ρ = density
τ = sampling interval

Mathematical Symbols

rank[ ] = rank of matrix
E[ ] = expectation

LITERATURE CITED

Burnett, R. L., H. L. Steinmertz, E. M. Blue, and J. J. Noble, "An analog computer model of conversion in a catalystic reformer," *The devision of Petroleum Chemistry, American Chemical Society*, Detroit, (Apr., 1965).

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Reduced-Order Steady-State and Dynamic Models for Separation Processes

Part I. Development of the Model Reduction Procedure

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One of the major difficulties with mathematical models of staged separation systems is the large dimensionality of the process model. This paper is concerned with simple (reduced-order) steady-state and dynamic models for processes such as distillation, absorption and extraction. The model reduction procedure is based on approximating the composition and flow profiles in the column using polynomials rather than as discrete functions of the stages. The number of equations required to describe the system is thus drastically reduced. The method is developed using a simple absorber system. In the second part of this paper, the application of the method to nonlinear multicomponent separation systems is demonstrated.

SCOPE

The literature on modeling of stage separation systems is quite extensive. A number of fast, efficient algorithms have been developed for solving the large set of equations resulting from a tray-by-tray model both in the steady state as well as in the dynamics. Yet there exists a need for reduced-order models for two reasons. In cases involving optimization of systems involving more than one column or a single large column, the computation involving the steady-state simulation of these columns can be extremely time-consuming. In the case of dynamic simulation, most of the integration packages deal with a single column. But in dynamic simulation the interaction with other units is very important and it is desirable to treat the column as part of a large network of units each described by a set of differential equations. Hence it is desirable to use a general purpose integration package for the dynamic simulation. In such instances, a reduced order model is preferable to making modifications to the integration package.

This paper is concerned with reduced-order approximations to the rigorous stage-by-stage models. Two approaches are developed in this paper. The first is based on approximating the tray-by-tray differential-difference equations by a set of partial differential equations. These partial differential equations are in turn solved by the orthogonal collocation method. In the second approach, the model reduction is achieved by a direct transition to polynomial representation of the composition and flow profiles in the column.

In this paper, we examine: (1) the accuracy of different approximation procedures used for generating the reduced-order models; (2) the significance of the type and degree of the polynomials used in the orthogonal collocation procedure; and (3) the ability of the reduced-order models to approximate the rigorous model both in the steady state and in the dynamics.

CONCLUSIONS AND SIGNIFICANCE

The number of equations required to describe the behavior of staged separation systems can be drastically reduced by the approximation procedure developed here. Preliminary experimentation using selected test examples show excellent agreement between the rigorous model and the simplified model both in the steady-state and in the dynamic response to identical step, sinusoidal and random input disturbances. The accuracy of the approximation can be improved by appropriate choice of the PDE approximation and the type of polynomials used in the model reduction.

The work is of considerable significance to practitioners involved in the modeling of staged separation systems. The reduced-order steady-state models are useful in the simulation and optimization of processes having large multicomponent distillation columns or interconnected separation trains. The reduced-order dynamic models would allow the study of dynamic systems hitherto considered difficult because of the large dimensionality of the equations involved. Application areas include the study of process interaction, analysis and troubleshooting of startup and shutdown operations, safety and reliability analysis, design and testing of control strategies, and process identification using transient responses.

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BACKGROUND

The literature on modeling of staged separation systems is quite extensive. A large number of well known texts exist in the area of steady-state modeling. Most of these books also address the problem of solving the resulting equations (for example, Holland, 1975). It is only recently that efficient procedures were developed to model the dynamic behavior of separation columns. Howard (1970) presents an excellent study of the simulation of unsteady-state behavior of multicomponent distillation columns and a comparison between theory and experimental results. Recently Ballard et al. (1978) and Seider and Prokopakis (1980) have presented efficient algorithms for the solution of these equations.

The need for reduced-order models is more important in dynamic simulation because of the large number of differential equations in a stagewise model and the stiffness associated with the widely differing time constants that exist in a column. A typical column may require well over 1,000 differential equations to describe its dynamics. Most of the time, the dynamic simulation is carried out using general purpose simulation packages which are limited in the number of differential equations that can be handled simultaneously. Even though one could design computers and software to deal with the problem, the average process engineer usually does not have access to such special purpose computer aids.

Process control engineers have traditionally used simple input-output models to represent the dynamics of complex chemical processes. This approach to developing simple models have largely been empirical. Step response or impulse response techniques are frequently employed. For distillation columns, Wahl and Harriot (1970) gave a set of correlation curves to obtain dominant poles and zeroes. More recently, Waller (1979) presented correlations in the frequency domain. Williams and his colleagues at Purdue University have developed methods for estimating the 60% response time of distillation columns (Weigand et al., 1972).

In this paper, we use an approach to model reduction based on the idea that a separation column can be approximated as a distributed system in which the composition and flow profiles can be represented as continuous variables along the length of the column. This allows the variables to be expressed as polynomials and leads to a wide variety of model reduction procedures.

The concept is derived from the use of partial differential equations to approximate column dynamics. Armstrong and Wilkinson (1958) used this approach to derive the response of binary distillation columns to upsets in feed composition. The partial differential equations were solved by the Laplace transform method. Brosilow and his colleagues (Holt, 1966; Brosilow et al., 1968) showed that one could derive many types of partial differential equations from the differential-difference model of the staged system. Friedly (1972) termed this approach "inverse quantization." He used it for obtaining the approximate response of staged extraction columns. Osborne (1971) used the partial differential equations in a dynamic simulation model of the column. The equations were solved by finite differencing in time and space. Osborne was motivated by the desire to keep the time step large enough (for explicit integration methods) and he achieved this by finite differenceing the spatial derivatives with step sizes smaller than the height of a tray.

Recently, Wong and Luss (1980) published a model reduction procedure based on the orthogonal collocation procedure. The method is applicable to equations of the form

$$\frac{dx}{dt} = Ax$$

where A is a tridiagonal matrix. Simple gas absorption problems can be reduced to this form with matrix A containing constant coefficients. One difficulty with this approximation procedure (as demonstrated later) is that it does not preserve material balance in the steady state. Even though the error incurred is small, it accumulates over a period of time and can cause serious difficulties especially when applied to nonlinear systems. Nevertheless Wong and Luss were able to demonstrate that considerable reduction in the number of equations can be achieved by this reduction procedure.

