Part II. Application to Nonlinear Multicomponent Systems

In Part I, a novel method for reducing the order of models for countercurrent staged separation systems was presented. In this paper, the method is applied to the modeling and simulation of nonlinear multicomponent distillation systems. Some additional properties of the model reduction procedure are derived. The accuracy of the approximation is established by comparison of the steady-state profiles and transient responses to that of rigorous dynamic models. The results indicate that the proposed technique is an effective way of reducing the number of equations needed to model stagewise multicomponent separation systems.

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SCOPE

The model reduction procedure developed in Part I is extended to nonlinear multicomponent staged separation systems. Attention is focused on reducing the number of equations required to model a section of a column with no intermediate feeds, side-draws or pump-arounds. In addition to preserving component and total mass balances across the entire column, the reduced-order model also incorporates the energy balance as well as the effect of tray hydraulics and tray efficiencies. The model reduction procedure is applied to example problems in binary and multicomponent distillation and comparisons are made with responses of rigorous tray-by-tray models.

CONCLUSIONS AND SIGNIFICANCE

Comparison between rigorous stage-by-stage calculations and the reduced-order models show excellent agreement both in the steady state as well as in the dynamics. The number of equations required to model the system can be drastically reduced, sometimes by as much as a factor of ten. The actual reduction achievable is a factor of: (1) the column size (the reduction being greater for larger columns); (2) the accuracy desired (greater accuracy is achieved by using more collocation points, but this also increases the number of equations); and (3) the nonlinearity of the column temperature, flow and composition profiles (the greater the nonlinearity, the greater the number of collocation points needed). In the examples tested, a maximum of four collocation points gave accurate results both in the steady state and in the dynamics.

The method developed is applicable to a wide range of problems in modeling of separation systems. These include steady state design, steady state optimization, dynamic simulation and the design and testing of on-line identification, control and on-line optimization strategies. By application of the model reduction procedure, the number of differential equations required to model large columns can be substantially reduced, thus allowing the use of common integration packages such as CSMP (IBM, 1972) to simulate the dynamics of interconnected columns and other processing equipment. The use of such general purpose packages are attractive to process engineers who do not want to get involved in setting up their own special purpose integration packages.

DEVELOPMENT OF EQUATIONS

The modeling of a simple column with a single feed, no sidestreams, pumparounds or other intermediate takeoffs is considered first. The model reduction technique developed in Part I is applicable to sections of a column where there are no abrupt changes in the vapor flow, liquid flow, temperature and composition profiles. For the column shown this amounts to reduced-order models for the stripping section and the enriching section.

We start by considering the rigorous, tray-by-tray model of a section of a column. In developing this model, we adopt certain basic assumptions which have been proved to be reasonable by earlier investigators (Howard, 1970; Ballard et al., 1978; Seider and Prokopakis, 1980). These are: (1) the liquid leaving a tray is well mixed; (2) the vapor holdup is negligible; (3) there is a definite relationship (not necessarily equilibrium) between the liquid and a vapor composition leaving a tray; and (4) vapor and liquid leaving a tray are in thermal equilibrium.

The dynamic model is obtained by writing the unsteady state mass and energy balances around the tray in conjunction with equilibrium and hydraulic relationships. The variables associated with a tray are shown in Figure 1. For convenience in later manipulations, we have deliberately chosen to give the same tray index to vapor and liquid variables *passing* each other on a tray. This is in contrast to the usual practice of giving the same index to liquid and vapor variables *leaving* a tray. The approximation procedure that we use will assume a continuous profile for vapor and liquid and hence the tray index j will disappear in the approximation. Thus, instead of x_j and y_j, we will have $x(z)$ and $y(z)$ where z is a distance variable.

Component balance around a stage yields (Figure 1)

$$\frac{d}{dt}(M_j x_{ij}) = L_{j-1}x_{i,j-1} + V_j y_{ij} - L_j x_{ij} - V_{j-1}y_{i,j-1} \quad (1a)$$

Total balances:

$$\frac{dM_j}{dt} = L_{j-1} + V_j - L_j - V_{j-1} \quad (1b)$$

Energy balance:

$$\frac{d}{dt}(M_j h_j) = L_{j-1}h_{j-1} + V_j H_j - L_j h_j - V_{j-1}H_{j-1} \quad (1c)$$

Flow hydraulics equation:

$$M_j = m(L_j) \quad (1d)$$

Vapor-liquid relationship:

