Dynamics and Control of Unstable Distillation Columns

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Abstract

The paper adresses dynamics and control of distillation columns which are operated at an open-loop unstable operating point. The fact that industrially operated distillation columns may be naturally unstable - even when the level and pressure loops are closed - has only recently been recognized. The main reason why this has been overlooked is that almost all work published in the field of distillation control has assumed the inputs (eg. reflux L and boilup V) to be on a molar rate basis. Several authors have claimed, using models of different complexity, that in this case the responses will always be stable. However, in real columns the inputs are usually not on a molar basis, but rather on a mass or volume basis. It is shown that the transformation from mass or volume inputs to molar inputs may be singular. The results are independent of thermodynamic complexity, and applies also to homogenous ideal distillation with constant molar flows. The singularity in this transformation implies that the column will have multiple steady-states, one of which will be unstable. In the paper we discuss the implications of unstable operating points with respect to distillation dynamics and control. It is shown that instability may be avoided by changing the control configuration. However, as we show, the instability will in most cases not cause any problems with regards to control. This is due to the fact that the unstable right half plane pole usually will be close to the imaginary axis ("goes slowly unstable"), thereby not affecting the high frequency behavior of the response which is most important for control. Results are also presented showing that previous results on distillation control design based on molar inputs in most cases will be valid for columns with other input units. This is true even for unstable operating points.

The paper includes an example showing that also models with molar inputs may exhibit multiple steady states and unstable solutions when the energy balance is included.

1 Introduction

Almost all work published on dynamics and control of distillation columns assumes the inputs, eg. reflux and boilup, to be given on a molar basis. The main reason for this is probably that it is the size of the molar flows that enters directly into the material balances in distillation, and thereby determines the separation. However, as discussed by Jacobsen and Skogestad (1990) in a recent paper, real columns will only in rare cases have molar rate measurements for all the manipulated flows. The measurements will rather be on a mass or volume basis. As shown in the paper by Jacobsen and Skogestad the transformation from mass or volume flows to molar flows may become singular, leading to multiple steady-state solutions for a given set of inputs. They also find that one of the solutions will be unstable, but do not provide rigorous evidence for this. Their results apply to ideal as well as non-ideal systems.

The multiplicity and instability found for columns with mass or volume inputs is in contradiction to what has been published previously for column models with molar inputs. Rosenbrock (1962, 1963) showed that for the case of ideal binary distillation with constant molar flows the solutions will always be unique. Doherty and Perkins (1982) studied models of different complexity and concluded that multiplicity and instability is impossible for any multistage homogenous binary separation. They did not include the energy balance in their study. Shridar and Lucia (1989) included the energy balance and found that binary homogenous distillation columns with molar inputs will exhibit unique and stable solutions also in this case. They did however only study a limited set of specifications (LB and $Q_D Q_B$). In this paper we include an example showing that multiplicity and instability also may exist for the case of molar inputs. The multiplicity is found for specifications of reflux and boilup, and is caused by the energy balance and not by vapor-liquid equilibrium.

The previous paper by Jacobsen and Skogestad (1990) treats the multiplicity only from a steady state point of view. In this paper we study the dynamics of columns with mass or volume inputs, and consider the implications for distillation control. The last point is of outmost interest since all previous work published on distillation control have assumed uniqueness and open-loop stability of the operating points. The most important question to be answered is whether the control design methods developed on the basis of molar inputs are valid for real columns which may have open-loop unstable operating points due to mass or volume inputs.

We start the paper by giving a brief summary of the previous results on steady state multiplicity for distillation columns with mass or volume inputs. The dynamics of these columns is then studied and we provide evidence for the instability found for one of the solutions. We then treat the control problem to see if any fundamental new control problems are introduced by the multiplicity and instability. At the end of the paper we give an example showing that steady state multiplicty and instability may be found also for the case of molar inputs when the energy balance is included. This will be of importance in simulations where specifications often are done on a molar basis, but will also influence the behavior of real columns as the molar flows determines separation.

In the following we will limit ourselves to discuss only one set of specifications (configuration), namely the case where mass reflux and molar boilup (corresponds to heat input, Q_B, for the case of constant molar flows) are used as independent variables. This is the most common configuration used on industrial distillation columns (ref. ..). Jacobsen and Skogestad (1990) found multiplicity also for several other configurations, but they concluded that multiplicity was most likely for the case we discuss in this paper.

All results presented are for ideal systems with constant molar overflows. The only exception will be the example of multiplicity for molar specifications where the energy balance is included.

2 Steady State Multiplicity

We give here a brief review of the results presented in Jacobsen and Skogestad (1990).

Consider the two-product distillation column in Fig.1. If the feed to the column is given there are at least four flows that may be specified: reflux L, boilup V, distillate D and bottoms flow B. However, for a given column there are only two degrees of freedom at steady state, that is, only two of these flows may be specified independently. In the following we will denote a specific choice of independent variables as a "configuration". This word comes from process control where these are the two independent variables from a control point of view. Doherty and Perkins (1982) have shown that for the case of ideal binary distillation with constant molar overflow the steady state solution found for any set of molar specifications will be unique and asymptotically stable, eg. the top composition $y_D = g(L, V)$ is a unique and stable function of L and V.