It is not necessary to derive the partial differential equations to apply the polynomial approximation procedure. In fact it may be more convenient to go directly to the polynomial approximation. As demonstrated later, this approach yields better results.

From our objective, that of obtaining simpler reduced-order models, this approach is very convenient. By varying the order of approximation (degree of polynomials), we can obtain solutions of varying accuracy and dimensionality. The number of equations is directly proportional to the order of approximation. There is another subtle, yet significant gain that is obtained by this model reduction procedure. In the process of approximation (as demonstrated below) the number of stages and the feed location are absorbed as continuous parameters.

Previously, these variables took on discrete values and the number of equations depended on these parameters. For example, if we wanted to design a column, the number of stages had to be specified first before the equations could be written and the other variables calculated. Thus, the calculation of the number of stages required for a given separation involves trial-and-error calculations.

From an optimization viewpoint, it is very inconvenient to have some variables that take on only discrete values and that influence the structure of the equation set. With the polynomial approximation, we can utilize the more efficient packages available for optimization of continuous variables. The designer could, for example, specify a certain separation and choose the number of stages and feed location to yield the least costly solution.

For the dynamic models, the polynomial approximation yields a reduced set of ordinary differential equations. More importantly, this reduced set of equations can be generated fully automatically on a digital computer without the user having any knowledge of the polynomial approximation procedure. Thus it becomes easy to simulate such models using general-purpose dynamic simulation packages.

DEVELOPMENT OF PDE APPROXIMATION PROCEDURES

The following development is based on a simple gas-absorption system (Figure 1). For this system, it is easy to derive some analytical results which are useful in making comparisons. The extension to complex, nonlinear systems is carried out in Part II of this paper. We make the simplifying assumptions of dilute gas and liquid solution so that liquid and vapor flows can be considered constant, constant molal holdup, isothermal operation with negligible heat effects and ideal stages. With these assumptions the component balance equation can be written as (Figure 1)

$$M_j \frac{dx_j}{dt} = L(x_{j-1} - x_j) + V(y_j - y_{y-1}) \tag{1a}$$

This must be solved in conjunction with the equilibrium relations

$$y_{j-1} = Kx_j \tag{1b}$$

with boundary conditions

$$x(j = 0) = x_0, \quad y(j = N) = y_N$$

The PDE approximation can be obtained by assuming that x and y are continuous variables of the spatial variable, z (Figure 1).

A first-order approximation can be obtained by expanding some of the terms in Eq. 1 using only the first-order terms in a Taylor series expansion:

$$x_{j-1} = x_j - \frac{\partial x}{\partial z}\Delta z \tag{2a}$$

$$y_{j-1} = y_j - \frac{\partial y}{\partial z}\Delta z \tag{2b}$$

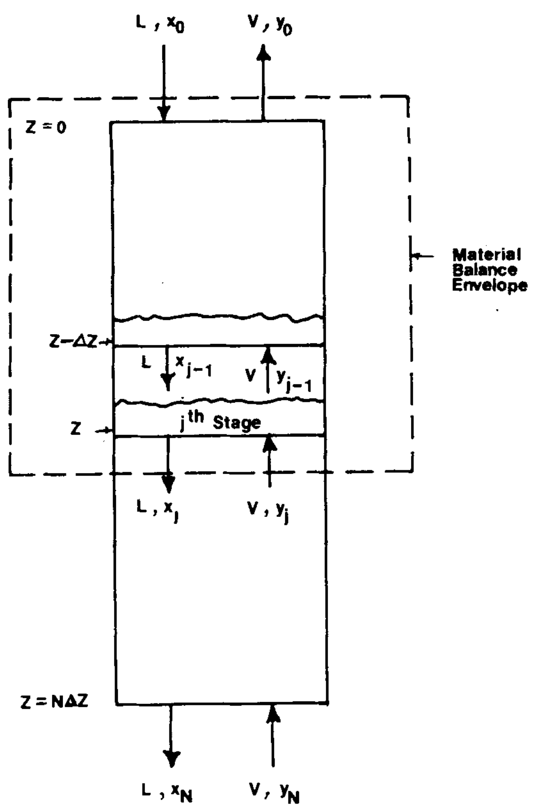

Figure 1. Variables used in modeling the absorber.

where Δz is the height of a stage. When these are substituted into Eq. 1 we get

$$M\frac{\partial x}{\partial t} = V\frac{\partial y}{\partial z} - L\frac{\partial x}{\partial z} \tag{3a}$$

where M is holdup per unit distance ($M = M_j/\Delta z$) and

$$y = Kx + \frac{\partial y}{\partial z}\Delta z \tag{3b}$$

with boundary conditions

$$x(z = 0) = x_0 \qquad y(z = N\Delta z) = y_N$$

To be mathematically rigorous, the variables x_j and y_j are discrete functions of position and the Taylor expansion is not strictly valid. However, this may be viewed as the inverse of finite differencing (inverse quantization). The difference equation then becomes one of the many possible approximations to the partial differential equation.

We can arbitrarily select $\Delta z = 1$. The steady state solution of Eq. 1 is given by the familiar Kremser equation (McCabe and Smith, 1976):

$$y_N = \frac{1 - A^{N+1}}{1 - A}y_0 - \frac{A - A^{N+1}}{1 - A}y_0^* \tag{4}$$

where $A = L/KV$, $y_0^* = Kx_0$
A more convenient form for comparison is obtained by solving for N from Eq. 4

$$N = \frac{\log[(y_N - y_N^*)/(y_0 - y_0^*)]}{\log A} \tag{5}$$

The steady-state solution to the PDE approximation (Eq. 3) is given by

$$N = \frac{\log[(y_N - y_N^*)/(y_0 - y_0^*)]}{(1 - 1/A)} \tag{6}$$

The two solutions differ in the denominator terms. The accuracy of the approximation may be estimated by expanding both terms in powers of $(A - 1)$,

$$\log A = (A - 1) - \frac{(A - 1)^2}{2} + \frac{(A - 1)^3}{3}\ldots$$

$$1 - \frac{1}{A} = (A - 1) - (A - 1)^2 + (A - 1)^3\ldots$$

Thus, the approximation is valid if $A - 1$ is small. Note that A is the ratio of the slope of the equilibrium line (K) to that of the operating line (L/V). The approximation is valid if the two lines are nearly parallel. This usually implies a large number of stages as is also evident from Eqs. 5 and 6 where N will be large if $A \approx 1$. Fortunately this is also the case that we are interested in (columns with many plates).

