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Dynamics and control of distillation columns—a critical survey

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Distillation column dynamics and control have 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 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

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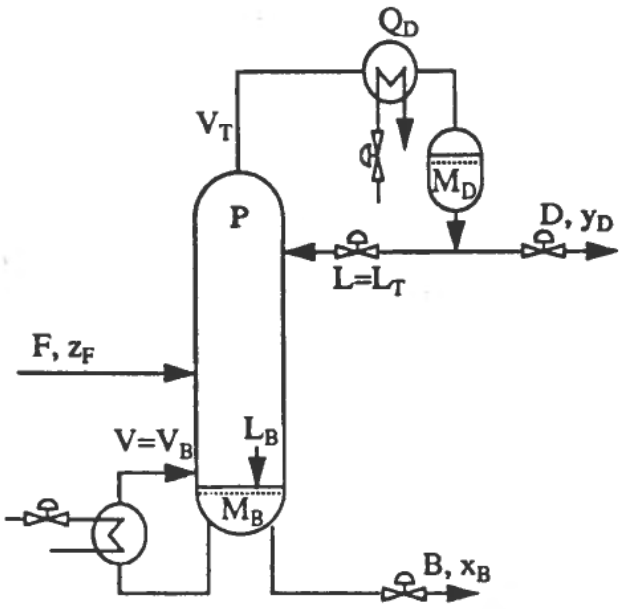

Figure 1. Typical simple distillation column, z_F, y_D and x_B are mole fractions.

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, 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 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. Shinskey (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 Shinskey (1984), but there is a good selection 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 binary high purity column with product compositions $x_B = 1 - y_D = 0{\cdot}01$ (Column A of Skogestad and Morari 1988a). It has $N = 40$ theoretical trays plus a total condenser. Thermodynamic data: Constant molar flows and constant relative volatility $\alpha = 1{\cdot}5$ between the two components. Vapor holdup neglected, constant pressure. Other column data: $z_F = 0{\cdot}5$, $N_F = 21$, $D/F = 0{\cdot}5$, $L/F = 2{\cdot}706$, $V/F = 3{\cdot}206$. Nominal liquid holdups: $M_i/F = 0{\cdot}5$ min on all 41 stages, except for Fig. 8 where condenser holdup $M_D/F = 32{\cdot}1$ min. Liquid flow dynamics: For $i = 2,40$:$\Delta L_i = \Delta M_i/\tau_L$ where $\tau_L = 0{\cdot}063$ min (i.e., $\theta_L = N\tau_L = 2{\cdot}46$ 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 stage differential equations may be formulated for,

(i) component material balances (composition dynamics) for components $j = 1, n_c - 1$

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

where: $N_{ij} = M_{Li}x_{ij} + M_{Vi}y_{ij}$

(ii) overall material balance (flow dynamics)

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

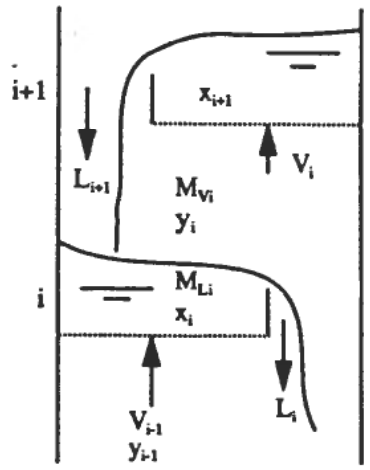

Figure 2. Stage in distillation column.

and

(iii) energy balance

$$\frac{dU_i}{dt} = L_{i+1}h_{L,i+1} + V_{i-1}h_{V,i-1} - L_ih_{Li} - V_ih_{Vi} \tag{3}$$

where: $U_i = M_{Li}u_{Li} + M_{Vi}u_{Li}$

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 $\Sigma_j N_{ij} = M_i$. In addition, there are algebraic relations for the tray hydraulics and pressure drop

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

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. The solution (integration) may proceed as follows:

(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_{Li}, M_{Vi}), phase compositions (x_i, y_i), temperature (T_i), pressure (p_i) and specific energies (h_{Li}, h_{Vi}).
(3) L_i and V_i are computed from the algebraic expressions for tray hydraulics and pressure drop in (4).
(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 computer 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 (e.g., 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_{Li}), 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 $h_{Li} = u_{Li}$.
(3) Compute L_i from the algebraic expression for the tray hydraulics.
(4) Use the energy balance (3) to compute V_i: Since $dU_i/dt = d(M_{Li}h_{Li})/dt$ 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_{Li}/dt numerically using previous time steps (Doukas and Luyben 1978), or
    (*b*) for cases with simple thermodynamic equations by evaluating dh_{Li}/dt analytically using expressions for $(\partial h_{Li}/\partial x_{ij})$, 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 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_{Vi}. 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, $M_{Vi} = 0$, and use the approximation $h_{Li} \approx u_{Li}$ which holds for liquids. The left hand side of the energy balance (3) then becomes

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

Case E1. Neglect changes in energy holdup, $dU_i/dt = 0$. This 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

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

Case E2. Neglect changes in liquid enthalphy. 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

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

The very commonly used 'constant molar flows' or 'equimolal 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

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

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 (e.g., Levy *et al.* 1969), and it may be used to obtain good estimates of the dominant response (see Section 2.3). 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).

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

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).

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

where

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

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 (e.g., 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 asymmetrical 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) (e.g., 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 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 (e.g., 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, e.g., 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 (e.g., 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 by $M_l = NM_i$. A typical value for trayed columns is that M_l is about 5–10% of the total column volume, or that M_l/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, as defined following (11), may be estimated from

$$\theta_L = nM_t/L \tag{12}$$

where typically $n = 0{\cdot}6$ for packed columns and $n = 0{\cdot}67\,f$ 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 (e.g., vapor pushes liquid off the tray), but it may also be negative (e.g., buildup of liquid in downcomer or buildup of liquid on tray if there is no downcomer). For $\lambda > 0{\cdot}5$ one may observe undesirable inverse response characteristics in level and composition for an increase in boilup (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 responses*

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), 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 perturbations to the column

$$\tau_1 = \frac{M_t/\ln S + M_D y_D(1-y_D) + M_B x_B(1-x_B)}{Bx_B(1-x_B) + Dy_D(1-y_D)} \tag{13}$$

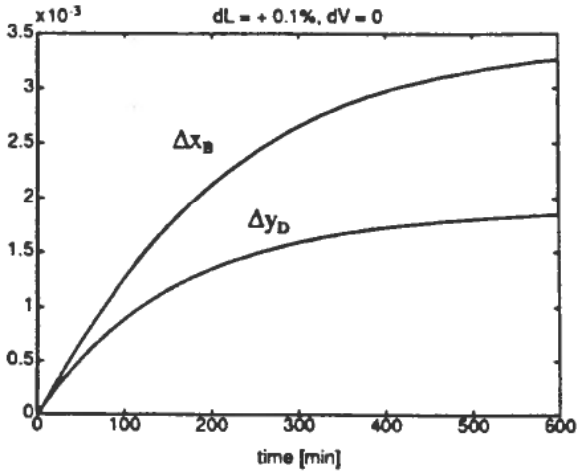

Figure 3. Typical response to a small change in external flows. One can observe the dominant time constant, τ_1, of about 194 min.

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 (Shinskey 1984). We therefore see from this expression that the time constant will 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 that 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_t/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.

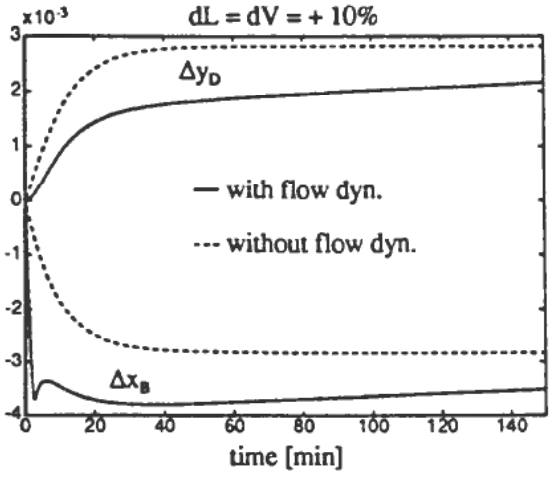

Figure 4. Response to an increase in internal flows (with D and B constant). For the case without flow dynamics one can observe the internal flows time constant, τ_2, of about 15 minutes.