$$y_{i,j-1} = y(x_{ij}, T_j^L) \quad (1e)$$

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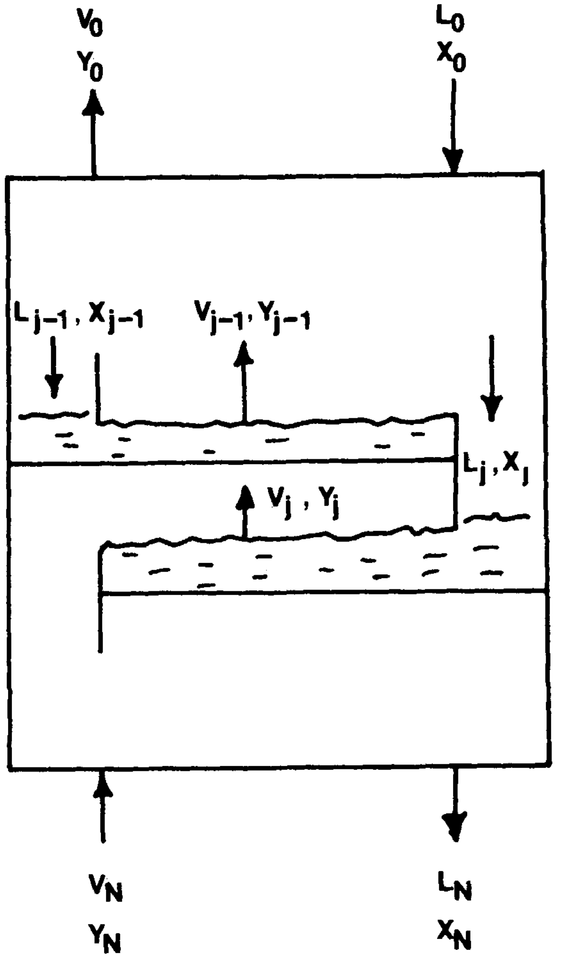

Figure 1. Definition of variables for writing material balance on a tray.

Bubble-point relation:

$$\sum_{i=1}^{c} y(x_{ij},T_j^L) = 1 \tag{1f}$$

A typical correlation used for tray hydraulics is the Francis-Weir equation:

$$M_j = A_s\rho(x_j)(L_w + \delta w_j) \tag{1d'}$$

$$\delta w_j = W_c L_d^{2/3}$$

Similarly typical vapor-liquid relationships are the Murphree tray efficiency:

$$y_{i,j-1} - y_{ij} = E_{ij}^M(y_{ij}^* - y_{ij})$$

and the vaporization efficiency

$$y_{i,j-1} = E_{ij}^V K_{ij} x_{ij} \tag{1e'}$$

Both equations can be used in the development that follows. For convenience we will select the vaporization efficiency relationship.

Although Eq. 1c is written as a differential equation in time, it is not an independent equation. As shown by Howard (1970) this can be reduced to an algebraic equation. Thus we have a set of state variables consisting of the liquid composition on each tray and the liquid holdup on each tray. Although it is possible to eliminate one equation for the liquid composition using the relationship $\Sigma x_{ij} = 1$, from a numerical standpoint it is advisable to carry all equations and to satisfy the summation by normalizing the composition at every time step. Otherwise, accumulated numerical round-offs can cause a mole fraction to go negative with disastrous results (Brosilow and Ballard, 1978).

PDE Approximation

Following the procedure outlined in the earlier paper, we first generate a set of partial differential equations which approximate the above set of differential difference equations. For this we assume that the variables x, y, L, V, M and T are smooth functions of the distance variable Z. Using this assumption we can write

$$x_{i,j-1} = x_{ij} - \frac{\partial x_i}{\partial z}\Delta z$$

where Δz is the spacing between trays. For convenience we can take $\Delta z = 1/N$ where N is the number of trays in the section that we are approximating (e.g., stripping or enriching section).

$$\frac{\partial}{\partial t}(Mx_i) = \frac{\partial}{\partial z}(Vy_i - Lx_i) \tag{2a}$$

$$\frac{\partial M}{\partial t} = \frac{\partial}{\partial z}(V - L) \tag{2b}$$

$$\frac{\partial}{\partial t}(Mh) = \frac{\partial}{\partial z}(VH - Lh) \tag{2c}$$

$$M\Delta z = m(L) \tag{2d}$$

$$y_i - \Delta z\frac{\partial y_i}{\partial z} = y(x_i,T^L) \tag{2e}$$

$$\sum_{i=1}^{c} y(x_i,T^L) = 1 \tag{2f}$$

Equations 2a and 2c can be simplified using Eq. 2b to give:

$$M\frac{\partial x_i}{\partial t} = \frac{\partial}{\partial z}(Vy_i - Lx_i) - x_i\frac{\partial}{\partial z}(V - L) \tag{2a'}$$

$$M\frac{\partial h}{\partial z} = \frac{\partial}{\partial z}(VH - Lh) - h\frac{\partial}{\partial z}(V - L) \tag{2c'}$$

In the above derivation we have used the definition

$$M_j = M\Delta z \tag{3}$$

Thus M can be looked upon as the holdup per unit length along the column.

The above equations have the property that certain steady state conditions are satisfied. At steady state we have

$$\frac{d}{dz}(V - L) = 0$$

$$\frac{d}{dz}(Vy_i - Lx_i) - x_i\frac{d}{dz}(V - L) = 0$$

The first equation has the solution

$$(V - L)_z = \text{Constant} = (V - L)_{z=0}$$

which is the requirement for overall mass balance. The second equation has the solution

$$Vy_i - Lx_i = \text{Constant} = (Vy_i - Lx_i)_{z=0}$$

which is the requirement for component balance at any section of the column. Likewise the energy balances are also satisfied. The importance of satisfying those equations on accuracy of the approximation will be demonstrated later. It was noted in Part I that the PDE representation is not unique. There exist other PDE approximations which may not satisfy the above steady-state conditions.