This approximation has another remarkable property. At steady state, Eq. 3 can be written as

$$V\frac{dy}{dz} - L\frac{dx}{dz} = 0$$

or

$$\frac{d}{dz}(Vy - Lx) = 0$$

with the solution

$$(Vy - Lx)|_z = (Vy - Lx)|_{z=0}$$

which can be seen to be the requirement for component balance written around the envelope shown in Figure 1. This equation is automatically satisfied by the original Eq. 1. Stage-by-stage material balance implies overall material balance.

It is interesting to note here that the error in approximation is closely related to the approximation used for the equilibrium relationship. For example, if the equilibrium relationship is written as

$$y = Kx$$

we get the following for x:

$$M\frac{\partial x}{\partial t} = KV\frac{\partial x}{\partial z} - L\frac{\partial x}{\partial z}$$

The steady-state solution of this equation is given by

$$x = \text{constant}$$

which is considerably in error.

Next, consider higher order approximations. The simplest way to obtain a higher order approximation is to eliminate the variables y_j in Eq. 1a using Eq. 1b to get

$$M\frac{dx_j}{dt} = Lx_{j-1} - (L + KV)x_j + KVx_{j+1} \tag{7}$$

The terms x_{j-1} and x_{j+1} are expanded by including the second order terms of the Taylor series

$$x_{j-1} = x_j - \Delta z\frac{\partial x}{\partial z} + \frac{(\Delta z)^2}{2}\frac{\partial^2 x}{\partial z^2}$$

$$x_{j+1} = x_j + \Delta z\frac{\partial x}{\partial z} + \frac{(\Delta z)^2}{2}\frac{\partial^2 x}{\partial z^2}$$

with the resulting equation (cf., Wong and Luss, 1980)

$$M\frac{\partial x}{\partial t} = \frac{1}{2}(KV + L)\frac{\partial^2 x}{\partial z^2} + (KV - L)\frac{\partial x}{\partial z} \tag{8a}$$

the steady-state solution of which is given by

$$x = x_0 - \frac{x_0 - x_{N+1}}{1 - e^{-\alpha}}(1 - e^{-\alpha z}) \tag{8b}$$

with

$$\alpha = \frac{2(KV - L)}{KV + L} \text{ and } x_{N+1} = y_N/K$$

This solution does not satisfy the equation

$$(Lx - Vy)|_z = (Lx - Vy)|_{z=0}$$

This causes some severe problems because mass is "lost" between stages. Even when the error introduced is small, it can accumulate over a period of time causing considerable error in the final answers if one is looking at the transient behavior of the system.

However, it is possible to generate higher-order approximations which do preserve the material balance property. We can rewrite Eq. 1a as

$$M_j\frac{dx_j}{dt} = (Lx_{j-1} - Vy_{j-1}) - (Lx_j - Vy_j) \tag{9}$$

consider the new variable

$$u = Lx - Vy \tag{10}$$

Then Eq. 9 becomes

$$M_j\frac{dx_j}{dt} = u_{j-1} - u_j \tag{11}$$

which can be approximated as

$$M\frac{\partial x}{\partial t} = -\frac{\partial u}{\partial z} + \frac{1}{2}\frac{\partial^2 u}{\partial z^2} \tag{12}$$

At steady state

$$\frac{1}{2}\frac{d^2u}{dz^2} - \frac{du}{dz} = 0 \text{ with } u\,(z = 0) = u(z = N) = \text{constant} \tag{13}$$

with the solution

$$u = \text{constant}$$

which implies overall material balance:

$$Lx - Vy = \text{constant}$$

Other second order approximations can be generated by using Eq. 2a and expanding y_{j-1} in a Taylor series involving higher derivatives. These also preserve overall material balance. We will consider some of these later in the example problems.

POLYNOMIAL APPROXIMATION USING ORTHOGONAL COLLOCATION

While the PDE approximation represents the model in compact form, it is difficult to solve analytically even for simple problems such as the one discussed above. Hence, we look for numerical solutions by discretization in space and time variable. Discretization by finite-differencing in space leads to large number of equations as shown by the studies of Holt (1968) and Osborne (1971). (The spatial step size must be kept small to retain accuracy.) The alternative here is to discretize using orthogonal collocation which is particularly suited for machine computation when compared with other approximation methods based on the method of weighted residuals (Finlayson, 1972).

The collocation approximation is obtained as follows. The variables x and y are expressed in terms of Lagrange polynomials $l_k\,(z), k = 1, 2, \ldots n + 2$

$$x(z,t) = \sum_{k=1}^{n+2} l_k(z)x_k(t) \tag{14}$$

where

$x_k(t)$ = value of x evaluated at collocation point $z = z_k$

The collocation points are chosen as the zeroes of orthogonal Jacobi polynomials $P_n^{(\alpha,\beta)}(z)$ defined by

$$\int_0^1 z^\beta(1 - z)^\alpha z^j P_n^{(\alpha,\beta)}(z)dz = 0 \tag{15}$$

$$j = 0, 1, \ldots n - 1$$

This particular selection of collocation points leads to approximations which are comparable in accuracy to the Galerkin method (Villadsen, 1978). The choice of α and β is discussed later.

Differentiating Eq. 14 we get:

$$\left.\frac{\partial x}{\partial z}\right|_{z=z_j} = \sum_{k=1}^{n+2} A_{jk}x_k(t) \tag{16}$$

where $A_{jk} = dl_k/dz\,|_{z=z_j}$ by definition. Similarly

$$\left.\frac{\partial^2 x}{\partial z^2}\right|_{z=z_j} = \sum_{k=1}^{n+2} B_{jk}x_k(t) \tag{17}$$

where $B_{jk} = d^2l_k/dz^2|_{z=z_j}$. Coefficients A_{jk} and B_{jk} are fixed once the collocation points are selected.

Substituting the derivative expansions (Eq. 16) into Eq. 3 gives:

$$M\frac{dx_j}{dt} = V\left(\sum_{k=1}^{n+2} A_{jk}y_k\right) - L\left(\sum_{k=1}^{n+2} A_{jk}x_k\right) \tag{18a}$$

$$j = 2, 3, \ldots n + 2$$

$$y_j = Kx_j + \left(\sum_{k=1}^{n+2} A_{jk}y_k\right) \tag{18b}$$

$$j = 1, 2, \ldots n + 1$$

Equation 18 represents the final reduced-order model for the original system. The state variables are the liquid mole fractions x_j evaluated at the collocation points. There will be a reduction in the order of the system if the number of collocation points is smaller than the number of stages N. There is reason to expect that this will generally be the case since collocation has been shown to work better than finite differencing for many problems in chemical reaction engineering.