However, as Jacobsen and Skogestad (1990) argue, in real columns one will only in rare cases be able to specify the flows on a molar basis. For instance, fixing the valve position in a pipe will normally correspond closely to fixing the volumetric flow-rate. For gases the ratio between volumetric rate and molar rate is usually only weakly dependent on composition, but for liquids the ratio between volume and molar rate is strongly dependent on the composition. In this case one would need continous composition measurements in order to determine the molar flow from the volume flow. If flow measurements are available these will usually be on a mass- or volume basis, and only in rare cases on a molar basis.

Jacobsen and Skogestad (1990) give a simulation example of steady state multiplicity in a column separating a mixture of ethanol and butanol. The column has mass reflux and molar boilup as independent variables. We will refer to this as the L_wV-configuration. Data for the column is given in Table 1. The simulation results are given in Table 2, and the multiplicity is graphically illustrated in Figure 2. The existence of solutions with negative slope between mass and molar reflux was confirmed experimentally on a pilot scale column.

The reason for the multiplicity is found in the transformation between the actual flow-rates (mass) and the molar flow-rates which determines separation. Assume that the boilup is kept constant on a molar basis, and that the reflux is given on a mass basis, ie. L_wV-configuration. The transformation between mass reflux, L_w, and molar reflux, L, is given by

$$L = L_w/M; M = y_D M_1 + (1 - y_D) M_2 \tag{1}$$

Here M_i denotes the mole weight of the individual components. One might expect the molar reflux to increase monotonically with the mass reflux, that is $(\delta L/\delta L_w)_V > 0$. However, because M is a function of composition, y_D, and thereby of L_w, this might not be the case. Assuming molar boilup V fixed and differentiating $L_w = LM$ on both sides with respect to L yields

$$\left(\frac{\delta L_w}{\delta L}\right)_V = M + L(M_1 - M_2)\left(\frac{\delta y_D}{\delta L}\right)_V \tag{2}$$

If $M_1 < M_2$, ie. most volatile component has the smallest mole weight (ideal case), the second term on the right hand side of Eq. (2) will be negative and the total differential may take either sign. The transformation will be singular when

$$M_1 y_D + M_2(1 - y_D) - L(M_2 - M_1)\left(\frac{\delta y_D}{\delta L}\right)_V = 0 \tag{3}$$

The singular point corresponds to a pitchfork bifurcation point, ie. one eigenvalue crosses the imaginary axis and the number of solutions changes from one to three. Jacobsen and Skogestad (1990) found that the solutions with a negative slope between L and L_w corresponds to unstable operating points, but did not provide rigorous proof of this. However, for pitchfork bifurcations the intermediate solution (branch II in Fig.2) will in most cases be unstable. In this paper we give evidence for the observed instability.

Jacobsen and Skogestad (1990) show that for ideal cases the probability of a negative slope in eq. (1) is increased when internal flows (ie. L and V) are increased. They find that for the L_wV- configuration one may divide column operation into three possible regions:

1. Internal flows low. No multiplicity, no instability.
2. Internal flows intermediate. Multiple steady states, one of which is unstable. In this case there will usually be three solutions, but there may also exist columns with only two solutions. The third "solution" would then correspond to a solution with one product flow being negative.
3. Internal flows high. No multiplicity, all operating points unstable.

Jacobsen and Skogestad also studied the D_wV-configuration, ie. mass distillate and molar boilup used as independent variables. They found that for singularity to be possible for this configuration one had to require that $M_1 > M_2$, ie. the most volatile component must have the largest mole weight. As this is the opposite requirement as compared to the L_wV- configuration it is possible to avoid multiplicity and instability by changing configuration. However, as we shall see later this will usually not be necessary as the unstable operating point may easily be stabilized by use of feedback control.

For further details on the steady state multiplicity we refer to the previous paper.

3 Dynamics

Fig.3 shows the maximum eigenvalue in different operating points for the ethanol-butanol column. From the figure we observe that the eigenvalues at branch I and III are negative, implying stability, while those at branch II are positive, implying instability. The open-loop instability is illustrated by the simulations in Fig.4. which shows the open-loop response in top composition y_D to an infinitesimal change in mass reflux L_w at operating point 3. The simulations indicate that the two stable solutions 2 and 4 have equally large area of attraction seen from the unstable solution. From Fig.3 we also observe that the eigenvalues at the singular points are zero, which is not surprising since these corresponds to bifurcation points. The purpose of this section is to give evidence for the observed instability at branch II and to compare the dynamics of columns with mass or volume inputs with the dynamics found in models with molar inputs. We start by explaining the observed instability, and then consider the effect of mass inputs on the overall dynamics.

3.1 Stability

One-stage Column. Consider the simple column in Fig.5 with one theoretical stage (the reboiler) and a total condenser. Of course, such a column will never be operated in practice because the reflux is simply wasting energy and has no effect on separation. However, we start by analyzing this column due to the simplicity of the dynamic model. As Jacobsen and Skogestad (1990) show, even such a simple column with ideal thermodynamics may have multiple steady state solutions and unstable operating points.