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 known for some time that logarithmic compositions make the response of distillation columns more linear (e.g., 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

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

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

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

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

$$X_i = \ln\frac{x_{Li}}{x_{Hi}} \tag{16}$$

where subscripts L and H denote light and heavy key component. This transformation also linearizes 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 $y_B \approx 1$ and $x_B \approx 0$ (16) becomes

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

These transformations are sometimes denoted 'relative' or 'scaled' compositions. A linearizing transformation in terms of temperatures is derived by Mejdell and Skogestad (1991a):

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

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 (e.g., McGreavy 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 (e.g., 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 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 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] $= L \cdot M$. Here $M = 34{\cdot}3y_D + 40(1 - y_D)$ [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 is reduced from 34·3 to 28·1 kg/kmol.

2.5.6 *Effect of energy balance on response*

When we neglect the 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). (The fact that for this column the steady state value of dL_{wB}/dL_{wT}

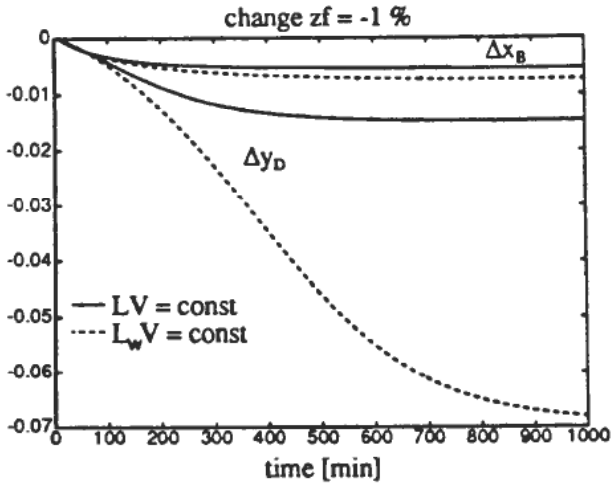

Figure 5. The use of mass flows may strongly affect the open-loop response; here shown for a decrease in feed composition. Solid line: constant L (kmol/min). Dotted line: Constant L_w (kg/min) and V (kmol/min).

with constant boilup is 0·25 rather than 1·0 (Häggblom 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, pp. 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)

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

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 $k_p = 0{\cdot}12$ and $\tau_p = 1{\cdot}1$ 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 $k_p = 1$ 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 probably rarely occurs in practice because there usually is some composition or temperature control system which keeps the temperatures from drifting away. Davidson (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 for the flow dynamics. Here we shall consider low-order models to be used for simulation or controller design.

2.6.1. *Linear low-order models*

One may attempt to combine the sub-models presented in the Section 2.5 in order to describe the overall behavior as suggested by Skogestad and Morari (1988a). However, as noted in Jacobsen (1991) and discussed further in Section 4 on identification, this may lead to fundamental inconsistencies such as two instead of one dominant pole at $-1/\tau_1$, and this may give incorrect responses, for example, when considering one-point control.

Another low-order model which is based on combining sub-models is that of Wahl and Harriot (1970). It was very popular for some time, but its use is *not* recommended. First, it contains the inconsistency noted above. Second, their values for the dominant

[1]For 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.

time constant, τ_1, are generally much too large as they apply to the special case $1 - y_D = x_B$ only (Skogestad and Morari 1987a).

A more realistic simplified linear model is proposed by Kapoor and McAvoy (1987). However, one might argue that this model is too complicated to be helpful for simulation and controller design. Therefore, at present it is suggested that low-order linear models are obtained from linearizing nonlinear model with subsequent model reduction. Jacobsen *et al.* (1991a) obtained very good results using the Hankel model reduction option from the Robust Control Toolbox in MATLAB.

2.6.2. *Nonlinear low-order models*

Compartment models (tray lumping). One simple and intuitive way of deriving a low-order nonlinear model is to lump stages together in compartments. Within each compartment steady-state relationships are used and the stages are assumed to have the same dynamic response. Typically, one gets a reasonable accuracy with three compartments in each column section. Compartmental modeling was recently considered by Benallou *et al.* (1986) who also provide a good review of low-order models in general, and it is also used by Lear *et al.* (1989) and by Levine and Rouchon (1991). Horton *et al.* (1991) propose some modifications in order to avoid incorrect inverse response predictions.

Orthogonal collocation. Another approach to obtain low-order nonlinear models is to start from a PDE model and use orthogonal collocation (Wong and Luss 1980, Cho and Joseph 1984, Stewart *et al.* 1985). This method has been applied recently by a number of authors (Drozdowicz and Martinez 1988, Kim *et al.* 1988, Pinto and Biscaia 1988). The main disadvantage with this approach compared to the compartmental model is that the resulting parameters do not have a physical meaning and cannot be easily adjusted.

Front models. A third possibility is the front or wave approach introduced by Gilles and Retzbach (1980) and used by Marquardt (1986) and Lang and Gilles (1991). However, this method is not as accurate and general, although it may be useful for some separations.

3. 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 columns with no flow dynamics, perfect manipulators (no model error) and no measurement delays. 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. Because of these issues there still are a lot of issues which need to be studied further within the area of distillation control.

There are some misunderstandings 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 slower. A convincing example is shown in Fig. 6. Here we have a disturbance in boilup which is to be counteracted by adjusting the reflux. Doing this is in an open-loop (feedforward) fashion by directly setting the reflux to its desired value yields a rather slow settling, with time constant equal to τ_1, towards the steady-state (solid line), whereas use of feedback (one-point control) yields a much faster response (dotted lines). This rather large difference in composition response is surprising since there is only a minor difference in the reflux flow rate. A similar example, but with two-point control is shown in Fig. 7.

3.1. *Inherent control limitations*

If we consider the linearized column model, $G(s)$, for the entire column or for various configurations, then we usually find that it is minimum phase (no RHP-zeros) and stable (excluding the levels). With the exception of robustness issues (sensitivity to model uncertainty) there are therefore no inherent control limitations, and to get a model which is useful for control studies one should always add time delays (or similar) for the inputs and outputs. The time delay on the inputs may be due to valve dynamics, reboiler dynamics (for V), etc., and those on the outputs due to measurement delays.

There are a few cases where one may get inverse responses (RHP-zeros) in the individual elements. This is undesirable if single-loop control is used. As discussed for the DV-configuration below (Fig. 8), one may find inverse responses in some cases if the levels are not tightly tuned. As discussed earlier one may for $\lambda > 0{\cdot}5$ experience inverse responses in level and in x_B to increase in boilup. For multicomponent mixtures one may experience inverse responses if one controls an intermediate component. This is shown by simulations for a depropanizer by Carling and Wood (1987). The problem is usually avoided by redefining the measurements, for example, by using the ratio between key components (Jacobsen and Skogestad 1991a). Instability may occur in some cases as discussed in Section 5.

A significant feature of distillation columns is the strong interactions caused by the fact that changes in external flows have a large effect on both components (see 2.5.2. *Effect of internal flows*). Furthermore, since the internal flows usually have a much smaller effect on composition, the plant models is usually ill-conditioned, and this may cause fundamental control limitations because of sensitivity to model uncertainty, in particular, to input gain uncertainty. Skogestad and Morari (1987c) considered this and found that plants with large Relative Gain Array (RGA)-elements in the frequency range corresponding to the closed-loop response time are fundamentally difficult to control. High-purity columns with large reflux are generally considered to be the most difficult to control, and indeed we find that the RGA-values of the most commonly used LV-configuration are large for such columns. In addition, when the internal flows (reflux) are large, it is difficult to use D and B for level control because of constraints (e.g., negative flows not allowed), and this presents additional limitations.