The discretization using orthogonal collocation introduces another level of approximation. It is important that overall mass balances be met by the new approximated set of equations as well. Again *only certain* types of collocations will meet this criteria. This is demonstrated next.

At steady state

$$V\left(\sum_{k=1}^{n+2} A_{jk}y_k\right) - L\left(\sum_{k=1}^{n+2} A_{jk}x_k\right) = 0 \tag{19}$$

$$j = 2, 3, \ldots n + 2$$

i.e.

$$\sum_{k=1}^{n+2} A_{jk}(Vy_k - Lx_k) = 0 \tag{20}$$

$$j = 2, 3, \ldots n + 2$$

Define

$$u_k = Vy_k - Lx_k$$

Then Eq. 20 becomes

$$\sum_{k=1}^{n+2} A_{jk}u_k = 0 \qquad j = 2, 3, \ldots n + 2 \tag{21}$$

It is proved in Appendix A that Eq. 21 has the unique solution

$$u_k = \text{constant}$$

or

$$Vy_k - Lx_k = \text{constant}$$

which satisfies the requirement for material balance written for every envelope of the type shown in Figure 1.

Choice of Polynomials

The location of the collocation points is determined by the choice of α and β in the Jacobi polynomials defined by Eq. 15. The best choice of α and β depends on the nature of the problem. For example if the variables are symmetric in z then $\alpha = 1, \beta = -0.5$ is the recommended choice. Since separation problems do not exhibit any symmetry in general, the choice of α and β will be governed by considerations of the accuracy of the solution. Choosing $\alpha = 1$, $\beta = 1$ gives symmetrically placed collocation points. Choosing β

> 1 puts more points closer to the boundary $z = 1$. Thus, if the composition profile shows stronger nonlinearity towards one end of the column, a choice of β greater than 1 would be recommended. This is borne out by the example studies below.

DIRECT REDUCTION USING POLYNOMIALS

The above reduction was based on the concept of first deriving a continuous approximation to the system of equations and then redescretizing 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 u are all continuous variables along the column. Modeling the column as consisting of discrete elements (trays) with discrete values of variables is just one way of modeling the system.

If we assume x is a continuous function of distance then polynomials can be used to approximate x. A convenient representation is using Lagrange polynomials $l_k(z)$. A polynomial function of degree $n + 1$ can be expressed in terms of Lagrange polynomials as

$$x(z) = \sum_{k=1}^{n+2} l_k(z)x_k \qquad (22)$$

where x_j represent x evaluated at $n + 2$ arbitrary points, z_j. The material balance equation for x can be written as:

$$M\left.\frac{\partial x}{\partial t}\right|_j = (Lx - Vy)_{z_j-\Delta z} - (Lx - Vy)_{z_j} \qquad (23)$$

Noting that Eq. 22 represents x in terms of $n + 2$ unknowns x_k, we only need $n + 2$ equations to solve for this approximation to the solution. Here we have a choice since Eq. 23 is valid at all trays ($j = 1$ to N). In the development that follows, we assume that Eq. 23 is valid at the $n + 2$ arbitrary points z_j selected to express the polynomials $x(z)$ in Eq. 22. Comparison with the development in the previous section indicates that choosing these points to be zeroes of orthogonal polynomials will improve the accuracy of the solution.

Application of Eq. 23 at points z_j, gives the following set of equations

$$M\frac{d}{dt}\left(\sum_{k=1}^{n+2} l_k(z_j)x_k\right) = \sum_{k=1}^{n+2} [l_k(z_j - \Delta z) - l_k(z_j)][Lx_k - Vy_k] \qquad (24)$$

But the Lagrange functions have the property:

$$\sum_{k=1}^{n+2} l_k(z_j)x_k = x_j$$

and Eq. 24 becomes

$$M_j\frac{dx_j}{dt} = \sum_{k=1}^{n+2} [l_k(z_j - \Delta z) - l_k(z_j)][Lx_k - Vy_k] \qquad (25)$$

Note that, once the points z_j are selected, the reduced-order model equations are obtained directly from Eq. 25. The Lagrange polynomials $l_k(z)$ determine the coefficients of the variables x_k and y_k on the RHS.

The advantage of this approach to model reduction is that it avoids the construction of an intermediate PDE. *Further*, the approximations obtained in the previous section can be derived from Eq. 25. The first-order approximation given earlier can be obtained by using a first-order expansion for $l_k(z_j - \Delta z)$:

$$l_k(z_j - \Delta z) = l_k(z_j) - \left.\frac{\partial l_k}{\partial z}\right|_{z=z_j}\cdot \Delta z$$

but

$$\left.\frac{\partial l_k}{\partial z}\right|_{z=z} = A_{jk}$$

as defined earlier. Hence the material balance equation becomes

$$\left(\frac{M_j}{\Delta z}\right)\frac{dx_j}{dt} = V\left(\sum_{k=1}^{n+2} A_{jk}y_k\right) - L\left(\sum_{k=1}^{n+2} A_{jk}x_k\right)$$

which is the same as Eq. 18a.

By introducing the approximation in Eq. 26, the accuracy of the reduced-order model is reduced. This is borne out further by the numerical example problems discussed below.

Equation 25 actually represents the highest order pde approximation possible using polynomials of degree $n + 1$. This is so because for a polynomial of degree $n + 1$, the derivatives of order $n + 2$ and higher vanish.

It is interesting to note that Eq. 25 is simpler to deal with computationally than the approximations given earlier. Using this approach the equilibrium relationship is approximated by:

$$y_{ij} = K\left[\sum_{k=1}^{n+1} l_k(z_j + \Delta z)x_k\right]$$

The material balance constraints are satisfied by this reduced-order model also.

EXAMPLES

It is difficult to derive analytical solutions to the dynamic equations either in the original form or after carrying out the model reduction procedure. Estimates of the accuracy of the approximation and the reduction in order achievable can be obtained by studying some example problems. First computer programs were written to solve the tray by tray equations as well as the reduced-order collocation approximation. The steady state profiles as well as transient response of the system to various input disturbances were then compared using the simulation models.