The boundary conditions for the above equations are obtained by considering the conditions at the top and bottom of the column section under consideration. The known values of input stream variables constitute the boundary condition (Figure 1):

$$x_i(z = 0) = x_{io} \tag{4a}$$

$$L(z = 0) = L_o \tag{4b}$$

$$T^L(z = 0) = T_o^L \tag{4c}$$

$$y_i(z=1) = y_{i,n} \tag{4d}$$

$$V(z=1) = V_N \tag{4e}$$

$$T^V(z=1) = T_N^V \tag{4f}$$

Collocation Approximation

The next step in the approximation procedure is to discretize the above PDEs by orthogonal collocation in the spatial direction. The functions x_i, y_i, etc. are, then, expanded in terms of Lagrange polynomials,

$$x_i(z,t) = \sum_{k=1}^{n+2} l_k(z) x_{ik}(t) \tag{5}$$

Substituting these expansions into the PDE's yield a set of ODE's as follows:

$$M_j \frac{dx_{ij}}{dt} = \sum_{k=1}^{n+2} A_{jk}(V_k y_{ik} - L_k x_{ik}) - x_{ij} \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) \tag{6a}$$

$$\text{for } j = 2, \ldots n+2$$

$$\frac{dM_j}{dt} = \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) \tag{6b}$$

$$\text{for } j = 2, \ldots n+2$$

$$M_j \frac{dh_j}{dt} = \sum_{k=1}^{n+2} A_{jk}(V_k H_k - L_k h_k) - h_j \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) \tag{6c}$$

$$\text{for } j = 2, \ldots n+2$$

$$M_j \Delta z = m(L_j) \tag{6d}$$

$$\text{for } j = 2, \ldots n+2$$

$$y_{ij} - \Delta z \sum_{k=1}^{n+2} A_{jk} y_{ik} = y(x_{ij}, T_j^L) \tag{6e}$$

$$\text{for } j = 1, \ldots n+1$$

$$\sum_{i=1}^{c} y(x_i, T^L) = 1 \text{ for } 0 \le z \le 1 \tag{6f}$$

It is important that these approximations preserve mass and energy balances in the steady state. Again, at steady state, we have:

$$\sum_{k=1}^{n+2} A_{jk}(V_k - L_k) = 0 \tag{6a$'$}$$

$$\sum_{k=1}^{n+2} A_{jk}(V_k y_{ik} - L_k x_{ik}) - x_{ij} \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) = 0 \tag{6c$'$}$$

The first equation represents a set of linear algebraic equations in the unknowns $V_k - L_k$. Recall that to maintain material balance

$$V_k - L_k = \text{const.}$$

This was proved in Appendix A of Part I. From Eqs. 6a′ and 6c′ we have

$$\sum_{k=1}^{n+2} A_{jk}(V_k y_{ik} - L_k x_{ik}) = 0$$

and hence

$$V_k y_{ik} - L_k x_{ik} = \text{const.}$$

by analogy with the overall balance. This proves that component balance is also satisfied by the polynomial approximation.

In the above derivations, Eqs. 6a and 6c can be decomposed to give simpler forms. Appendix A shows the difference in collocations between the form in Eq. 6a or 6c and its decomposed form. However, these decomposed forms do not conserve mass and energy at steady state.

The boundary conditions associated with these equations are:

$$x_{i1} = x_{io} \tag{7a}$$

$$L_1 = L_o \tag{7b}$$

$$T_1^L = T_o^L \tag{7c}$$

$$y_{i,n+2} = y_{iN} \tag{7d}$$

$$V_{n+2} = V_N \tag{7e}$$

$$T_{n+2}^V = T_N^V \tag{7f}$$

Solution Procedure

The reduced order model can be reduced to a set of equations in the state variables x and L evaluated at the collocation points, z_j, $j = 2, 3, \ldots, n+2$. This is done as follows. The total mass balance can be combined with the Weir equations to give

$$\frac{dL_j}{dt} = \frac{\Delta z}{(\partial m/\partial L_j)} \left(\frac{dM}{dt}\right)_j$$

$$= \frac{\Delta z}{(\partial m/\partial L_j)} \sum_{k=1}^{n+2} A_{jk}(V_k - L_k)$$

The energy balance can be reduced to the form

$$V = R \cdot L - S \cdot V_{n+2}$$

as shown in Appendix B. For the case where a vaporization efficiency is used, the equilibrium relationship becomes

$$y_{ij} - \sum_{k=1}^{n+2} A_{jk} y_{ik} = E_{ij} K_{ij} x_{ij}$$

which can be solved to give

$$y_i = F^{-1} x_i$$

The derivatives of L_j and x_{ij} are calculated as follows (given L_j and x_{ij}).

(1) Compute the temperature T_j by the bubble point relationship.
(2) Compute the y_{ij} and V_i using above equations.
(3) Compute the derivatives from Eqs. 6a and 6b.