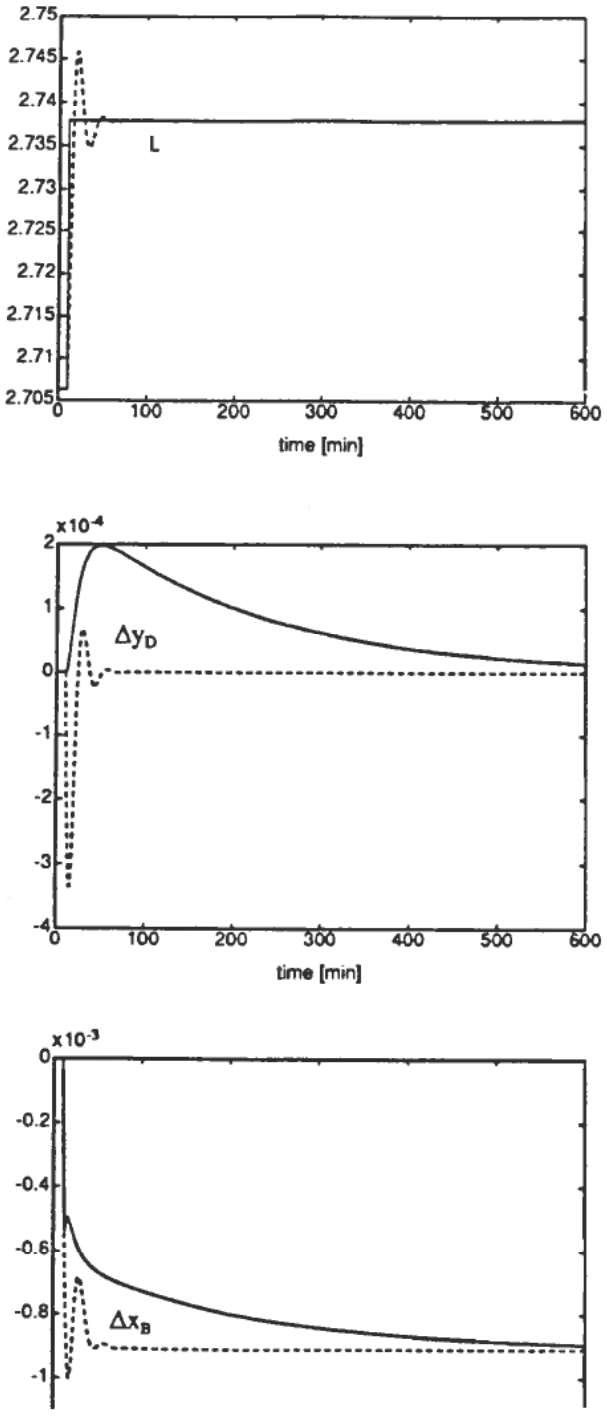

Figure 6. Response to a 1% step increase (disturbance) in V. Solid line ('open loop'): Simultaneous increase in reflux to keep y_D constant at steady-state. Dotted line ('one-point control'): Feedback control using L to keep y_D constant; PI-settings: $k = 0{\cdot}45$, $\tau_I = 3{\cdot}6$ min.

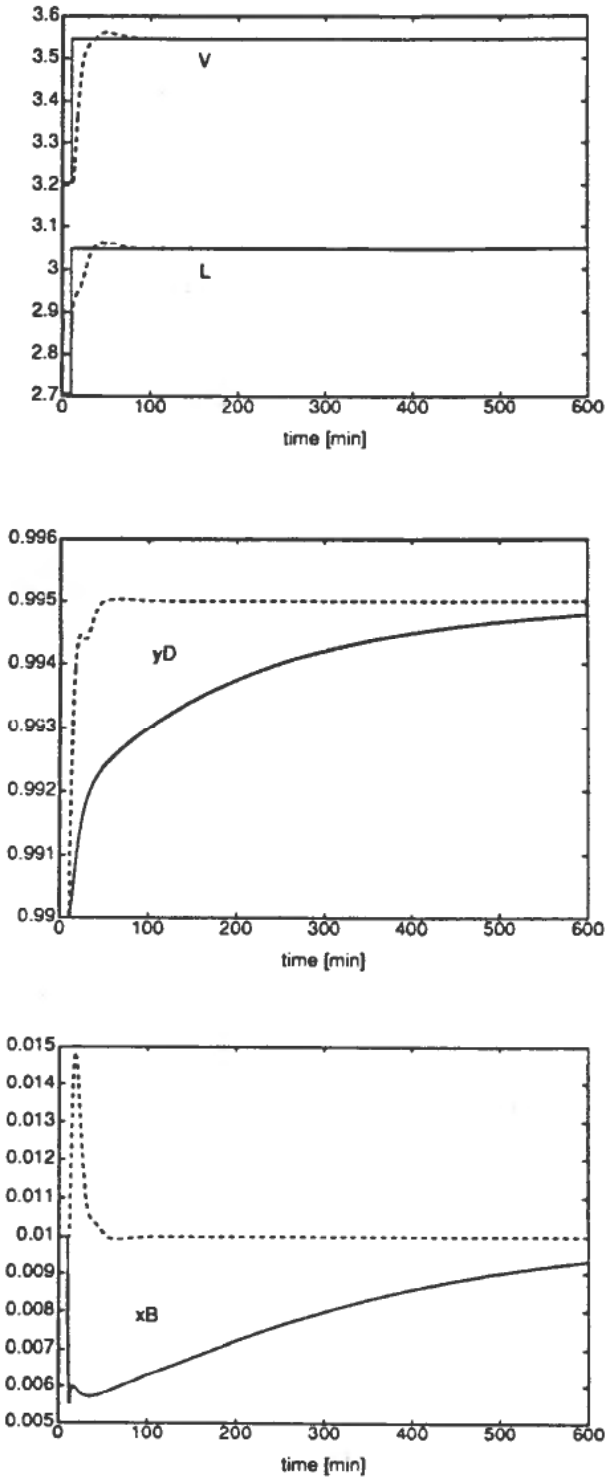

Figure 7. Change in top composition from $y_D = 0{\cdot}99$ to $y_D = 0{\cdot}995$ with x_B constant solid line: Open-loop approach where L and V are increased simultaneously to their new steady-state values. Dotted line: Two-point feedback control using the LV-configuration. PI-settings for $Y_D - L$ and $X_B - V$-loops: $k = 0{\cdot}22$, $\tau_I = 3{\cdot}6$ min.

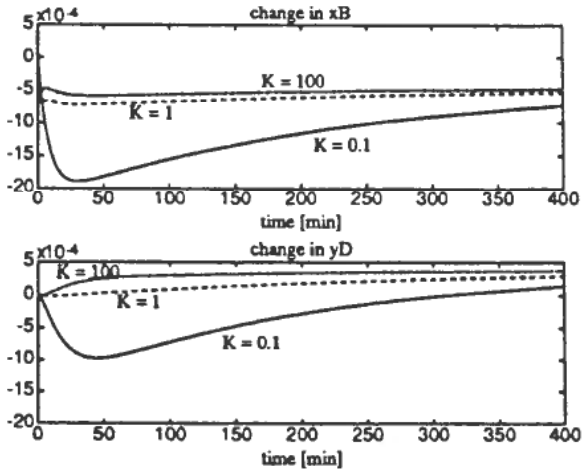

Figure 8. Tuning of the condenser level controller may strongly affect the 'open-loop' response for the DV-configuration. Response is shown for a 1% increase in V. Level controller: $\Delta L = K\Delta M_D$.

3.2. *Control configurations*

Most distillation columns may be treated as 5×5 control problem. We have $dy(s) = G^{5\times5}(s)du(s)$ where typically, the manipulated inputs u and controlled outputs y are

$$u = \begin{pmatrix} L \\ V \\ D \\ B \\ V_T \end{pmatrix}; \; y = \begin{pmatrix} y_D \\ x_B \\ M_D \\ M_B \\ M_V(p) \end{pmatrix} \tag{20}$$

In some cases we may use some other composition indicator, such as temperature, and in most cases V and V_T can only be manipulated indirectly through heating and cooling. In the following we assume that the inventory loops are closed; usually with three single-loop controllers. We assume that pressure is tightly controlled using the condensing rate, V_T, and that the two levels, M_D and M_B, are controlled using some combination of the flows, L, D, B and V. What remains is a 2×2 composition control problem, and the two manipulators left for this correspond to a particular control 'configuration' or 'structure'. It is the inventory control system which determines the configuration, and up to quite recently it was not widely acknowledged how different characteristics the various configurations have, although some authors, notably Shinskey (1967, 1977, 1984) stressed this point.