Two example problems were studied, the first consisting of nine theoretical stages and the second consisting of 20 theoretical stages. The operating conditions of these simple gas absorbers are shown in Table 1. A semi-implicit Runge-Kutta method was used to integrate the equations (Ballard et al., 1979).

Comparison of Steady-State Profiles

Figure 2 compares the steady-state profiles of the reduced-order models with that of the rigorous solution. Different polynomial approximations (Direct Reduction) were tried, Figure 2, and all polynomials gave excellent agreement in the steady state. There is a slight improvement in using higher values of β which tends to move the collocation points closer to the region of high nonlinearity but this improvement is small. The important conclusion from this study is that the reduction procedure is remarkably accurate in the steady state. These reductions utilized three collocation points. In example 2 this implies a reduction in the number of equations by a factor of five.

Step Response Studies

Figures 3 and 4 compares the step-response of the rigorous model with different reduced-order models. The disturbance was a step increase in feed liquid concentration. The rigorous model exhibits a time delay (due to the 20 plates) and then a second-order response.

TABLE 1. STEADY-STATE OPERATING CONDITIONS OF EXAMPLES

	Example 1	Example 2
No. of Stages	9	20
Liquid Flow Rate, kmol/h	2.4×10^5	1.8×10^5
Vapor Flow Rate, kmol/h	1.5×10^5	2.4×10^5
Equilibrium Constant	1.0	0.6
Step Disturbance	Increase x_0 by 0.1	Increase x_0 by 0.1
Initial Profile	$x = 0$ for all z	$x = 0$ for all z

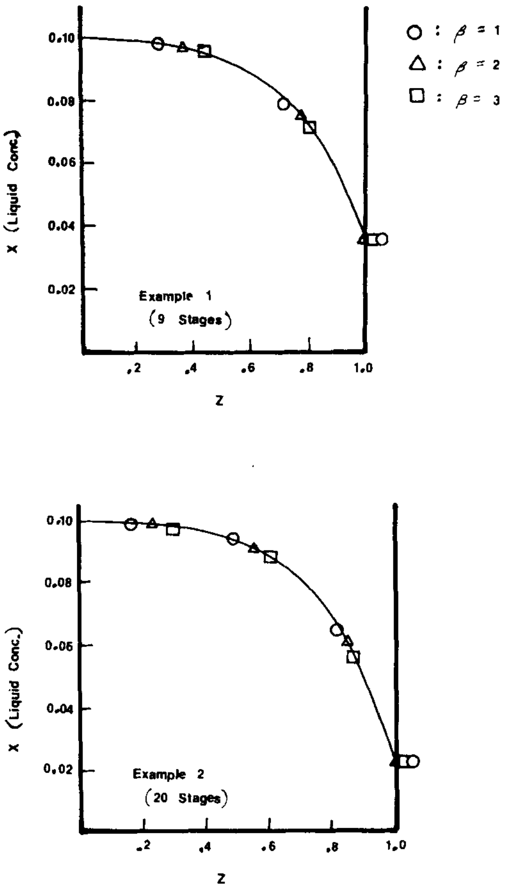

Figure 2. Comparison of steady-state profiles obtained from stage-by-stage calculations with that of the reduced-order model using three-point collocation.

TABLE 2. ERROR IN STEP RESPONSE FOR DIFFERENT PDE APPROXIMATION (USING 3-POINT COLLOCATION, $\alpha = 1$, $\beta = 3$, EXAMPLE PROBLEM 2)

Approximation	Max. Error % of Steady-State Value	Steady-State Error
1. $M\frac{\partial x}{\partial t} = V\frac{\partial y}{\partial z} - L\frac{\partial x}{\partial z}$ $y = Kx + \Delta z\frac{\partial y}{\partial z}$	6.6%	3.9%
2. $M\frac{\partial x}{\partial t} = V\frac{\partial y}{\partial z} - L\frac{\partial x}{\partial z}$ $y = Kx + \Delta z\frac{\partial y}{\partial z} - \frac{(\Delta z)^2}{2}\frac{\partial^2 y}{\partial z^2}$	4.5%	3.1%
3. $M\frac{\partial x}{\partial t} = V\frac{\partial y}{\partial z} - L\frac{\partial x}{\partial z}$ $y = Kx + K\Delta z\frac{\partial x}{\partial z}$	7.5%	4.2%
4. $M\frac{\partial x}{\partial t} = V\frac{\partial y}{\partial z} - L\frac{\partial x}{\partial z}$ $y = Kx + K\Delta z\frac{\partial x}{\partial z} + \frac{K(\Delta z)^2}{2}\frac{\partial^2 x}{\partial z^2}$	4.9%	0.2%
5. Direct Reduction $M\frac{dx_j}{dt} = \sum_{k=1}^{n+2}[l_k(z_j - \Delta z) - l_k(z_j)][Lx_k - Vy_k]$ $y_j = K\left[\sum_{k=1}^{n+2} l_k(z_j + \Delta z)x_k\right]$	0.5%	0.2%