Direct Reduction to Polynomial Approximation

The above reduction was based on the concept of first deriving continuous approximation to the system of equations and then rediscretizing in space. However, it is not necessary to go through the PDE approximation to get the reduced order equations. The important factor in the approximation is the recognition that the variables like x, L, and V are all continuous variables along the column. Consider the component balance equation.

$$\frac{d}{dt}(M_j x_{ij}) = (L_{j-1} x_{ij-1} - L_j x_{ij}) + (V_j y_{ij} - V_{j-1} y_{ij-1}) \tag{8}$$

Define new variables

$$u_j = L_j x_{ij} \quad w_j = V_j y_{ij}$$

Then

$$\frac{d}{dt}(M_j x_{ij}) = (w_j - w_{j-1}) - (u_j - u_{j-1})$$

If u and w were continuous function of z, a polynomial approximation could be used to represent them.

$$u(z) = \sum_{k=1}^{n+2} l_k(z) u_k \tag{9a}$$

where u_k are evaluated at discrete intervals of z given by z_k, $k = 1, 2, \ldots n+2$

Then

$$u_{j-1} = u(z_j - \Delta z) \tag{9b}$$

$$= \sum_{k=1}^{n+2} l_k(z_j - \Delta z) u_k$$

Hence

$$\frac{d}{dt}(M_j x_{ij}) = \sum_{k=1}^{n+2} l_k(z_j - \Delta z) L_k x_{ik} - \sum_{k=1}^{n+2} l_k z_j L_k y_{ik}$$
$$+ \sum_{k=1}^{n+2} l_k(z_j) V_k y_{ik} - \sum_{k=1}^{n+2} l_k(z_j - \Delta z) V_k y_{ik} \tag{10}$$

The reduced order model is obtained by assuming that Eq. 10 holds

TABLE 1. OPERATING CONDITIONS OF EXAMPLES

	Example 1	Example 2	Example 3
No. of Stages	10	10	20
No. of Components	2	3	3
Operating Pressure	1.702 MPa	1.702 MPa	1.702 MPa
Mole Fractions in Liquid Feed			
Comp. 1 (Ethane)	None	0.01	0.2
Comp. 2 (Propane)	0.98	0.97	0.75
Comp. 3 (N-Butane)	0.02	0.02	0.05
Liquid Feed Flow Rate	1,260 kmol/h	1,260 kmol/h	1,980 kmol/h
Liquid Feed Temperature	324.0 K	323.0 K	359.7 K
Mole Fractions in Vapor Feed			
Comp. 1	None	0.02513	0.14
Comp. 2	0.72	0.69950	0.40
Comp. 3	0.28	0.27537	0.46
Vapor Feed Flow Rate	1,800 kmol/h	1,800 kmol/h	1,800 kmol/h
Vapor Feed Temperature	349.0 K	347.0 K	371.1 K
Cross-Sectional Area (A_s)	0.0021 m^2	0.0021 m^2	0.0021 m^2
Weir Height	0.04 m	0.04 m	0.04 m
W_c (in Weir's Equation) (for all three)	0.013 m (kmol/h)$^{-2/3}$		
Vaporization Efficiencies			
Comp. 1	None	1.0	0.2
Comp. 2	1.0	1.0	0.5
Comp. 3	1.0	1.0	1.0

TABLE 2. COMPARISON OF STEADY-STATE PROFILES FOR EXAMPLE 1

	Rigorous Model		Reduced Model*	
Tray No.	X1	L	X1	L
Inlet	0.98	21.0	0.98	21.0
1	0.97905	20.7436	0.97913	20.8192
2	0.97738	20.7432	0.97853	20.7257
3	0.97382	20.7422	0.97578	20.6993
4	0.96634	20.7387	0.96776	20.7117
5	0.95092	20.7268	0.95065	20.7265
6	0.92039	20.6848	0.91994	20.6992
7	0.86458	20.5516	0.87041	20.5772
8	0.77577	20.2118	0.79615	20.3000
9	0.66100	19.5843	0.69054	19.7989
10	0.54632	18.9974	0.54627	18.9972

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* Tray values were obtained by Lagrangian interpolation of the results from three-point collocation.

at n arbitrarily selected interior points, z_j. Although, other approximations could be obtained by combining the stage Eq. 10 in various ways, the choice of satisfying it only at selected collocation points is shown to be quite accurate in the following example problems. This representation of the reduced order model is in a form that can be conveniently programmed on a digital computer.

EXAMPLES

The accuracy of the approximation was tested using three example problems. The operating conditions of the three columns are shown in Table 1. Column 1 is a binary column with 10 stages. Column 2 is a ternary column also having 10 stages. Column 3 has the same components as column 2 but consists of 20 trays.

For comparison purposes, the rectification section of the column was selected and a model reduction procedure was carried out. At the same time a rigorous tray-by-tray simulation was carried out using the semi-implicit second-order Runge-Kutta algorithm due to Brosilow and Ballard (1978).

In addition, the physical properties were estimated using

(1) Ideal solution and Antoine equation for K and

(2) $H_j = \sum_{i=1}^{c} y_{ij}H_{ij}, \quad h_j = \sum_{i=1}^{c} x_{ij}h_{ij},$

$$H_{ij} = A + BT + CT^2 \quad h_{ij} = a + bT + CT^2$$

where, coefficients, A, B, C, etc. are given in Amundson and Pontinen (1958).