The standard configurations, as used by Shinskey (1984), include the flows L, D, V, B, and their ratios. Use of these manipulated variables have the advantage of being relatively easy to implement and simple to understand for the operators. Skogestad and Morari (1987d) show that the use of ratios does not have any linearizing effect, but introduces multivariable controllers which may be tuned as single-loop controllers. Usually combinations of L and D are used for the top, and combinations of V and B are used for the bottom.

In some papers on distillation control it may not be obvious what configuration is used. For a given column one can obtain the configuration by identifying the valves

which are either in manual ('flow control' only) or used for control of some composition dependent variable. For example, in industry one often finds columns where heat input is used to control some temperature and with reflux in manual; this corresponds to the LV configuration.

Since L and V are the flows that affect compositions, whereas D and B can only indirectly affect compositions through affecting L and V, it may be at first seem like there is no difference between the control properties of various configurations. The simplest way to realize that there indeed is a difference is to study what happens to flow disturbances. For example, consider an increase in feed vapor flow with the composition loops open. Then for the LV-configuration this will eventually result in an increase in D, for the DV-configuration in an increase in B, for the (L/D V/B)-configuration in an increase in both D and B, and for the DB-configuration it will fill up the column as both D and B remain constant. Obviously, the composition responses are entirely different in these cases. Similar differences apply to changes in the other flows.

3.2.1. *Transformation between configurations*

With the level loops closed one gets a 2×2 model for the remaining control problem. For example, the models for the LV- and DV-configurations may be written

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G^{LV}(s) \begin{pmatrix} dL \\ dV \end{pmatrix}; \quad \begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G^{DV}(s) \begin{pmatrix} dD \\ dV \end{pmatrix} \tag{21}$$

Assuming constant molar flows, immediate vapor response and perfect level control the following transformation holds between these models for the case with flows in molar units (e.g., Skogestad *et al.* 1990c)

$$G^{DV}(s) = M^{DV}(s) G^{LV}(s); \quad M^{DV}(s) = \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \tag{22}$$

Surprisingly, systematic methods for making such transformations have been developed only recently. Independently, Häggblom and Waller (1986, 1988), Skogestad and Morari (1987b) and Takamatsu *et al.* (1987) developed transformations for the steady-state case. Häggblom and Waller (1988) use the most general formulation and allow, for example, flows on a mass basis. Older experimental data are often not consistent with transformations such as (22). For example, this is shown by Häggblom and Waller (1988) for the data of McAvoy and Weischedel (1981). The transformations may be extended in a straightforward manner to the dynamic case (Takamatsu 1987, Skogestad *et al.* 1990c, Yang *et al.* 1990), but care must be taken to include flow and level dynamics which determine the transformation $M(s)$ in (22). The LV-configuration is probably the best choice for a 'base configuration' since the model in this case is almost independent of the level tuning. In addition to the consistency relationship between configurations, there also exists consistency relationships between the gain elements for a given configuration. These may be derived from the component material balance (Häggblom and Waller 1988, Skogestad and Morari 1987c) and for the feed disturbance gains from the invariance with respect to scaling of all flows (Skogestad 1991a). The last relationship may be used to demonstrate some inconsistency for the steady state gains of the widely used Wood and Berry (1973) model.

For someone coming from the outside to the distillation control field, the use of separate models for specific configurations and transformations between these probably seems somewhat unnecessary. After all, one may easily formulate a 5×5 model,

$G^{5\times5}(s)$, for example by linearizing the dynamic model presented in Section 2, and the model for any specific configuration may easily be derived by closing the appropriate level loops (Lee and Park 1991). The justifications for using the separate models for the various configurations is at least twofold:

(1) During identification on real columns the level loops are always closed.
(2) It gives insight into the relative merits of the various configurations.

Nevertheless, it seems fair to state that the issue of transformations has been somewhat over-emphasized in the distillation literature.

3.2.2. *Differences between configurations*

Disturbance rejection. As already mentioned there is a large difference with respect to the *open-loop* disturbance sensitivity (here 'open loop' refers to the case with the inventory loops closed, but with the composition loops open). The difference may be analyzed rigorously, for example, by plotting the open-loop disturbance gains, e.g., $(\partial y_D/\partial z_F)_{L,V}$ for the LV-configuration, as a function of frequency (e.g., Skogestad *et al.* 1990c). Alternatively, since the initial response is of primary interest for feedback control, it is simpler to consider the frequency where these gains cross 1 in magnitude, which is identical to the sensitivity parameter K_w/T_w used by Waller *et al.* (1988a) and Sandelin *et al.* (1991b). Since the composition are mainly affected by changes in external flows, an even simpler, but less accurate approach is to consider the sensitivity of D/F to flow disturbances (see Table 3 of Skogestad *et al.* 1990c). The latter method yields useful insight and shows that the (L/D V/B)-configuration is a good choice, in particular, if the reflux is large.

All the above measures are related to the self-regulating properties when no feedback is used. However, these measures may not correlate well with the disturbance rejection properties when using feedback control, because they do not take into account how the disturbance direction is aligned with the plant. Skogestad and Hovd (1990) introduced the frequency-dependent Closed-loop disturbance-gain (CLDG) as an improved measure for the case of *two-point control.*

For *one-point control* it is important that the uncontrolled product is not too sensitive to disturbances. Luyben and coworkers (Luyben 1975, Muhrer *et al.* 1990) use steady-state 'rating curves' which show how the flows must be adjusted to keep the compositions constant. It is recommended that flows which need only small adjustments should be kept in manual when using one point control. Skogestad *et al.* (1990c) consider the steady-state gains, for example, for one-point control of the bottom it may be acceptable to have L in manual if $(\partial y_D/\partial z_F)_{L,x_B}$ is small. Based on results for some typical columns they conclude that the LV-configuration seems to be good choice for one-point control. Waller and coworkers (Waller *et al.* 1988, Sandelin *et al.* 1991b) found that also the one-point control properties correlated well with their open-loop disturbance parameter, K_w/T_w. However, this does not always hold, for example, the LV-configuration is quite sensitive to disturbances in boilup when no control is used, but rather insensitive with one-point control (Skogestad *et al.* 1990c).

Interactions and the RGA. Other important differences between configurations are related to interactions when using single-loop controllers (Shinskey 1984) and sensitivity to input gain uncertainty when using decouplers for two-point control (Skogestad and Morari 1987d). For both these items large values of the relative gain

array (RGA), in the frequency range corresponding to the closed-loop response time, signal serious problems. The RGA is easily computed from the gain matrix G for a given configuration. The diagonal RGA-elements are given by

$$\lambda(G) = 1/\left(1 - \frac{g_{12}g_{21}}{g_{11}g_{22}}\right) \tag{23}$$

which may also be used to compute the RGA as a function of frequency. For the LV-configuration Skogestad and Morari (1987b) derive the following approximation at *steady state*:

$$\lambda(G^{LV}) \approx \frac{(2/N)L(L+1)}{Bx_B + D(1-y_D)} \tag{24}$$

(here all flows are scaled with respect to F). $\lambda(G^{LV})$ is large for high-purity columns with large reflux. On the other hand, for the DV-configuration the RGA-elements are always small. We have steady-state (Shinskey 1967)

$$\lambda(G^{DV}) \approx 1/\left(1 + \frac{D(1-y_D)}{Bx_B}\right) \tag{25}$$

which is close to one for columns with a pure bottom product and close to zero for a column with a pure top product. The RGA for the (L/D)(V/B)-configuration is reduced relative to the LV-configuration when the internal flows are large since (Skogestad and Morari 1987b)

$$\lambda(G^{(L/D)(V/B)}) \approx \lambda(G^{LV})/\left(1 + \frac{L}{D} + \frac{V}{B}\right) \tag{26}$$

Convenient worksheets for estimating the steady-state RGA for other configuration are given by Shinskey (1984). Some fundamental steady-state RGA relationships are presented by Häggblom and Waller (1988) and Häggblom (1988). Estimates of the frequency-dependent RGA, including the frequency where the magnitude approaches one, are given by Skogestad *et al.* (1990c).