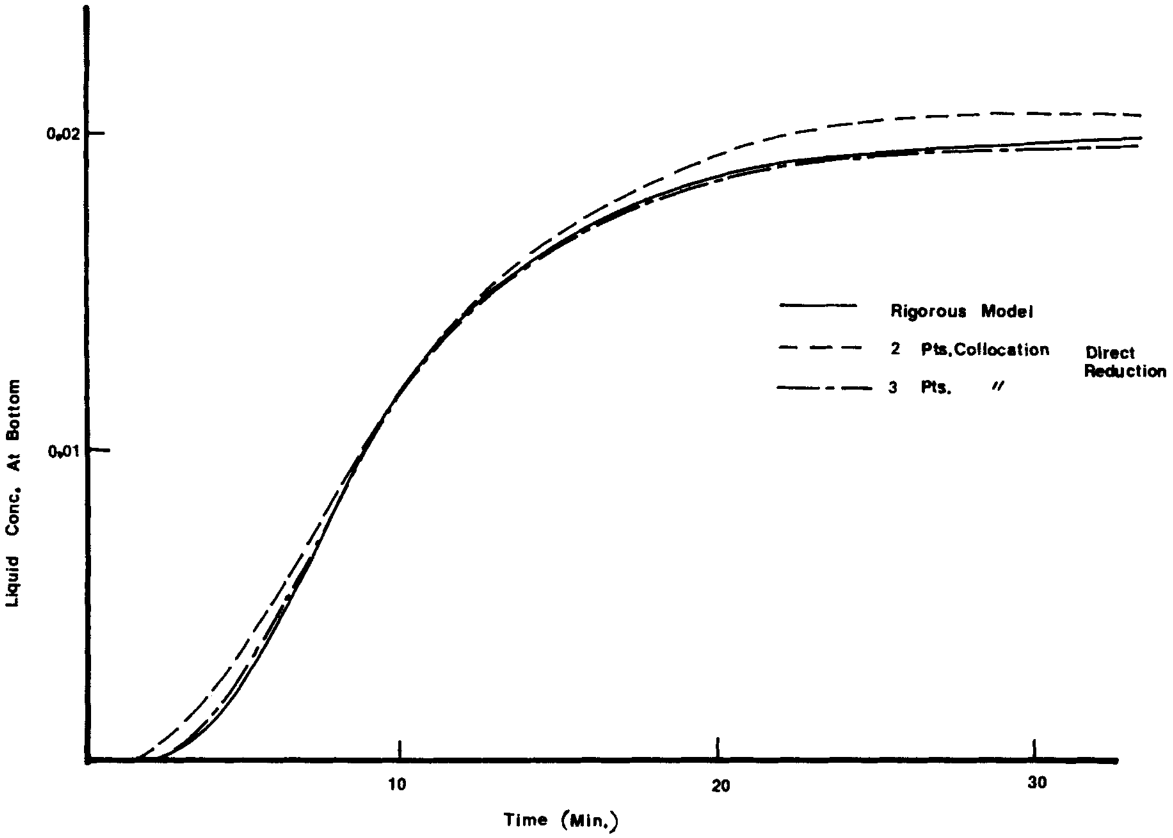

Figure 3. Responses of the liquid concentration at bottom of the absorber to a step change in the liquid feed concentration for example 2.

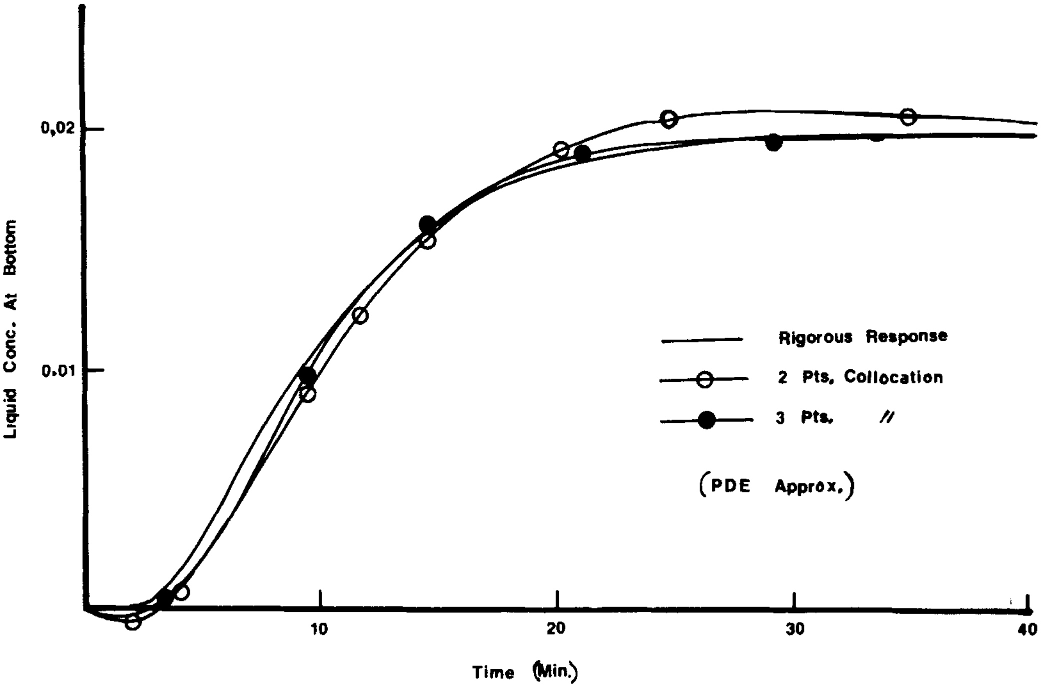

Figure 4. Responses of the liquid concentration at bottom of the absorber to step change in feed concentration (example 2).

Figure 3 compares the step response of the models obtained by direct reduction procedure with the response of the rigorous model. With two points there is some error in the transient as well as in the steady state. With three collocation points the agreement between the two models is quite good, in the transient as well as in the steady state.

Figure 4 compares the responses obtained from the PDE approximation models. While the agreement is good in the steady state, there is a disturbing inverse response. This inverse term is a result of the attempt to approximate the time delay term. The inverse term tended to decrease with increasing order of approximation. It was also found to be sensitive to the choice of β in the polynomial approximation.

Table 2 compares the maximum error as well as steady-state error during the transient for various types of approximations. All these approximations preserve material balance in the steady state.

The conclusions to be drawn from these comparisons are: (1) the direct reduction procedure preserves the accuracy even in the dynamic case for this example; and (2) the PDE approximation procedures tend to give higher errors both in the transient and steady state.

One-point collocation was also tried on these example problems. The errors incurred were of the order of 15%. It was noted that two point collocation was sufficient to model the column in example 1 whereas three points modeled the column in example 2 quite well. The actual choice of the number of collocation points to be used will be guided by the size of the column, the accuracy desired

