}^{-1}$ for a typical column operating at 1 bar where cooling is self-regulated (e.g., using cooling water). However, Choe and Luyben (1987) report success in using (19) with $k=1$ and $1/\tau_p = 0$ as a simple means for tracking the pressure when studying heat-integrated distillation systems. Also note that (19) applies to the initial response and does not include the effect of composition on temperature and thereby on the self regulation in the condenser or reboiler. As reported by Rademaker et al. (1975, p. 162) this effect may yield an inverse response. For example, consider an increase in boilup with reflux constant (LV configuration). This will first increase pressure according to (19). However, the slow composition drift with time constant τ_1 will yield an additional temperature increase and the self-regulation in the condenser may eventually result in a negative pressure change. This may signal a serious control problem, but it is probably rarely occurs in practice because there usually is some composition or temperature control system which keeps the temperatures from drifting away. Davison (1967) noted that if the DV-configuration was used instead of the LV-configuration then no inverse response occurred. The reason is that in this case the increase in boilup, V , corresponds to an increase in internal flows which has much less effect on composition.

Another issue which does not seem to have been carefully studied is how pressure variations affect the composition dynamics through the VLE. For example, an increase in pressure will usually reduce the relative volatility and make separation more difficult. These effects will obviously be most important for difficult separations with relative volatility close to one and for low-pressure columns. Overall, it seems that the pressure dynamics and their effect on the column behavior is not well understood.

2.6 Low-order dynamic models

Low-order models may serve several purposes. Simple models that may be used to obtain analytical expressions are extremely valuable in order to obtain insight into the dynamic behavior. In the previous section, we presented a few such sub-models, for example, for the dominant composition dynamics and

¹For example, Skogestad (1991b) find $\tau_p \approx C_V/UA$ where C_V is the overall heat capacity of the column and UA applies to the self-regulating heat exchanger in question. Hajdu et al. (1978) derive similar formulas for the case with constant top pressure and varying pressure drop.