3.2.3. *Selection of configuration*

There is probably no single configuration which is suitable for all columns. This was noted already by Boyd (1946) who states: 'It would be impossible to give a control system that would be a panacea for all fractionation control problems'. Because of the large number of possible control configurations for a given column, there is clearly a need for tools which may assist the engineer in selecting the best control configurations. Luyben (1979, 1989) emphasizes the large diversity of columns, processes and plants, and seems to doubt that a simple tool may be found. This is partly supported by a recent paper by Birky *et al.* (1989). They compared the rules of Page Buckley and Greg Shinskey, who both are well-known industrial experts on distillation column control, on a set of example columns and found that they agreed in only 3 out of 18 cases. There may be a number of reasons for these differences, but the most important one is probably that Buckley considers mostly level control and one-point composition control, whereas Shinskey also addresses two-point control.

In spite of these differences, it is clear that Shinskey's (1984) worksheets for computing the steady-state RGA for various configurations present a step forward towards a systematic procedure. His rule is to choose a configuration with a diagonal steady-state RGA-value in the range from about 0·9 to 4 (Shinskey 1984). However,

the steady-state RGA contains no information about disturbances and dynamic behavior, both of which are crucial for evaluating control performance. The fact that this measure has proved to be so useful for distillation columns is because it for most configurations correlates well the RGA-behavior at higher frequencies (Skogestad *et al.* 1990c) and because it also correlates with the open-loop disturbance sensitivity (Skogestad 1988). Thus the steady-state RGA-tables of Shinskey (1984) may be useful as a screening tool, but they should be used with care. Other papers which discuss control configuration selection are McCune and Gallier (1973), Waller (1986), Skogestad *et al.* (1987d, 1990c) and Waller (1992). The L/D V/B-configuration seems to be a good overall choice, but it has the disadvantage of being somewhat difficult to implement.

3.2.4. *The DB-configuration*

One counterexample which demonstrates that the steady state RGA is generally *not* reliable is the DB-configuration. This control scheme has previously been labeled 'impossible' by most distillation experts (e.g., Perry and Chilton 1973, p. 22.123, McCune and Gallier 1973, Shinskey 1984, p. 154, Skogestad and Morari 1987d, Takamatsu *et al.* 1987, Häggblom and Waller 1988) because it seems to violate the steady-state material balance and because the RGA is infinite at steady state. Yet, Finco *et al.* (1989) have shown both with simulation and with actual implementation that the scheme is indeed workable. Skogestad *et al.* (1990b) found that the DB-configuration works because of the liquid flow dynamics. They show how to derive a model from the LV-configuration, and derived RGA-values as a function of frequency. They found that the RGA-value for the DB-configuration comes down to a value of one (no two-ways interaction) at a much lower frequency than for the LV-configuration, in particular, for columns with two pure products. For such columns the internal flows are often very large, and this also favors the DB-configuration since level control using L and V is preferable in this case. The main disadvantage with the DB-configuration is that it works only when both composition loops are closed.

3.2.5. *The LV-configuration*

This is the most common configuration in industry. Its main advantage is that the manipulated inputs directly affect composition, and that it is almost independent of level tuning. It also usually performs well for one-point control. For high-purity columns the model is strongly interactive with large RGA-values, at least at low frequencies. The large RGA-values imply that one cannot use decoupling (inverse-based) controllers (Skogestad and Morari 1987c, 1988b). The physical reason is that a decoupling controller wants to make large changes in the L and V (the internal flows) without affecting D and B (the external flows). This is practically impossible using L and V as manipulators since the exact input values are never exactly known. Skogestad and Lundström (1990) found that PID control may yield good performance with closed-loop time constant less than 10 minutes provided the measurement delay is not too large (less than 1–2 min). Performance deteriorates drastically if the loops for some reason are detuned, because interactions are much stronger at lower frequencies. To avoid measurement delay one may use a temperature measurement and cascade this with a composition measurement (e.g., Luyben 1973), or alternatively, estimate the composition using multiple temperaures (e.g., Mejdell and Skogestad 1991b). Andersen et al. (1988) present a comparison of various PI controller tunings, including use of the BLT-method of Luyben (1986).

The LV-configuration is probably the best choice in many cases because it is simple. However, if fast control is not possible, or if there are very strong interactions, or if the internal flows are large such that level control using D or B becomes difficult, then one should consider other configurations.

3.2.6. *The importance of inventory (level) control*

Whereas the behavior of the LV-configuration is almost independent of the tuning of the level loops, it makes a large difference for other configurations. Generally, the responses are significantly worse when level control is slow. For example, for the DV-configuration with condenser level not tightly controlled a step change in V (internal flows) may result in an inverse response for y_D (Yang *et al.* 1990, Lee and Park 1991) and a serious overshoot for x_B ('almost inverse response', Shinskey 1984, p. 157) which cannot be counteracted by a PID controller. The reason is that the slow level dynamics cause the increase in V to initially act as a change in external flows (it acts as an increase in D which is stored in the condenser). This is illustrated in Fig. 8 for three values of the level gain K. These effects limit the allowable closed-loop time constant.

To avoid the dependency of the level control tunings on the choice of configuration one may let the condenser level control set the sum $L + D$, and the reboiler level controller set $V + B$. This may also improve the dynamic responsiveness in some cases. For example, for the DV-configuration, a change in D will then directly affect L, and the level controller will only act as a correction (Shinskey 1984, p. 128 calls this a feedforward scheme).

Often we do not want to have tight level control, for example, to avoid abrupt changes in the products rates D and B. However, the key issue is not that level control is perfect, but that the response in internal flows, L and V, are similar to those for the case with perfect level control. For example, consider the L/D-manipulator. If the level control is slow a change in boilup V will not yield an immediate change in L and we may get inverse responses similar to those discussed for the DV-configuration above. One way to avoid this problem is to note that with perfect level control $L/D = L/(V_T - L)$ so specifying L/V_T is equivalent to specifying L/D. However, from a dynamic point of view L/V_T is preferred because it avoids the dependency of the level tuning. One problem here is that V_T is usually difficult to measure, but it may be estimated from the level measurement, e.g., one may let the output from the level controller be V_T (Shinskey 1984, pp. 160–161). This is the scheme proposed by Ryskamp (1980) although he used a flooded accumulator so that the column-pressure controller was used to set V_T. Another way to avoid the dependency on level control tuning is to move the accumulator and use it as a storage tank for the product stream D.

3.2.7. *Use of decouplers*

Decoupling. The possible use of decouplers, $G^{-1}(s)$, to counteract interactions for a given configuration has been discussed extensively in the distillation literature (e.g., Luyben 1970), and it was found that in some cases the results were very sensitive to decoupler errors (e.g., Weischedel and McAvoy 1980). Skogestad and Morari (1987c) found that decouplers should never be used when the model has large RGA-elements compared to one. First, as just noted, the response is very sensitive to element uncertainty (decoupler errors). Second, and more importantly, the response is very sensitive to small errors in the input gains, and such errors can never be avoided. Thus, using a more exact, or even nonlinear decoupler as indicated by Alsop and Edgar (1990)

will not help. Consequently, decouplers should never be used for high-purity columns using the LV-configuration, whereas they may be helpful for the DV-configuration where the RGA-values are always small. Unilateral (one-way) decouplers (Shinskey 1981) may be used even for cases with large RGA-values (Skogestad and Morari 1987c).