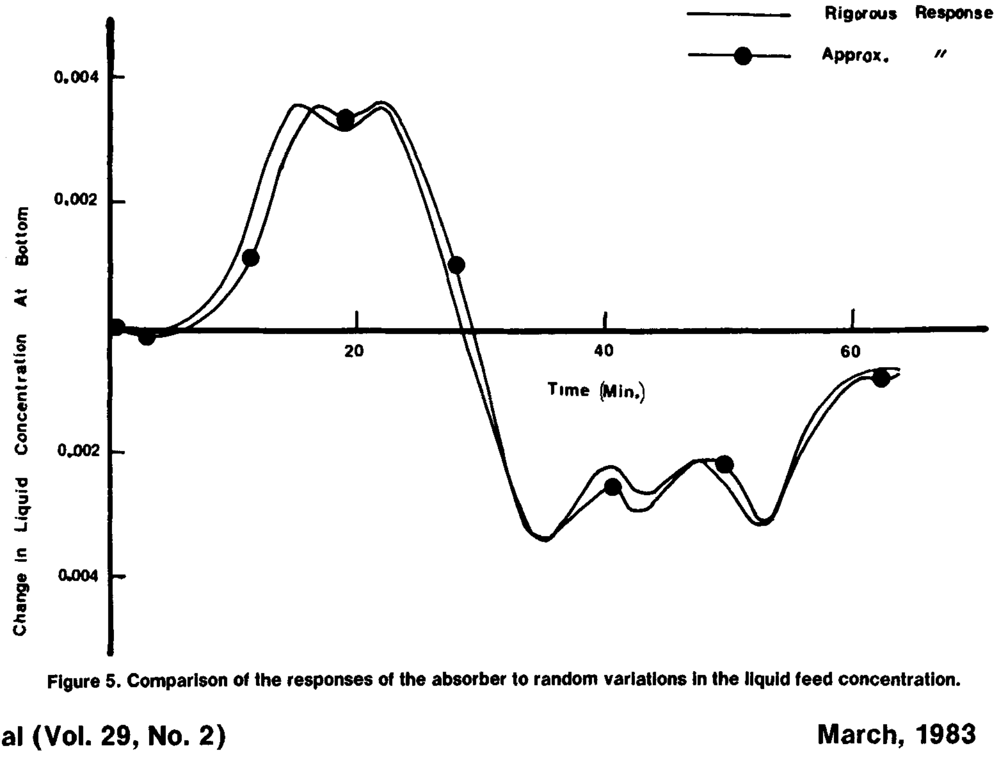

Figure 5. Comparison of the responses of the absorber to random variations in the liquid feed concentration.

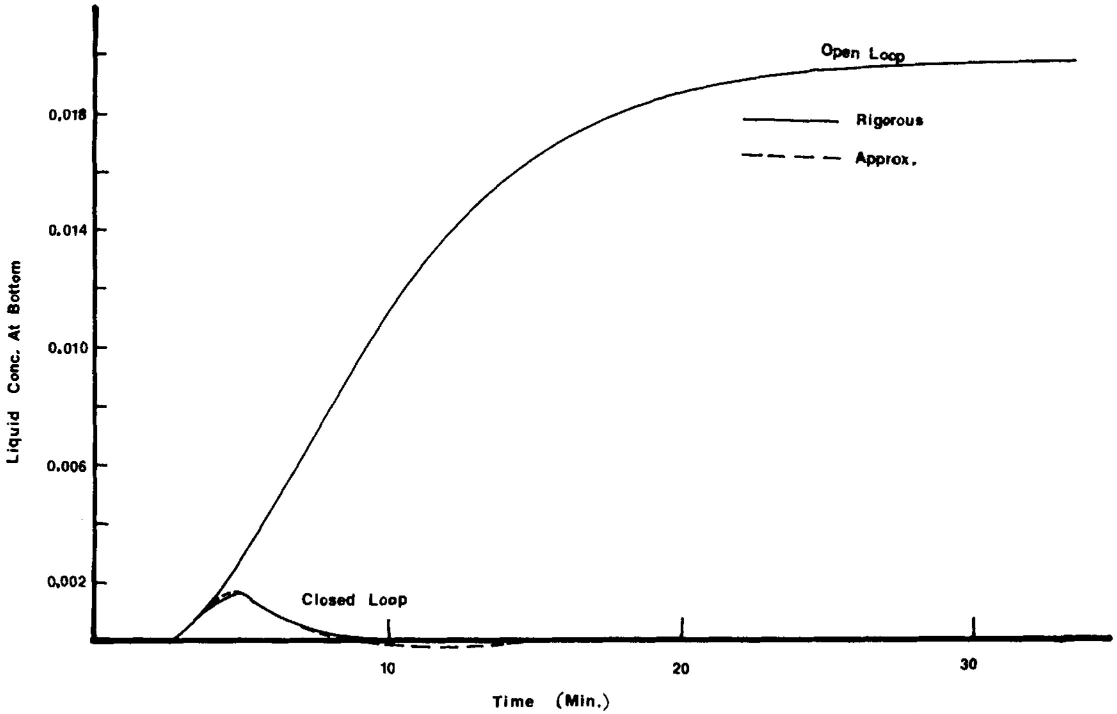

Figure 6. Results of a control study. The liquid concentration at bottom was controlled using the vapor flow input.

and, if the information is available, comparison of steady state profiles.

Response to Random Disturbances

From a dynamic simulation point of view, the ability of the model to predict the response to randomly changing inputs is important. To this end, both the rigorous model and the approximation model (no. 4, Table 2) was subjected to random-step input disturbances. The approximation model is able to track the variations in the output remarkably well, Figure 5.

Control System Studies Using Reduced Model

To further demonstrate the use of the reduced model, the response of the models were compared in a closed-loop system. The attempt here was to control the liquid concentration at the bottom. Figure 6 shows the response of the closed-loop system using the rigorous model and the reduced model. Identical proportional-integral controller was used in both cases. The responses compare well, although the reduced-order model exhibited a longer tail before reaching steady state.

Discussion

The example problems discussed above, while simple in nature, bring out the basic characteristics of the approximation procedure. The tests indicate that: (1) a large decrease in model dimensionality can be achieved without sacrificing the model accuracy; (2) two or three collocation points are generally sufficient to approximate the system; (3) the approximation is better for larger columns since as the number of stages increased the system approaches a truly distributed nature; (4) among all the approximation procedures studied, the direct reduction gives the best results; and (5) the accuracy of the approximation is improved by placing the collocation points where the nonlinearity is more pronounced.

It is to be recognized that this model reduction procedure is not intended as a substitute for rigorous models, but as a supplement in dealing with columns that require a large amount of computation. Packages do exist that can simulate steady-state or dynamic behavior of such columns which may be reasonable to use if a large number of simulations are not contemplated. The reduced-order models proposed here will be valuable when the computational time becomes the limiting factor, as in the optimization or dynamic testing of large process systems.