Assume binary separation, liquid feed, constant holdup in the reboiler (M_L) and negligible holdup in the condenser. The dynamic model of the column becomes:

$$M_L \frac{dx_B}{dt} = Fz_F - Dy_D - Bx_B \tag{4}$$

With L and V as independent variables we get

$$M_L \frac{dx_B}{dt} = F(z_F - x_B) + L(y_D - xB) + V(xB - yD) \tag{5}$$

Linearization, Laplace transformation and introducing deviation variables assuming F, z_F and V constant yields

$$sM_L \Delta x_B(s) = -D\Delta y_D(s) - B\Delta x_B(s) + (y_D - x_B)\Delta L(s) \tag{6}$$

Assuming constant relative volatility α we get the following relation between $\Delta y_D(s)$ and $\Delta x_B(s)$

$$\frac{\Delta y_D(s)}{\Delta x_B(s)} = K = \frac{\alpha}{(1 + (\alpha - 1)x_B)^2} \tag{7}$$

Equation 6 then becomes

$$\Delta x_B(s) = \frac{y_D - x_B}{M_L s + a} \Delta L(s) \tag{8}$$

where

$$a = KD + B \tag{9}$$

As all the elements in Eq.9 are positive the pole will always be negative, implying that an operating point always will be stable when reflux and boilup are given on a molar basis.

Now consider mass reflux L_w as an input instead of molar reflux L:

$$L = \frac{L_w}{M} \tag{10}$$

where M is as defined previously. By linearizing Eq.10 we obtain:

$$\Delta L = \frac{1}{M}\Delta L_w + L\frac{M_2 - M_1}{M}K\Delta x_B \tag{11}$$

Substituting Eq. 11 into Eq. 8 we obtain the following transfer-function between liquid composition, $\Delta x_B(s)$, and mass reflux $\Delta L_w(s)$:

$$\Delta x_B(s) = \frac{y_D - x_B}{M_L s + a_w}\frac{\Delta L_w(s)}{M} \tag{12}$$

where

$$a_w = KD + B - (y_D - x_B)LK\frac{M_2 - M_1}{M} \tag{13}$$

We see that if the last term on the right hand side of Eq.13 becomes dominating the operating point will be unstable. This may be shown to be equivalent to having a negative slope in Eq.2, and we conclude that for the single stage column we will have instability whenever there is a negative slope between molar and mass reflux.

When boilup V is kept constant the molar reflux L may be varied between $L_{min} = V - F$ (for the case of $B = 0$) and L_{max}=V (for D=0). The behavior of the pole as reflux is varied may be divided into three different cases depending on the size of the internal flows (L and V):

1. Internal flows low: In this case the pole starts in the left half plane for L_{min} and moves toward the imaginary axis as L is increased, but does never cross it. This implies that we have no singular points (uniqueness) and only stable operating points.
2. Internal flows intermediate: At L_{min} the pole is in the left half plane and moves towards the imaginary axis as L is increased. At a certain value of L the pole crosses the imaginary axis and we get instability. However, as L increases further K will decrease and the contribution from B in Eq.13 will dominate causing the pole to move back to the left half plane as L approaches L_{max}. In this case we get three solutions, one of which is unstable.
3. Internal flows high: At L_{min} the pole is already in the right half plane since the last term in Eq. 13 is dominating. As L is increased the pole will go further out in the right half plane. At a certain value of L it will turn as K decreases, but it never crosses the imaginary axis, implying that we have no singular points (uniqueness) and only unstable operating points. The "missing" branches in this case will correspond to nonphysical values of D negative (missing upper branch) and B negative (missing lower branch).

The three different regions of operation is illustrated in Fig.6.

Multistage Columns The high order of the dynamic model of a multistage distillation column makes it difficult to do an analysis similar to the one for the single-stage column. However, in spite of the high model order, it is well known that the overall composition dynamics in distillation columns may be well approximated by a first order response (eg. Moczek et.al. (1963), Skogestad and Morari (1988)). This implies that we may approximate the transferfunction from molar reflux to top composition with

$$\left(\frac{\delta y_D}{\delta L}\right)_V (s) = \frac{g_{11}}{1+\tau_1 s} \tag{14}$$

where g_{11} ($= \left(\frac{\delta y_D}{\delta L}\right)_V$ in Eq.2) is the steady state gain and τ_1 is the dominant time-constant. In order to study the stability problem consider a step change in L_w while the boilup V is kept constant on a molar basis. Dynamically the effect of changing L_w may be divided into three effects: 1) Changing L_w immediately changes L since y_D is unchanged. The gain is given by

$$\left(\frac{\delta L}{\delta L_w}\right)_V = y_D^* M_1 + (1-y_D^*)M_2 \tag{15}$$

where y_D^* is the initial value of the top composition. 2) Due to the change in molar reflux L, the top composition y_D will start to change. The dynamics is given by Eq.14 3) While mass reflux L_w is kept constant the molar reflux L will undergo new changes due to the change in the top composition. This gain is given by

$$\left(\frac{\delta L}{\delta y_D}\right)_{Lw} = \frac{L_w(M_2-M_1)}{[y_D M_1 + (1-y_D)M_2]^2} \tag{16}$$