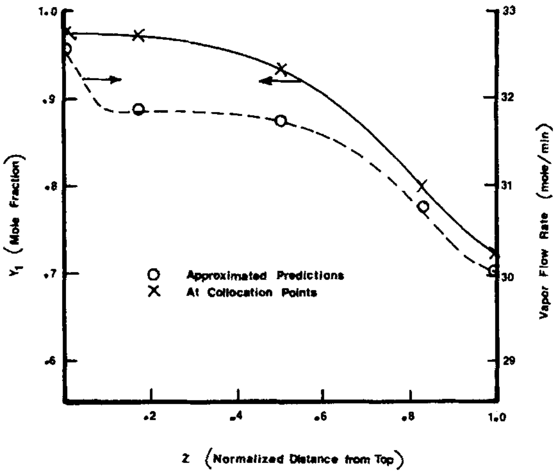

Figure 2. Steady-state profiles of y_1 and V for example 1.

Nature of Tests

The approximation accuracy was tested in two different ways. First by comparing the steady state profiles predicted by the rigorous model was compared with that of the reduced order model. Secondly the column was subjected to step disturbances in the feed flow rates and the transient responses of the two models were compared.

There are many choices to make in the selection of the reduced order model. First is the order of the approximation. In these tests we have used the second-order approximations that were derived earlier. Second there is the choice of the polynomial to be used. Both α and β were set equal to 1 and this gave collocation points evenly distributed across the column.

Comparison of Steady-State Profiles

Table 2 and Figures 2 and 3 compare the steady-state profiles of example 1. Three collocation points are used in this approximation. The accuracy is quite remarkable. The difference between the two models is not noticeable in the graphs. As seen from Table 2, the two models agree up to three significant digits. (Compare the location $z = 1.0$ which corresponds to $n = 10$.)

This agreement in steady-state profiles was true also for example 2 which required four collocation points (Figures 4 and 5). The collocation predictions fall exactly on the curves predicted by the rigorous model.

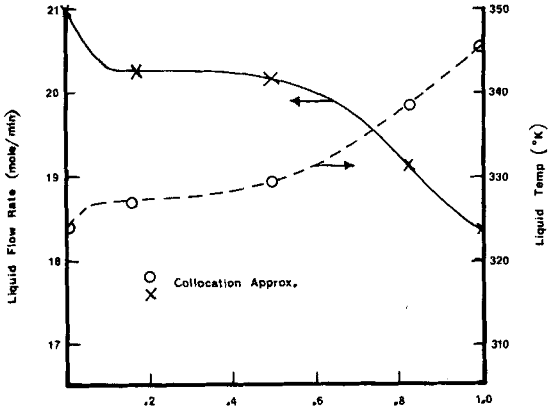

Figure 3. Steady-state profiles of L and T for example 1.

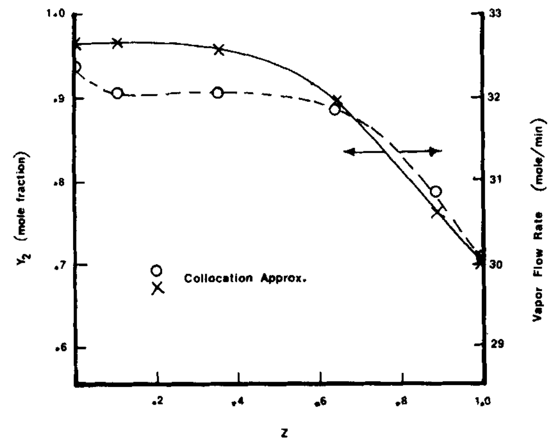

Figure 4. Steady-state profiles of y_2 and V for example 2.

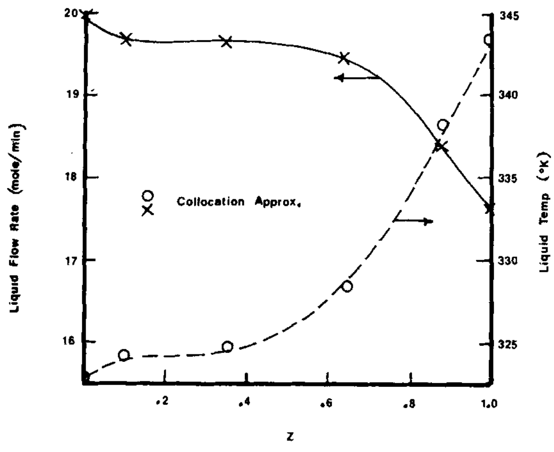

Figure 5. Steady-state profiles of L and T for example 2.

The reduction in order is most pronounced in example 3 with 20 trays (Figures 6 and 7). Here four collocation points was sufficient to approximate the column effectively reducing the order of the system by a factor of four. Note that component 1 is a trace component present in very small quantity through the column (for example 2). The agreement was excellent for the composition profile of this component as well.

Comparison of Transient Response to Input Disturbances

Each of the three columns was subject to changes in input flow rates or composition.