Physical input and output compensators. We here consider for a given control configuration the use of simple transformations (combinations) of the input and output variables. These may form the basis for a robust multivariable controller[2]. Waller and Finnerman (1987) present a survey of various output compensators, for example, taking sums and differences of compositions or temperatures. Bequette and Edgar (1988) show for the DV configuration that this idea and several other schemes proposed is equivalent to a SVD output compensator. A SVD compensator, which is based on well-conditioned input and output compensators plus two single-loop controllers, may be a good scheme in many cases. From physical considerations it is known that the strong direction (largest singular value) of the column corresponds to changing the external flows, $D - B$, which mostly affects the average composition, $y_D + x_B$, while the weak direction corresponds to changing the internal flows, $L + V$, which mostly affects the difference in composition, $y_D - x_B$ (e.g., Skogestad and Morari 1988a). Thus, for all configurations the SVD compensator will approximately yield $y_D + x_B$ and $y_D - x_B$ as inputs to the single-loop controllers and $D - B$ and $L + V$ as controller outputs[3]. The latter is very similar to using D and V, and thus the DV-scheme (and similarly, the LB-scheme) is 'naturally' decoupled at the plant input (Skogestad *et al.* 1988). For columns with different purities in the two column ends, the proper output directions are not quite 'sums' and 'differences' of compositions (Häggblom and Waller 1988), and one should instead use logarithmic compositions, i.e., use $Y_D + X_B$ and $Y_D - X_B$ where $Y_D = -ln(1 - y_D)$ and $X_B = lnx_B$ (this follows by combining the results by Häggblom and Waller (1988) with the estimate (25) of the RGA for the DV-configuration). The arguments above have a strong intuitive appeal and may be understood by operators, but they apply mainly the steady-state. Further research is needed to test these ideas.

3.2.8. *Feedforward control*

Feedforward control has the possible advantage of allowing for fast control action without introducing stability problems. In distillation columns it is common to use simple ratio feedforward schemes without dynamics, e.g., use L/F to adjust for disturbances in F. However, this method gives a dynamic imbalance because of the level and flow dynamics, and this may produce rather large changes in composition because

[2]The input combinations we are referring to here may be used as part of the *composition* controller for a given control configuration. They should not be confused with the transformations between various control configuration, such as (22), which are actually due to changes in the *level control system.* For example, use of L/D as a composition manipulator means that a change in condenser level, through the action of the level controller, will yield a change in *both* L and D, but such that their ratio is constant. The use of control configurations with low interaction is sometimes denoted "implicit" decoupling (Ryskamp 1982), but in this subsection we consider "explicit" decoupling.

[3]Exact decoupling with the SVD controller is obtained if the ratio between the two controller gains is equal to the ratio of the gains in the strong and weak direction of the plant (which is the plant condition number). However, for configurations with large RGA values this will be very sensitive to small input gain errors and should not be used in practice.

high-purity distillation columns are so sensitive to small imbalances. This is illustrated by Fig. 6 which compares 'perfect' (at least at steady-state) feedforward control (solid line) with one-point feedback control (dotted line). The use of dynamic compensation in the feedforward loop (Shinskey 1984) would hardly help in this example, and in practice the pure feedforward response would be much worse because of additional errors caused by measurement errors and controller gain errors. This does not mean that feedforward control should not be used, but it must in most cases be combined with feedback control.

3.2.9. *Non-standard configurations*

The only combination of flows used by the standard configurations is ratios. From a linear point of view the composition manipulator $u = L/D$ corresponds to $du = c_1 dL + c_2 dD$ with $c_1 = 1/D$ and $c_2 = -L/D^2$. Häggblom and Waller (1990) generalize this by allowing arbitrary linear combinations of all flows.

$$du = c_1 dL + c_2 dD + c_3 dV + c_4 dB \tag{27}$$

They use these additional degrees of freedom, combined with the transformations by Häggblom and Waller (1988), to specify that the open-loop model at steady state has

(1) perfect open-loop disturbance rejection and
(2) decoupled response from the new manipualators to the outputs (DRD configuration).

The physical reason for how one may obtain open-loop disturbance rejection is that one may use the information from the level measurement to estimate the disturbances (Waller 1988). Since there are only two level measurements, one can only estimate two disturbances, and the DRD structure can give perfect disturbance rejection only for two disturbances. Note that the conventional configurations also yield perfect disturbance rejection for some disturbances, for example, the LV-configuration for disturbances in D and B, and the DB-configuration for disturbances in L and V. Häggblom and Waller (1990) consider disturbances in F and z_F for their DRD-scheme. However, in many cases, at least for mixtures with similar components and thus similar molecular weights, it will be difficult to detect changes in z_F using level measurement, and one may get close to singularity in the transformations leading to the DRD-configuration. Also, as discussed by Häggblom and Waller, the disturbance rejection will not be perfect in practice because of dynamic interactions and sensitivity to parameter variations. Since the transformations leading to the decoupled response is an 'implicit decoupling' due to the level control system (see footnote 2), it may avoid the strong sensitivity to input gain uncertainty that one often finds when using decouplers as part of the composition controller. However, this needs to be investigated further. The physical reasoning behind the DRD-structure of extracting information from the level measurements is clever. However, it yields a rather complex multivariable controller, and may thus not satisfy the main idea behind using simple control configurations which is to make the controller simple to understand and tune.

A related non-standard configuration which uses only combinations of L and D as the top manipulator (e.g., $du = k_1 dL + k_2 dD$), and only combinations of V and B in the bottom, is presented by Yang *et al.* (1991). The parameters, such as k_1 and k_2, are adjusted to minimize open-loop disturbance sensitivity and interactions in terms of the RGA. They found that their results were strongly influenced by the tuning of the level controllers.

3.2.10. *Experimental results on control configurations*

There has been numerous industrial reports on the success of various control configurations. However, the only detailed experimental *comparisons* have been published by Waller and coworkers (Waller *et al.* 1988a, Sandelin *et al.* 1991b) using a pilot-scale column separating ethanol-water and using mass flows as inputs. Their results confirm the theoretical calculations, and show that the ratio configurations may perform well. However, care should be taken to generalize these results based on experiments from one specific column. Their experimental results indicate that the static DRD structure may work well for one-point control.

3.3. *Control papers using distillation as a* 2×2 *example*

Most 'distillation control' papers start from a given control method, and use distillation as a convenient example. Very few papers start from a given column, and compare various control methods in order to get the best performance. Most papers consider the 2×2 composition control problem and use the LV-configuration.

Single-loop control. Distillation columns provide a nice example of a strongly interactive system, and a number of papers use distillation columns as an example for interaction analysis and design of single-loop controllers. Balchen (1990) presents a frequency-domain method for designing single-loop controllers for 2×2 interacting plants with application to distillation control.

Robust control. High-purity distillation columns are always ill conditioned and may therefore be sensitive to modeling errors. Skogestad *et al.* (1988) use a very simplified distillation model to study this for the LV- and DV-configuration. They used the structured singular value to study robust performance, and found that input gain uncertainty should always be included. Skogestad and Morari (1988b) and Skogestad and Lundström (1990) extend the results using more realistic column models. Arkun (1988) and Scali *et al.* (1987) also apply structured singular value analysis. McDonald *et al.* (1988) attempt to treat nonlinearity as model uncertainty, but this is generally very conservative, and it did not work very well. Sandelin *et al.* (1991a) consider a multimodel approach to design robust controllers.

Multivariable control. Kümmel and Andersen (1987) use geometric control with additional feedback from two internal stages (states) and achieve improved performance compared to PI control with the same robustness. Lang and Gilles (1989) compared several design approaches on a pilot plant coupled distillation column and found that H_∞-controllers worked well when provision was made for input saturation. Model predictive control has also been used on the composition control problem. McDonald and McAvoy (1987) and Georgiou *et al.* (1988) present simulation studies using DMC with the LV configuration. Patwardhan and Edgar (1991) describe the experimental application of nonlinear model predictive control with online estimation for a packed bed distillation column.

Nonlinear control. There are a few papers on nonlinear control, e.g., Alsop and Edgar (1990) who use global input/output linearization for the DV configuration, and Castro *et al.* (1990) and Levine and Rouchon (1991) who use nonlinear geometric control. However, none of these include a robustness analysis (e.g., with respect to input gain

errors), and none include comparisons with simpler methods, such as linear controllers combined with the logarithmic transformations in (17) and (18). Logarithmic transformations are used by Shinskey (1977, 1984) (he calls it adaptable gain) and both Skogestad and Morari (1988b) and Georgiou *et al.* (1988) found in simulation studies that they work well.

Adaptive control. Dahlqvist (1981) obtained good results using adaptive control on a pilot plant distillation column with the LV-configuration. Similar studies have been performed by Rhiel and Krahl (1988), Kim *et al.* (1989), and Woinet *et al.* (1991).