The total effect may be considered in a feedback manner. This is illustrated by the blockdiagram in Fig.7. If we consider the transfer-function from dL_w to dy_D we get (note that we have positive feedback):

$$\left(\frac{dy_D}{dL_w}\right)_V = \frac{\left(\frac{\delta L}{\delta L_w}\right)_{y_D}\left(\frac{\delta y_D}{\delta L}\right)_V}{1-\left(\frac{\delta L}{\delta y_D}\right)_{Lw}\left(\frac{\delta y_D}{\delta L}\right)_V} \tag{17}$$

Inserting the expressions for the gains and simplifying yields

$$\left(\frac{dy_D}{dL_w}\right)_V = \frac{g_{11}(M_1 y_D + (1-y_D)M_2)}{1+\tau_1 s - \frac{g_{11}L(M_2-M_1)}{y_D M_1 + (1-y_D)M_2}} \tag{18}$$

The pole of the system becomes

$$\lambda_{max} = -\frac{1}{\tau_1}\left(1 - \frac{g_{11}L(M_2-M_1)}{y_D M_1 + (1-y_D)M_2}\right) \tag{19}$$

The pole will be in the right half plane when

$$\frac{g_{11}L(M_2-M_1)}{y_D M_1 + (1-y_D)M_2} > 1 \tag{20}$$

This is exactly the same criterion as Jacobsen and Skogestad (1990) found for a negative slope between mass and molar reflux. Thus, a necessary and sufficient condition for instability due to change in units is

$$\left(\frac{\delta L}{\delta L_w}\right)_V < 0 \tag{21}$$

In other words, branch I and III will always be stable and branch II unstable provided the column is stable on a molar basis. This result is in accordance with numerical results and also with what one would expect for a pitchfork bifurcation.

Eq.19 gives an approximate way of calculating the dominating pole for the L_wV-configuration from data computed for molar inputs. The expression gives a correct value of zero λ_{max} at the singular points. From Eq.19 we also see that we get qualitatively the same behavior of the pole when L is varied in a multistage column as discussed for the single stage column above. This means that also in the multistage case we may experience the three different regions of operation illustrated in Fig.6.

In the general case with more complex thermodynamics, Eq.14 may be replaced by

$$\left(\frac{\delta y_D}{\delta L}\right)_V (s) = \frac{g_{11}(1 + b_1 s + b_2 s^2 + ... + b_{n-1}s^{n-1})}{1 + a_1 s + a_2 s^2 + ... + a_n s^n} \tag{22}$$

and we may use Routh-Hurwitz stability criterion (all coefficients in the pole polynomial should have the same sign) to conclude that Eq.21 is a sufficient condition for instability.

3.2 Overall Dynamics

The analysis above shows that the dominant pole, and thereby the <u>l</u>ow frequency dynamics, is heavily influenced by the transformation between mass and molar flows. The multiplicity and instability is caused by this pole crossing the imaginary axis. However, it is not clear what the effect on the <u>h</u>igh frequency dynamics will be. For feedback control the high- frequency behavior is of more interest than the low-frequency behavior

Skogestad and Morari (1988) have studied the dynamics of several ideal two-product distillation columns assuming molar inputs. We will use one of these columns (column A) to study the effect on the overall dynamics of introducing mass-reflux. Data for the column is given in Table 1. The nominal operating point have reflux $L = 2.706$ kmol/min and boilup $V = 3.206$ kmol/min. We assume a mole weight ratio $M_2/M_1 = 5.0$. This makes the nominal operating point open-loop unstable when operated with the L_wV-configuration, and the rhp pole will be $\lambda_{max} = 0.042$. In order to compare the dynamics we consider the frequency dependent gains between the inputs, ie. L and V respectively L_w and V, and the outputs, ie. top and bottom composition.

$$\begin{pmatrix} dy_d \\ dx_B \end{pmatrix} = \begin{pmatrix} g_{11}(s) & g_{12}(s) \\ g_{21}(s) & g_{22}(s) \end{pmatrix} \begin{pmatrix} du_1 \\ dV \end{pmatrix}, du_1 = dL \ or \ du_1 = dL_w \tag{23}$$

The full dynamic model used here includes 2 states on each tray, ie. liquid holdup and composition. For the column studied this implies a total of 82 states. Figure 10 shows the amplitude and phase as a function of frequency for the four transfer-functions using the LV- and L_wV-configurations. The transfer functions were found by linearizing the full models around the nominal operating point. In order to compare the two responses we have scaled the gains from L_w by M. The frequency plots in Fig.10 show that the low-frequency behavior of the two configurations differs significantly. From the phase plots it is clear that the column with L_wV-configuration is open-loop unstable. Note that the phases for the molar boilup gains are shifted with 180 degrees due to the negative effect on compositions. The large difference at low frequencies is as expected since we know that the dominant pole is strongly affected by the transformation between molar and mass flows. However, the plots also show that the high-frequency behavior is similar in the two cases. In other words, the open-loop initial response is similar for the two configurations. This is not really surprising as the main difference between the two configurations depends on the slow composition dynamics. Initially we will only have a scaling between the two configurations.