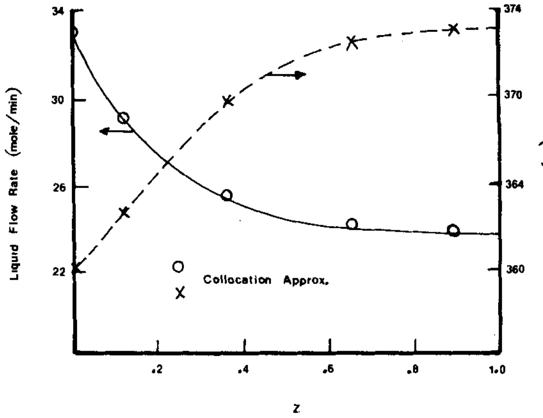

Figure 6. Steady-state profiles of L and T for example 3.

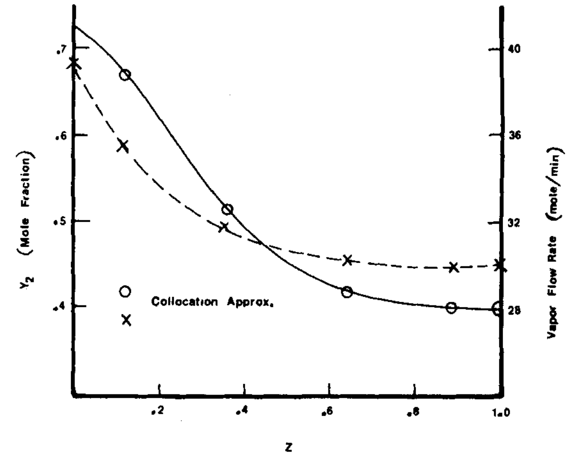

Figure 7. Steady-state profiles of y_2 and V for example 3.

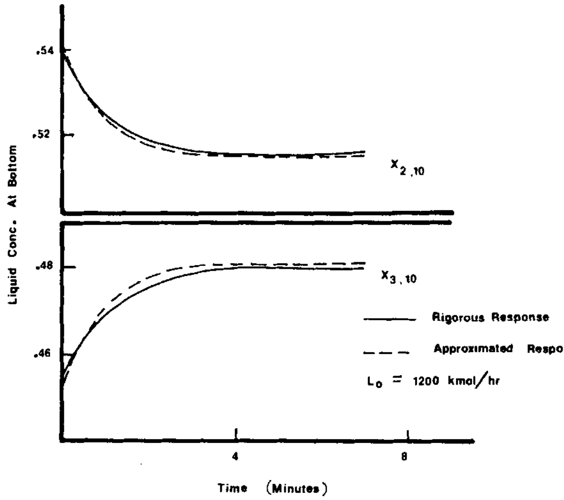

Figure 8. Step responses of x_2 and x_3 at bottom of the column for a step decrease in liquid feed rate (example 2).

Due to space limitations only some selected test results are given. Figure 8 gives the response of the liquid concentration at bottom to a step change in liquid flow to column 2. Good agreement is obtained in the dynamics as well as in the final steady state. Figure 9 compares the response of liquid and vapor flow rates for the same test. Again the agreement is good.

Figure 10 gives part of the responses to a step increase in vapor flow to column 3. The output compositions of liquid and vapor are given. The agreement is quite good.

Similar trends were observed in other variables.

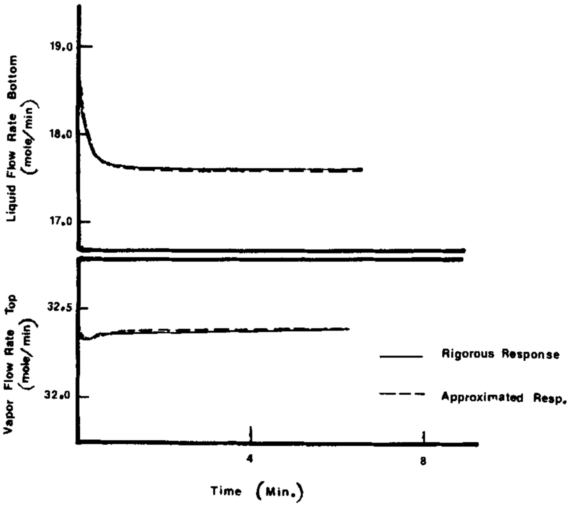

Figure 9. Step responses of L and V for a step decrease in liquid feed rate (example 2).

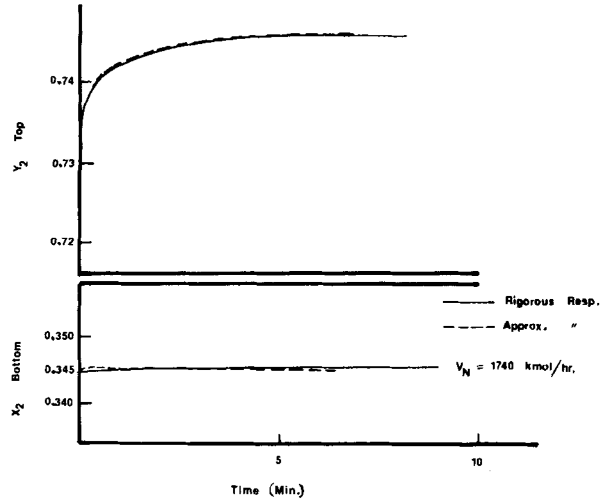

Figure 10. Step responses of y_2 at top and x_2 at bottom for a step decrease in vapor flow rate (example 3).