3.4. *Optimizing, supervisory and constraint control*

This is usually at a level above the control scheme discussed above, for example, the DMC-controller by Tran and Cutler (1989) adjusts the setpoint for a tray temperature. Constrained control is discussed by Maarleveld and Rijnsdorp (1970). Lear *et al.* (1989) consider optimizing control using single loops. Industrial applications of Dynamic Matrix Control (DMC) are presented by Hokanson *et al.* (1989) for the combined level and composition control in the top part of demethanizer column, and by Tran and Cutler (1989) for supervisory control of benzene and toluene towers.

3.5. *Control of the column as a 5×5 problem*

No papers have been found which deal with this issue. Even though such controllers probably rarely will be used, it is interesting from a theoretical point of view to find what performance can be achieved (Skogestad 1989). Since constraints are important for distillation columns, model predictive control (MPC) seem to be a good alternative. However, there are two problems:

(1) To find appropriate weights that give a reasonable solution for the two fundamentally different problems of inventory and quality control,
(2) To achieve robustness.

Preliminary results with a MPC-controller with no robustness considerations included (Lundström and Skogestad 1991) yields a controller similar to a LV-configuration with a decoupler, which we know is a poor controller for this process. The present work of Lundström is aimed at first finding a *robust* 5×5 MPC controller with satisfactory performance. The problem here is that the standard MPC formulation does not allow model uncertainty to be included explicitly. The idea is then to combine this robust linear controller with the constraint formulation.

3.6. *Inferring compositions*

Product composition measurements are often expensive, unreliable and with delays. The most popular means of product control is therefore to control a temperature (e.g., Kister 1990). However, there are several problems with this approach.

(1) The location of the temperature measurement is discussed by Tolliver and McCune (1980), Yu and Luyben (1987) and Moore *et al.* (1987). To make the measurement sensitive it is usually located at a tray at some distance away from the column ends (e.g., Shinskey 1984), and it may not correlate very well with the product composition. To solve this one may use a fast temperature loop cascaded with an analyzer (e.g., Luyben 1973, Kister 1990).

(2) However, the most sensitive temperature location may move. To avoid this problem Luyben (1971) suggested to use a weighted average of many temperatures. Johnson (1984) implemented this on a deethanizer, a demethanizer and a C2-splitter and Whitehead and Parnis (1987) on a C2-splitter. Bozenhardt (1988), Marquardt (1988) and Wozny *et al.* (1989) suggest various methods for locating the temperature front using multiple measurements.
(3) The relationship between product composition and tray temperature also depends on feed composition, z_F, and Rovaglio *et al.* (1990b) use a measurement of z_F to adjust the setpoint for the tray temperature (this may be viewed as a feedforward scheme or as a simple estimator).
(4) Fast setpoint changes in compositions are difficult to make.

An alternative procedure which may solve all of the above problems is to use a composition estimator based on all available measurements. Several approaches have been suggested, e.g., the inferential estimator of Brosilow and coworkers (Joseph and Brosilow 1978), but this estimator is very sensitive to model errors for high-purity columns. Mejdell and Skogestad (1991ab) found both from simulations and implementation of high-purity example columns that very good results could be obtained by directly regressing compositions and temperatures. They used a linear static partial-least-squares (PLS) regression estimator, $y_D = y_D^o + \Sigma_i k_i T_i$, which provides a robust way of obtaining the parameters k_i. The estimator may also provide pressure compensation. Another important advantage with this approach is that measurement delays are almost eliminated, and they found that the estimator may actually provide a lead compared to the true composition which may improve feedback performance compared to using exact measurements. Logarithmic transformations on compositions and temperatures were used to reduce the effect of nonlinearity. Typically, about five temperature measurements evenly spaced along the column are needed. They found that flow measurements did not improve the estimate, but filtered feed composition measurements may probably help.

3.7. *Interactions between process design and control*

The control characteristics are affected by the design. The difference between trayed and packed columns have already been discussed. Jacobsen and Skogestad (1991c) have considered various design modifications for high-purity columns. They found the most effective to be to add more trays to the column. This yields a pinch region in the middle of the column which decouples the response and reduces the interaction. They also found that the active use of a feed preheater to control an intermediate tray temperature had a similar effect. Lewin (1991) presents similar ideas and suggests the active use of the feed rate and feed preheat temperature.

4. Identification

For control purposes it is often desirable to obtain a model directly from observations. Consider obtaining a model for the LV-configuration

$$\begin{pmatrix} dy_D \\ dx_B \end{pmatrix} = G^{LV}(s) \begin{pmatrix} dL \\ dV \end{pmatrix} \tag{28}$$

It has been common to identify models for $G^{LV}(s)$ by fitting the observed response using simple models, e.g. first-order-plus-deadtime, for the individual transfer function

elements, $g_{ij}^{LV}(s)$. At least for high-purity columns this is often a poor approach, and three problems are outlined below.

Problem 1. It is difficult to observe the low-gain direction (Skogestad and Morari 1988a, Andersen *et al.* 1989a), and for high-purity columns with large RGA-values one may easily get the wrong sign of RGA (and the determinant) of the steady-state gain matrix. The model will then be useless for feedback control purposes. This may be corrected by performing separate experiments for changes in internal flows (e.g., by using the DV-configuration as suggested by Skogestad 1988, Alsop and Edgar 1990, Andersen and Kümmel 1991, Kuong and McGregor 1991), or by adjusting the steady-state gains to match an estimated steady-state RGA-value as suggested by Jacobsen *et al.* (1991a), or by using a 'perturbed model' (Kapoor *et al.* 1986) based on steady-state where the RGA-elements are smaller. The basis for the two last suggestions is that the steady-state behavior is not of primary importance, but rather the initial response.

Problem 2. One may get a poor model of the initial response, and in particular of the decoupling that should result from the liquid flow dynamics. Again, as suggested by Jacobsen *et al.* (1991a) one may avoid this problem by carefully correcting the model.

Problem 3. A fundamental problem, that does not seem easy to correct, is discussed by Jacobsen (1991). The full column model, at least for high-purity distillation, contains a one single 'slow' pole (mode) located at $-1/\tau_1$, but since this mode dominates all the open-loop responses it will appear in all the identified elements, $g_{ij}^{LV}(s)$. Thus, the overall model $G^{LV}(s)$ will contain at least two slow poles, and this will result in an inconsistent model that is generally poor for feedback control (Jacobsen 1991): The inconsistency is often most clear when studying partial (one-point) feedback control. The feedback will affect the single slow mode of the column, and also the uncontrolled output should have a fast response (see Fig. 6). However, when an inconsistent model with two slow poles is used (e.g., Wahl and Harriot 1970, Skogestad *et al.* 1990a, Sandelin *et al.* 1991a) one gets an incorrect slow settling in the uncontrolled output, as may be observed from their figures.

The above discussion shows that fitting the individual elements will most likely fail, at least for high-purity columns. One must therefore look for a multivariable model structure that explicitly takes into account the physical couplings in the column. One example is the simple model, N2, introduced by Skogestad and Morari (1988a) that models the column explicity in terms of the external and internal flows and has a realization with only one slow pole. However, this model does not include the flow dynamics which are crucial for feedback control studies, and attempting to add these on in a simple fashion (model F2) gives incorrectly two slow poles. Also, it is difficult to include disturbances in a consistent fashion to model N2 (Jacobsen 1991).

At present, there does not seem to be any good low-order model structure for distillation columns, at least not for high-purity columns, and this is clearly an important issue for future research. The preferred approach at present therefore seems to be to fit parameters (typically, N, and θ_L and λ for the flow dynamics) to a nonlinear column model and linearize this to obtain a model for control purposes.

5. Complex dynamic behavior for simple columns with ideal thermodynamics

The consensus within the distillation community has been that distillation columns respond in a sluggish manner much like a large mixing tank, and that there, with the exception of nonideal multicomponent mixtures, does not exist any complex dynamic behavior. For example, McAvoy and Wang (1986) state in their review paper: 'Doherty and Perkins point out that multiple steady states can only arise when one has more than two components and more than a single stage'. Actually, for someone entering the distillation field, this would probably seem quite surprising because of the often large number of coupled nonlinear differential equations. Indeed, the recent results of Jacobsen and Skogestad (1991a, 1992) show that complex behavior such as open-loop instability, limit cycles and multiple steady states may occur even for simple columns separating ideal binary mixtures with constant relative volatility, and it is likely that new complex phenomena will be discovered for distillation columns in the future. Jacobsen and Skogestad have identified two possible sources for the instability and multiplicity:

(1) Multiplicity with mass or volumetric flows as independent variables instead of molar flows as is usually assumed (see Section 2.5.4).
(2) Multiplicity with molar flows as independent variables for systems where the constant molar flows assumption is invalid and the energy balance must be included.