From this we conclude that while the low-frequency dynamics are strongly affected by the transformation between mass and molar flows, the high-frequency dynamics is only slightly affected. This will be true in most cases where the composition dynamics are slow compared to other effects. In cases where the composition dynamics are relatively fast, for instance in columns with small liquid holdups, the conclusions may be different.

4 Feedback Control

4.1 Stabilization.

As seen from the above analysis, columns operating with mass or volume inputs may be unstable and will require feedback control (in addition to level and pressure control) for stabilization. From control theory it is well known that right half plane poles in itself does not put limitations on the achieveable performance. Problems only arise if there are right half plane zeros at frequencies comparable to the right half plane pole ("The system goes unstable before we are able to observe what is happening") or if there are constraints ("we can not counteract the instability"). In distillation right half plane zeros are only rarely observed and the main control limitations are deadtimes in measurements and actuators. The bandwith, ω_B, is limited by the deadtime, θ_d

$$\omega_B \approx< \frac{1}{\theta_d} \tag{24}$$

In order to stabilize the rhp pole, λ_{max} we must require a certain bandwidth

$$\omega_B \approx> \lambda_{max} \tag{25}$$

From this we may conclude that it will be difficult to stabilize an open-loop unstable column if

$$\lambda_{max} \approx> \frac{1}{\theta_d} \tag{26}$$

The right half plane pole in distillation columns with mass or volume inputs will usually be close to the origin (goes slowly unstable). In our previous example $\lambda_{max} = 0.042 min^{-1}$ and we would require $\theta_d \approx< 24min$. Typically composition measurement delays in industrial columns may be up to 30 min. (GC-analysis). In this case one could cascade the composition measurements with temperature measurements, and thereby avoid the problem.

Good control of distillation columns requires two-point control, ie. feedback control of both product compositions. However, in order to stabilize an open-loop unstable column one-point control will suffice. This is also the way most industrial columns are operated. An unstable column operating with the L_wV-configuration may be stabilized by controlling the top or bottom composition, or any other variable related to composition, eg. a temperature inside the column. The rhp pole will be common for all transfer-functions involving composition dependent variables. If the open-loop dynamics is approximated by

$$\frac{dyj}{dui} = \frac{g_{ij}}{s-a} \tag{27}$$

where a is an unstable pole, one may stabilize the plant by a pure proportional controller with gain

$$K > \frac{a}{g_{ij}} \tag{28}$$

Simulations Nonlinear simulations of the ethanol-butanol column are shown in Fig.8 . The simulation shows a setpoint-change in top composition from operating point 2 (see Table 2), which is open-loop stable, to operating point 3 which is open-loop unstable and then further on to operating point 4 which is open-loop stable. The mass-reflux L_w was used to control the top composition y_D by use of a constant PI-controller while molar boilup V was kept constant. The controller parameters are given Table 3. Logarithmic measurements was used in the controller as this reduces the non-linearity between the operating points. A measurement delay of 1 min. was used in the simulations. As expected there are no problems of stabilizing operating point 3 where the right half plane pole, $\lambda_{max} = 0.116$. The simulations also show that the same controller may be used in these three very different operating points. The fact that these operating points have the same inputs is illustrated by the plots of the mass reflux L_w which shows a zero steady state change. The reason why the same controller may be used in both the unstable and stable operating points is simply that the initial response in similar for all three operating points.

If the controller gain is set too low one will experience that the controller is not able to stabilize the open-loop unstable operating point. However, if there exists solutions above and below the unstable point the column will not necessarily go totally unstable, but may instead go into limit cycles. Figure 9 a) shows the result of a setpoint change from operating point 2 to operating point 3 when the controller gain has been reduced by a factor of two compared to the simulations in Fig.8. We see that the controller is no longer able to stabilize the unstable operating point, but is instead oscillating around the setpoint. One might believe that the oscillations are due to a critical gain (closed-loop eigenvalues on the imaginary axis), but the phenomena experienced here is purely nonlinear. Initially the controller correctly increases L_w in order to increase y_D, but due to the low controller gain L_w does not decrease again fast enough to stabilize the setpoint. This leads to y_D increasing far beyond the setpoint and almost up to the upper solution branch III where the column settles somewhat because it is close to a stationary solution. Now the controller decreases L_w and the solution this time "jumps" almost down to the lower solution branch I where it settles somewhat again. This behavior continous in a limit cycle. If the controller gain is reduced further the limit cycles will continue but now with a longer period of each cycle, due to a slower change in L_w. This is illustrated in Fig.9 b) where the controller gain now has been reduced by a factor of ten. In this case the trajectory almost follows the steady state multiplicity curve around, jumping catastrophically at the singular points. There will as stated earlier exist cases where there are no solutions either above or below the unstable operating point (in fact the solutions then would correspond to one of the product-flows being negative). In this case the column would go globally unstable as either the condenser or the reboiler would go dry.