Discussion

The model reduction procedure developed here appears to be quite promising based on the test results obtained on binary and multicomponent columns studied so far. Even in presence of strong nonlinearities in the profile, model reduction procedure worked quite well both in the steady state as well as in the dynamics. Future testing will include nonideal solutions as well as wider range of test problems.

The reduction in order is quite remarkable. This reduction in order will result in much less computation both in the steady state as well as in the dynamics. The reduced model developed here is most effective for column sections with large number of trays. For the column with 20 trays the order of the system was reduced by a factor of four and still gave excellent agreement with the rigorous model. Some further reduction can be obtained by using fewer collocation points if one is willing to give up on the accuracy. For example using three instead of four collocation points the s.s. error is increased to 3.5%. One would expect that if the profiles in the column show severe nonlinearities then the number of collocation points required would increase and the reduction in order possible would be smaller. For high purity columns with large numbers of trays the reduction in order would be substantial.

The extension of the model reduction procedure to columns with feeds and sidedraws is still under investigation. One simple approach would be to model the column in sections which has no feed or sidedraws. Each of these sections could be modeled using the approach presented here and the final model is obtained by combining the individual sections. This is comparable to spline fitting methods employed to deal with discontinuous profiles (Villadsen, 1975).

Another approach under investigation involves redefining variables to maintain approximate continuity in the column and then applying polynomial approximation to the entire column.

ACKNOWLEDGMENT

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NOTATION

A_{jk} = numerical value of $\frac{dl_k}{dz}$ evaluated at collocation point z_j
= Where l_k denotes Lagrange polynomial for collocation point z_k
A_s = cross-sectional area of the column, m^2
B = bottom product rate, kmol/h
C = number of components in the separation unit
D = distillate rate, kmol/h
E_{ij} = stage efficiency for component i on jth plate
h = liquid enthalpy, kcal/mol
H = vapor enthalpy, kcal/kmol
L = liquid flow rate, kmol/min
L_w = weir height, m
M_j = liquid holdup on jth plate, kmol
n = number of collocation points
N = number of stages in the separation unit
R = reflux rate, kmol/h
T^L = liquid temperature, K
T^V = vapor temperature, K
t = time, h
V = vapor flow rate, kmol/h
x_i = mole fraction of ith component (liquid)
y_i = mole fraction of ith component (vapor)
z = spacial variable, m
Δz = spacial increment for PDE approximation, m
$\delta(x_i)$ = average molar density of liquid, kmol/m^3
δw = height of liquid over the Weir, m

APPENDIX A: DIFFERENCES IN COLLOCATION APPROXIMATIONS

Consider the steady-state component balance equation:

$$\frac{d}{dz}(Lx_i - Vy_i) = 0 \tag{A1}$$

The equation can be expanded to give

$$L\frac{dx_i}{dz} + x_i\frac{dL}{dz} - V\frac{dy_i}{dz} - y_i\frac{dV}{dz} = 0 \tag{A2}$$

Although the two equations are mathematically identical, collocation approximation will yield different solutions. In particular, collocation using Eq. A2 will violate the steady-state mass balance requirement.

For example, consider the problem

$$\frac{d}{dz}(Lx) = 0, \quad L = 1 + z \tag{A3}$$

with boundary condition

$$x(z = 0) = 3$$

which has the solution

$$L(z)x(z) = L(0)x(0) = 3 \tag{A4}$$

Applying the orthogonal collocation method we get

$$\sum_{k=1}^{n+2} A_{jk}L_k x_k = 0 \tag{A5}$$

which has the solution (as proved in the previous paper)

$$L_k x_k = L(0)x(0) = 3 \tag{A6}$$

Hence, collocation here gives the exact solution. Now consider the decomposed form of equation.

$$L\frac{dx}{dz} + x\frac{dL}{dz} = 0 \tag{A7}$$

Applying collocation to this equation, we get

$$L_j \sum_{k=1}^{n+2} A_{jk}x_k + x_j \sum A_{jk}L_k = 0$$

which is different from Eq. A6. Equation A8 is a poor approximation to the solution as can be seen from the solution to one point collocation. Choosing $\alpha = 1$, $\beta = 1$ for the Jacobi polynomial gives

$$\underline{A} = \begin{bmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{bmatrix} \text{with collocation point at } z = 0.5$$