By combining these sources they have found cases where for a fixed mass reflux and molar boilup there exists five coexisting multiple steady-states. The paper of Doherty and Perkins (1982) referred to above is correct, but it does not consider these two cases. In both these cases one may get the surprising result that increasing reflux makes separation worse in the top part of the column.

It is difficult to predict the practical impact of this on the operation of distillation columns. Most columns have a sluggish response that almost resembles that of a pure integrator, and in most cases it is probably not too important whether the response actually is stable or not. However, in some columns it may be significant as reported in the control study of Jacobsen and Skogestad (1991b). Also, there has always been reports both from industry and from pilot-scale columns of 'strange behavior'. Usually this has been attributed to some measurement problem or poor level control, but it may be possible that some of these observations may be explained by these new results on instability and multiple steady states. Jacobsen and Skogestad (1991a) found that the instability may be avoided by switching from the LV-configuration to the DV-configuration. However, if the level loops are not tightly tuned the instability may appear as limit cycles for the DV-configuration (Jacobsen and Skogestad 1992).

6. Dynamics and control for more complex cases

The word complex here refers to

(1) mixtures with complex (nonideal) thermodynamics and possible reactions, and
(2) complex column configurations (arrangements).

Although significant new results have been obtained over the last ten years, these areas give almost unlimited possibilities for future research. A general introduction to the possible complex behavior of azeotropic distillation, reactive distillation and interlinked columns is found in the general review papers on nonlinear analysis by Seider *et al.* (1990, 1991).

Homogeneous azeotropic distillation. In azeotropic extractive distillation an extra component (entrainer) is added to the column in order to split the azeotrope. In the homogeneous case we have only one liquid phase. Andersen *et al.* (1991) present some interesting new results for the dynamic behavior of such columns. For example, they found regions of operation where it is almost impossible to operate because of serious inverse responses. Jacobsen *et al.* (1991b) review the literature on control of azeotropic distillation. Some recent references are Abu-Eishah and Luyben (1985), Retzbach (1986), Andersen (1986) and Bozenhardt (1988). Jacobsen *et al.* discuss the possibility of operating in the economic optimal region close to minimum entrainer feed which usually is avoided in industry. They find that it is possible to operate in this region by use of feedback control if the measurements are sufficiently fast and if the entrainer feed is carefully adjusted. Bloch *et al.* (1991) present a simulation study for a benzene extraction plant and used tray lumping to reduce the order of the model.

Heterogeneous azeotropic distillation. For the case with potential liquid/liquid phase split the existence of multiple steady states and instabilities have been reported. Magnussen *et al.* (1979) found multiple steady states for the nonideal mixture of water-ethanol-benzene. Their results have been studied and reproduced in several other papers (e.g., Prokopakis and Seader 1983, Kovach and Seider 1987). Rovaglio and Doherty (1990) found complex dynamic behavior due to the multiple steady states, and Rovaglio *et al.* (1991) indicate that chaotic responses may be obtained when feedback is applied to the entrainer makeup. Wong *et al.* (1991) found that the formation and disappearance of the second liquid phase was critical to the dynamic behavior. Multiplicity for other heterogeneous systems have also been reported (e.g., Widagdo *et al.* 1989).

Reactive distillation. A recent paper on the dynamic modeling and simulation of reactive distillation with references to previous works is by Alejski (1991). Alejski presents a model which includes mixing on the plates and also refers to previous work on liquid flow patterns on trays in ordinary distillation. There does not yet seem to be any reports on complex behavior for reactive distillation, but this is clearly an area where almost anything is possible in terms of complexity.

Periodic distillation. Toftegård and Jørgensen (1987, 1988) present a review of periodic cycled operation, and derive a dynamic model. A periodic scheme for a horizontal distillation system is presented by Baron and Barbe (1987).

Double-effect (dual pressure) distillation. Control and dynamics of such columns are studied by Al-Elg and Palazoglu (1989) but no flow dynamics are included, and an industrial study is presented by Morrison and Laflamme (1990). Mandler *et al.* (1989) present a dynamic model for a double-pressure air separation column with an Argon side column.

Heat pump columns. Identification and control of an experimental column with vapor recompression (heat pump) is studied by Jørgensen and coworkers (Nielsen *et al.* 1988ab, Rasmussen *et al.* 1990, Hallager *et al.* 1990). In a simulation study Muhrer *et al.* (1990) find that the control problem is similar to that of a conventional column, except that the compressor is used as a heat source. Naka and O'Shima (1986) consider in a simulation study a side cooler with heat pump.

Secondary reflux and vaporization (SRV). This is studied by Shimizu and Mah (1983) and Shimizu *et al.* (1985).

Complex column configurations. Chavez *et al.* (1986) and Lin *et al.* (1987) have found multiplicity for interlinked columns with ideal thermodynamics, and dynamic responses are presented by Rovaglio *et al.* (1990a). A number of references on control of complex column configurations are given by Ding and Luyben (1990). Heat-integrated distillation is studied by Chiang and Luyben (1985), Elaahi and Luyben (1985) and Chiang and Luyben (1988). Columns with prefractionators and sidestreams are considered by Doukas and Luyben (1981) and Alitiqi and Luyben (1986). Sidestream distillation is studied by Papastathopoulou and Luyben (1991).

Crude oil distillation and fractionators. Sourander and Gros (1986) present an on-line optimizing strategy in a refiner. Shakouri (1986) consider the viscosity control of a high-vacuum distillation unit. Grosdidier and Kennedy (1990) use model predictive control to regulate two temperatures in the bottom of a fractionator. Industrial applications of control of crude distillation are given by Hoffman *et al.* (1988) and Muske *et al.* (1991). Hsie and McAvoy (1991) present a comparison of SISO and QDMC control for a crude column. The 'Shell Control Problem' (Prett and Morari 1987) provides a control problem formulation and a simple experimental model of a heavy-oil fractionator, and has been studied by numerous authors, especially as a case for model predictive control.

7. Needs for future work

The dynamic behavior for columns with varying pressure, non-constant molar flows (energy balance is needed) or non-ideal thermodynamics is not well understood. The same applies to interlinked column configurations and to the possible difference between trayed and packed columns. In terms of control there is a need for simple model structures which can be used for identification, and the possible improvements and problems of considering the control problem as a multivariable 5×5 problem are not well understood.

APPENDIX 1

Derivation of constant molar flows assumption

This derivation is included because no rigorous derivation of this common assumption was found in the recent literature (A rather complicated and different derivation where pressure variations are allowed is given by Roffel and Rijnsdorp 1982, and an interesting discussion is found in King 1971). Assume:

(1) Reference state for energy is pure components as saturated liquids at a given reference pressure;
(2) The column pressure is constant and equal to the reference pressure;
(3) Negligible heat of mixing such that $h_{Li} = \Sigma_j x_{ij} c_{PLj}(T_i - T_{bpj})$ where T_{bpj} is the boiling point of pure component j at the reference pressure;
(4) All components have the same value of the liquid molar heat capacity c_{PLj};
(5) The tray temperature T_i is the average of the component boiling points, $T_i = \Sigma_j x_i T_{bpj}$.

These assumptions give $h_{Li} = 0$ and thus $dh_{Li}/dt = 0$ on all stages.

The constant molar flow case is derived by assuming in addition that

(6) the vapor phase is ideal and all components have the same heat of vaporization, $h_j^{vap} = h^{vap}$, where h_j^{vap} is the heat of vaporization of pure component j at the column pressure. Then $h_{Vi} = h^{vap} + \Sigma_j x_{ij} c_{PVj}(T_i - T_{bpj})$;

(7) c_{PVj} is equal for all components such that the last term is zero (as for the liquid).

Then we have on all stages $h_{Vi} = h^{vap}$, and the energy balance yields $V_i = V_{i-1}$.

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