4.2 Two-point Control

As pointed out above one-point control is sufficient to stabilize an unstable column, but high performance control requires control of both compostions. There exist a large amount of literature on two-point control of distillation columns, but almost all the work has been based on molar inputs. The question we attempt to answer here is whether a controller designed for molar inputs will perform well on a real column where the inputs are in other units.

In process control in general there has been a long tradition for using steady state data for analyzing control properties. Many controllability measurements like the Relative Gain Array (Bristol, 1966) have usually been used in a steady state context. However, we stress again that it is the high-frequency behavior that is most important for feedback control unless there are severe bandwidth limitations like rhp-zeros close to the origin, large deadtimes, large model uncertainties or difficult multivariable properties like interaction between the loops. It is the frequency response around the expected closed loop bandwidth which is of most interest for feedback control. Skogestad et.al. (1990) studied the control of several ideal columns including column A (Table 1). They found that one may have good and robust performance, including high bandwidth, by using two single loop controllers. The main reason for this was the low interaction between the loops at high frequencies due to flow dynamics (liquid lag from top to bottom of column). In fact, they found that because of severe interaction between the loops at low frequencies the bandwidth of the controllers should be high to achieve reasonable performance. In light of this and the fact that the high-frequency dynamics for the LV- and L_wV-configuration differs only slightly we would expect that a well tuned controller for the LV-configuration should perform well also with the L_wV-configuration.

Simulations Skogestad et.al. (1990) designed robust decentralized PI-controllers for column A with the LV-configuration. The control parameters are given in Table 3. Figure 11 shows the response to a 20 % increase in feed flow rate using the LV- and the L_wV-configurations. The nonlinear simulations include a 20 % input uncertainty and 1 min. deadtime in each loop. The gain in the mass reflux loop was scaled by M compared to the molar reflux loop. The simulations show that we get a somewhat larger deviation from the setpoint when using mass reflux, but overall it is only a small detoriation in the performance when using mass reflux instead of molar reflux. This is as expected since the bandwidth is about $10 min^{-1}$, and around this frequency there are only small differences in the dynamic behavior of the two configurations (see Fig.10). Note that the new steady state reached have the same dynamic properties as the nominal point since an increase in the feed flow rate only leads to a scaling of all extensive variables when the compositions are kept constant. This means that the new steady state for the L_wV-configuration is still open-loop unstable.

5 Multiple Steady States and Instability for Molar Inputs

To this point we have only discussed multiplicity and instability in distillation due to input units other than molar. This is also the type of multiplicity studied by Jacobsen and Skogestad (1990). Models of binary distillation columns with molar inputs and not including any energy balance will always exhibit unique and asymptotically stable solutions (Doherty and Perkins, 1982). However, here we provide an example showing that when the energy balance is included one might get multiple steady states and instability also for molar inputs. In light of the arguments of real columns not having molar inputs the results on molar multiplicity might seem to be of more theoretical interest. However, these results will be of interest in simulations as the specifications here most often are done on a molar basis. Secondly, even though the inputs are on a mass or volume basis in real columns, the separation will depend on the molar rates and the multiplicity shown here may give new and interesting results when combined with mass or volume inputs.

Example. We will again study the ethanol-butanol column . We now include an energy balance in the model where we previously assumed constant molar flows. We assume no energy-dynamics, ie. immediate responses for the energy-balance. This has of course no effect on the steady state solutions, but will affect the overall dynamics somewhat. The energy-balance on each tray is given by:

$$Q_i + V_{i-1}H^V_{i-1} + L_{i+1}H^L_{i+1} - V_iH^V_i - L_iH^L_i + F_iH^F_i = 0 \tag{29}$$

where subscript i denotes tray number (trays are numbered from the bottom). Equlibrium data was computed using the Van Laar activity coefficient model.

Consider keeping the molar boilup V constant at 3.5 kmol/min and varying the molar reflux between 3.5 kmol/min and 3.6 kmol/min. Some solutions are given in Table 4. From the table we see that for L=3.54 we get the three different solutions 2, 3 and 4. Solution 3 is found to be unstable. The multiplicity is graphically illustrated in Fig.12. This example shows that for the LV-configuration we may have multiplicity even in ideal binary separation.

The reason for the multiplicity in this case is found in the opposing effects between compositions and flows inside the column. The heat of vaporization will in general depend on the composition and because of this the vapor and liquid flows, which determines separation, will depend on the composition on each tray. In the ethanol-butanol system the heat of vaporization decreases with the fraction of most volatile component (ethanol). When molar reflux is increased the amount of ethanol will increase throughout the column and (while molar boilup is kept constant) the vapor flows upwards in the column will increase. The effect of the increased vapor flows have an opposing effect on compositions compared to the increase in reflux. When the effect of increased vapor flows equals the effect of increased reflux we will have singularity. If the effect of increased vapor flows becomes greater than the effect of increased reflux we will have instability.