Thus, the collocation equations can be written

$$L_2(-x_1 + x_3) + x_2(-L_1 + L_3) = 0 \tag{A9a}$$

$$L_3(x_1 - 4x_2 + 3x_3) + x_3(L_1 - 4L_2 + 3L_3) = 0 \tag{A9b}$$

Solution to these equations is

$$x_2 = 2.3684$$

$$x_3 = 1.5789$$

The exact solution is given by $x_2 = 2$, $x_3 = 1.5$

APPENDIX B: ALGEBRAIC EXPRESSION FOR ENERGY BALANCE EQUATION

The energy balance equation at collocation point z_j is given by

$$M\frac{dh_j}{dt} = \sum_{k=1}^{n+2} A_{jk}(H_k V_k - h_k L_k) - h_j \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) \tag{B1}$$

Expansion of the term $\frac{dh_j}{dt}$ by the chain rule gives:

$$\frac{dh_i}{dt} = \frac{\partial h_j}{\partial T}\frac{dT_j}{dt} + \sum_{i=1}^{c} \frac{\partial h_j}{\partial x_{ij}}\frac{dx_{ij}}{dt} \tag{B2}$$

where c is the number of components.

To obtain $\frac{dT_j}{dt}$, differentiating the bubble point relation gives:

$$\begin{aligned} \frac{d}{dt}\left(\sum_{i=1}^{c} K_{ij}x_{ij}\right) &= \sum_{i=1}^{c}\left[x_{ij}\frac{dK_{ij}}{dt} + K_{ij}\frac{dx_{ij}}{dt}\right] \\ &= \sum_{i=1}^{c}\left[x_{ij}\frac{\partial K_{ij}}{\partial T}\frac{dT_j}{dt} + K_{ij}\frac{dx_{ij}}{dt}\right] \\ &= 0 \end{aligned} \tag{B3}$$

Solving for $\frac{dT_j}{dt}$ from Eq. B3, we get:

$$\frac{dT_j}{dt} = -\frac{\sum_{i=1}^{c} K_{ij}\frac{dx_{ij}}{dt}}{\sum_{i=1}^{c} x_{ij}\frac{\partial K_{ij}}{\partial T}} \tag{B4}$$

Substituting Eq. B4 into Eq. B3 yields:

$$\frac{dh_j}{dt} = -\frac{\partial h_j}{\partial T}\frac{\sum_{i=1}^{c} K_{ij}\frac{dx_{ij}}{dt}}{\sum_{i=1}^{c} x_{ij}\frac{\partial K_{ij}}{\partial T}} + \sum_{i=1}^{c}\frac{\partial h_j}{\partial x_{ij}}\frac{dx_{ij}}{dt} \tag{B5}$$

where $\frac{dx_{ij}}{dt}$ is given in the text by

$$M\frac{dx_{ij}}{dt} = \sum_{k=1}^{n+2} A_{jk}(V_k y_{ik} - L_k x_{ik}) - \sum_{k=1}^{n+2} A_{jk}(V_k - L_k) \tag{B6}$$

Combining Eqs. B1, B5 and B6

$$\begin{aligned} &\sum_{k=1}^{n+2} A_{jk}\left(\sum_{i=1}^{c} \alpha_{ij}y_{ik} + H_k - B_j\right)V_k \\ &\qquad = \sum_{k=1}^{n+2} A_{jk}\left(\sum_{i=1}^{c} \alpha_{ij}x_{ik} + h_k - B_j\right)L_k \end{aligned} \tag{B7}$$

where the coefficients α_{ij}'s and B_j's are given by

$$\alpha_{ij} = \frac{\partial h_j/\partial T}{\sum_{i=1}^{c} x_{ij}\frac{\partial K_{ij}}{\partial T}} K_{ij} - \frac{\partial h_j}{\partial x_{ij}} \tag{B8}$$

$$B_j = \sum_{i=1}^{c} \alpha_{ij}x_{ij} + h_j \tag{B9}$$

Equation B7 can be restated using a simple splitting to give (noting that boundary conditions give V_{n+2} and $y_{i,n+2}$):

$$\begin{aligned} &\sum_{k=1}^{n+1} A_{jk}\left(\sum_{i=1}^{c} \alpha_{ij}y_{ik} + H_k - B_j\right)V_k \\ &\qquad = \sum_{k=1}^{n+2} A_{jk}\left(\sum_{i=1}^{c} \alpha_{ij}x_{ik} + h_k - B_j\right)L_k \\ &\qquad - A_{j,n+2}\left(\sum_{i=1}^{c} \alpha_{ij}y_{i,n+2} + H_{n+2} - B_j\right)V_{n+2} \end{aligned} \tag{B10}$$

Equation B10 can be rewritten in matrix form

$$\boldsymbol{GV} = \boldsymbol{PL} - V_{n+2}Q$$

where

$\boldsymbol{G}$ is a $(n + 1)x(n + 2)$ matrix,

$\boldsymbol{P}$ is a $(n + 1)x(n + 2)$ matrix,

$\boldsymbol{L}$ is a $(n + 2)$ vector, and

V and Q are $(n + 1)$ vectors

Solving Eq. B11 for V_j, we have

$$\begin{aligned} \boldsymbol{V} &= \boldsymbol{G}^{-1}\boldsymbol{PL} - \boldsymbol{G}^{-1}\boldsymbol{O}V_{n+2} \\ &= \boldsymbol{RL} - \boldsymbol{S}V_{n+2} \end{aligned} \tag{B12}$$

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