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NOTATION

A_{jk} = numerical value of $\frac{dl_k}{dz}$ evaluated at collocation point z_j

B_{jk} = numerical value of $\frac{d^2l_k}{dz^2}$ evaluated at collocation point z_j

K = vapor-liquid equilibrium constant
l_k = Lagrange polynomial for collocation point z_k
L = liquid flowrate (kmol/min)
M = Liquid holdup per unit length of the column ($M_j/\Delta z$)
M_j = liquid holdup on jth plate (kmol)
N = total number of stages
V = vapor flowrate (kmol/min)
x_j = liquid mole fraction of first component on jth plate
y_j = vapor mole fraction of first component on jth plate
Δz = spacial increment for PDE approximation (m)

APPENDIX A: EFFECT OF COLLOCATION APPROXIMATION ON STEADY-STATE MASS BALANCE

For the absorber problem treated in this paper, the steady-state mass balance requires that

$$Lx_i - Vy_i = \text{constant} \tag{A1}$$

at each section of the absorber. Consider the PDE approximation:

$$M\frac{\partial x}{\partial t} = \frac{\partial}{\partial z}(Lx) - \frac{\partial}{\partial z}(Vy) \quad \text{(A2)}$$

At steady state

$$\frac{d}{dz}(Lx) - \frac{d}{dz}(Vy) = 0 \quad \text{(A3)}$$

which can also be written as

$$\frac{d}{dz}(Lx - Vy) = 0 \quad \text{(A4)}$$

Obviously, the equation satisfies condition A1. Let

$$u = Lx - Vy$$

Then at steady state

$$\frac{du}{dz} = 0 \quad \text{(A5)}$$

Applying orthogonal collocation

$$\sum_{k=1}^{n+2} A_{jk}u_k = 0 \qquad \text{for } j = 2, \ldots n+2 \quad \text{(A6)}$$

$$\sum_{k=2}^{n+2} A_{jk}u_k + A_{j1}u_1 = 0 \qquad \text{for } j = 2, \ldots n+2 \quad \text{(A7)}$$

This can be looked upon as $n + 1$ equations in $n + 1$ unknowns. In expanded form

$$\mathbf{B}\mathbf{u} + \boldsymbol{\alpha} u_1 = 0 \quad \text{(A8)}$$

where

$$\mathbf{B} = \begin{bmatrix} A_{22} & A_{23} & A_{2,n+2} \\ A_{32} & A_{33} & A_{3,n+2} \\ \vdots & & \\ A_{n+2,2} & A_{n+2,3} & A_{n+2,m+2} \end{bmatrix} \text{ and } \boldsymbol{\alpha} = \begin{bmatrix} A_{21} \\ A_{31} \\ \vdots \\ A_{n+2,1} \end{bmatrix}$$

A general relation for Lagrange polynomials is given by

$$\sum_{k=1}^{n+2} l_k(z) = 1 \qquad 0 \le z \le 1 \quad \text{(A9)}$$

Differentiating Eq. A9 with respect to z yields:

$$\sum_{k=1}^{n+2} \frac{d}{dz} l_k(z) = 0 \quad \text{(A10)}$$

At collocation point z_j

$$\sum_{k=1}^{n+2} \frac{d}{dz} l_k(z)|_{z=z_j} = 0 \quad \text{(A11)}$$

which implies

$$\sum_{k=1}^{n+2} A_{jk} = 0 \quad \text{(A12)}$$

since

$$A_{jk} = \frac{d}{dz} l_k(z)|_{z=z_j}$$

Equation A12 can be split into

$$B \cdot 1 + \alpha = 0 \quad \text{(A13)}$$

$$\text{where } 1^T = [1\ 1\ 1 \ldots 1]$$

combining Eq. A13 with Eq. A8 we get

$$B[u - u_1 \cdot 1] = 0 \quad \text{(A14)}$$

Since matrix B is nonsingular in general we conclude that

$$u_i = u_1 \qquad \text{for } i = 2, 3, \ldots n+2$$

Hence

$$(Lx - Vy)_i = (Lx - Vy)_0 \quad \text{(A15)}$$

which is the requirement for steady-state mass conservation.

LITERATURE CITED

Ballard, D., C. B. Brosilow, and C. Kahn, "Dynamic Simulation of Multicomponent Distillation Columns," Paper No. 42a, AIChE Meeting, Miami (Nov., 1978).

Finlayson, B. A., "The Method of Weighted Residuals and Variational Principles," New York, Academic Press (1972).

Friedly, J. C., "Dynamic Behavior of Processes," Prentice Hall, NJ (1972).

Holland, C. D., "Fundamentals and Modeling of Separation Processes," Prentice-Hall (1975).

Howard, G. M., "Unsteady State Behavior of Multicomponent Distillation Columns," *AIChE J.*, **16**, No. 6, 1022 (1970).

Holt, A. V., "Simplified Approximations to Countercurrent Stage Processes," M. S. Thesis, Case Western Reserve University (Nov., 1966).

McCabe, W. L., and J. C. Smith, "Unit Operations of Chemical Engineering," 3rd ed., McGraw-Hill (1976).

Osborne, A., "The Calculation of Unsteady State Multicomponent Distillation Using Partial Differential Equations," *AIChE J.*, **17**, 3, 696 (1971).

Seider, W. D., and P. G. J. Prokopakis, "Dynamic Simulation of Distillation Towers," Paper No. 2c, AIChE Meeting, Chicago (1980).

Villadsen, J. V., and M. L. Michelsen, "Solution of Differential Equations by Polynomial Approximation," Prentice-Hall, NJ (1978).

Wahl, F. F., and P. Harriot, "Understanding and Prediction of the Dynamic Behavior of Distillation Columns," *I & EC PDD*, **9**, No. 3, 396 (1970).

Waller, K. V., "Simple Models for Distillation Dynamics," Paper 36d, AIChE Meeting at Houston (April, 1979).

Weigand, W. A., A. K. Jhawar, and T. J. Williams, "Calculation Method for the Response Time to Step Inputs for Approximate Dynamic Models of Distillation Columns," *AIChE J.*, **18**, 6, 1243 (Nov., 1972).

Wilkinson, W. I., and W. D. Armstrong, "An Approximate Method for Predicting Composition Response of a Fractionating Column," *Chem. Engng. Sci. Genie Chemique*, **7**, No. 1 (1958).

Wong, K. T., and R. Luus, "Model Reduction of High-Order Multistage Systems by the method of Orthogonal Collocation," *Can. J., Chem. Eng.*, **58**, 382 (June, 1980).

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