Similar results have been found for several other columns, and the multiplicty and instability found here is in principal possible in any ideal as well as non-ideal system.

We do not provide any rigorous evidence for the multiplicity and instability here. This will be included in a later version of the paper.

6 Discussion

Global stability. We have derived conditions, e.g. (21), to check the local stability of a certain operating point. However, it is not easy to tell if it is globally stable, that is, if it is at a point where we have uniqueness. To be specific, recall Example 1 and Table 2. It is easily shown using (21) that operating point 3 is unstable, and that operating points 1, 2, 4 and 5 are (locally) stable. It is clear from Figure 3 that operating points 1 and 5 are globally stable (with the given L_w and V), whereas 2 and 4 are not. However, there exists no simple method to check this directly. To do this analytically one would have to apply some kind of Lyapunov function to the dynamic model, which is not at all straightforward due to the high order and complexity of a dynamic model of a distillation column. In fact, the easiest way to check for global stability is to obtain solutions in the whole range of operation using molar inputs in a steady-state simulator, and then convert the results to the actual input units, that is, to generate a figure similar to Fig.2.

Subcooling. In this paper we have not discussed all issues that may be important for multiplicity and instability in distillation. For instance, subcooling of the reflux may be important as the degree of subcooling may depend on the temperature and thereby on composition. The separation in the column is determinded by the effective reflux $L_{eff} > L$ which takes into account the additional internal reflux caused by subcooling. The degree of subcooling will usually decrease as y_D increases because the top part of the column cools down. With subcooling the second term in (2) is thererfore reduced in magnitude, and we conclude that subcooling makes instability somewhat less likely for the L_wV-configuration.

Multicomponent mixtures. Introducing additional non-key components will generally make multiplicity and instability less probable. The reason is that the “dead weight” of the non-key components generally will reduce the effect of changes in the compositions of the key components on mole weight, M, and heat of vaporization, ΔH_{vap}.

Volume basis. We have not discussed volume inputs in particular, but the results obtained for mass inputs will in general apply to the volume case. For the case with ideal mixing we need only substitute the molecular weights with the molar volumes in the equations presented. For example, consider the $L_q V$-configuration. Similar to the mass case, $V_2 > V_1$ is necessary for instability, and in this case the instability condition becomes

$$y_D + L\left(\frac{\partial y_D}{\partial L}\right)_V > \frac{V_2}{V2 - V_1} \tag{30}$$

For non-ideal mixtures the volume of mixing must also be accounted for.

Instability during industrial operation. As we have discussed above, instability for the $L_w V$-configuration is likely to occur during operation if the reflux is large. Since the $L_w V$-configuration is common in industry, it is surprising that there has been no previous experimental reports of instability. One possible reason is that multiplicity and instability always have been believed to be impossible in distillation, and consequently observations of instability during operation have been explained in other ways. Another possible explanation is that most columns in industry would be operated with one-point control. In this case one may identify an open-loop unstable operating point by observing that the steady state effect of increasing purity is to decrease mass reflux L_w.

Other Configurations In this paper we have only discussed the $L_w V$-configuration, ie. mass-reflux and molar boilup as manipulated inputs. As stated previously this is the most interesting configuration as it is most widespread in industry. Jacobsen and Skogestad (1990) found that multiple steady states and instability is likely for several other configurations as well. For all these configurations the rhp poles found was usually small (slowly unstable) and we would therefore expect the control problem to be similar for these configurations. That is, with a reasonably high bandwidth the change in input units does not create new control problems compared with what is found for molar inputs.

7 Conclusions

1. Two-product distillation columns may have multiple steady state solutions as well as unstable operating points. These results are independent of complex thermodynamics.
2. The multiplicity and instability is caused by the possible singularity in the transformation between actual inputs and the molar flows which determines the separation in distillation.
3. The probability of instability for the $L_w V$-configuration will increase when internal flows (eg. L and V) are increased.
4. A necessary and sufficient condition for an operating point to be unstable due to change in units is a negative slope between the actual reflux and molar reflux.
5. The right half plane pole will usually be close to the imaginary axis (slowly unstable) and the unstable operating point may then easily be stabilized by using feedback control of one composition or temperature in the column.

6. The high-frequency dynamics for the L_wV- and LV-configuration will usually be similar. Because of this a well designed controller based on molar inputs will perform well when applied to a column with mass-inputs.
7. New results are presented showing that models with molar inputs may also exhibit multiple steady states and unstable solutions. These results are also found for ideal systems and depends on the presence of an energy balance in the model.

NOMENCLATURE (see also Fig.1)

B - bottoms flow (kmol/min)
D - distillate flow (kmol/min)
F - feed rate (kmol/min)
H^L - liquid phase enthalpy (kJ/kmol)
H^V - vapor phase enthalpy (kJ/kmol)
L - reflux flow rate (kmol/min)
M - mole weight, usually of top product (kg/kmol)
M_1 - pure component mole weight of most volatile component (kg/kmol)
M_2 - pure component mole weight of least volatile component (kg/kmol)
M_L - Liquid holdup (kmol).
N - no. of theoretical stages in column
N_F - feed stage location (1-reboiler)
Q_D - heat input to reboiler (kJ/min.)
Q_B - heat input to condenser (kJ/min.)
V - boilup from reboiler (kmol/min) (determined indirectly by heating Q)
V_1 - pure component molar volume of most volatile component (m^3/kmol)
V_2 - pure component molar volume of least volatile component (m^3/kmol)
x_B - mole fraction of most volatile component in bottom product
y_D - mole fraction of most volatile component in distillate (top product)
z_F - mole fraction of most volatile component in feed

Greek symbols

$\alpha = \frac{y_i/x_i}{(1-y_i)/(1-x_i)}$ - relative volatility (binary mixture)
λ_{max} - maximum eigenvalue / dominant pole
ω_B - bandwidth (min^{-1})
θ_d - deadtime (min)

Subscripts

w - flow rate in kg/min
q -flow rate in m^3/min

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Table 1. Data for example columns.

Example	z_F	F	α	N	N_F	M_1	M_2
1.Ethanol – butanol	0.50	1	4.35	8	4	46.1	74.1
2.One – stage column	0.50	1	4.0	1	1	20	40
3.Column A	0.50	1	1.5	40	21	1	5

Feed is saturated liquid
Total condenser with saturated reflux
Liquid holdups are $M_{Li}/F = 0.5$ min, including reboiler and condenser.
*) α varies since non-ideal thermodynamics are used

Table 2. Steady-state solutions for ethanol-butanol column with V=2.5 kmol/min and L_w in the range 92 to 98 kg/min.

	L kmol/min	D kmol/min	L_w kg/min	y_D	x_B
1	1.550	0.950	92.00	0.526	$9.48e-4$
2	1.689	0.812	96.00	0.616	$1.14e-3$
3	1.920	0.581	96.00	0.860	$1.61e-3$
4	2.082	0.418	96.00	0.9995	$1.41e-1$
5	2.125	0.375	98.00	0.9996	$2.01e-1$

Table 3. Control parameters used in closed-loop simulations. $C(s) = \frac{k}{1+\tau_I S}$.

	k_y	τ_{Iy}	k_x	τ_{Ix}
ethanol – butanol column	5	21.21		
columnA	0.49	11.21	0.34	7.27

gains are for logarithmic compositons, ie. $log(1-y_D)$ and $log(x_B)$.

Table 4. Steady-state solutions for Ethanol-Butanol column with $V = 3.5$ kmol/min and L in the range 3.5 to 3.6 kmol/min.

	L kmol/min	D kmol/min	$log10(1-y_D)$	x_B
1	3.51	0.480	-3.33	$3.889e-2$
2	3.54	0.465	-3.486	$6.570e-2$
3	3.54	0.420	-3.670	$1.381e-1$
4	3.54	0.275	-3.854	$3.104e-1$
5	3.56	0.220	-3.899	$3.590e-1$

Figure Captions

1. **Figure 1**. Two product distillation column.
2. **Figure 2**. Multiple steady states for mass reflux L_w for the ethanol-butanol column. Boilup $V = 2.5$ kmol/min.
3. **Figure 3**. Eigenvalues for different operating points of the ethanol-butanol column. Boilup $V = 2.5$ kmol/min
4. **Figure 4**. Nonlinear simulation of ethanol- butanol column at unstable operating point 3. a) Infinitesimal increase in mass reflux L_w. b) Infinitesimal decrease in mass reflux L_w. Boilup $V = 2.5$ kmol/min.
5. **Figure 5**. One-stage column with total condenser.
6. **Figure 6**. Steady state solutions as a function of mass reflux L_w for one-stage column with $\alpha = 4$. a) $V = 3.0$ kmol/min - Unique stable solution. b) $V = 4.7$ kmol/min - multiple solutions. c) $V = 6.0$ kmol/min - Unique unstable solution.
7. **Figure 7**. Blockdiagram showing the effect of increasing mass reflux L_w on top composition y_D when molar boilup V is kept constant.
8. **Figure 8**. Nonlinear simulation of ethanol- butanol column with one-point control of top-composition y_D using mass reflux L_w. Setpoint changes from operating point 2 to 3 and from 3 to 4. Boilup $V = 2.5$ kmol/min. Controller parameters are given in Table 3.
9. **Figure 9**. Nonlinear simulation of ethanol- butanol column with one-point control of top-composition y_D using mass reflux L_w. a) Controller gain reduced by a factor of 2 compared to Table 3. b) Controller gain reduced by a factor of 10 compared to Table 3.
10. **Figure 10**. Frequency responses for column A with LV- and L_wV-configurations.
11. **Figure 11**. Nonlinear simulation of column A with two-point control using LV- and L_wV-configuration. Response to a 20 % increase in feed flowrate using single-loop PI controllers. PI-settings from Table 3.

12. **Figure 12**. Multiple steady states for ethanol- butanol column (including energy-balance) for molar reflux L. Boilup V = 3.5 kmol/min.