Analytic Reduced-Order Dynamic Models for Large Equilibrium Staged Cascades

A model reduction technique based upon modal analysis is presented for modeling the dynamics of general, large equilibrium staged cascades encountered in chemical processes. The analysis is general enough to encompass quite complex cascades involving multiple feed and/or product streams with nonideal thermodynamic behavior. The low-order models proposed have a number of desirable features: the state variables have physical significance and model parameters are clearly related to the fundamental process parameters which are easily obtainable from steady-state plant data. Quantitatively it is shown that the low-order models proposed are in excellent agreement with the complete (high-order) dynamic models on a range of problems some of which involve complex, nonideal cascades.

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SCOPE

The development of low-order dynamic models of equilibrium staged processes is desirable for a number of reasons including the development of on-line advanced control schemes, the training of plant personnel, and flowsheet dynamic simulation. A number of papers have addressed this topic in the past, however few have addressed the general problem involving complex cascades with multiple feed and/or product streams and nonideal thermodynamic behavior. Our approach encompasses such cascades and is based upon a modal analysis of the linearized dynamic equations of the complete system model.

One feature of the analysis is that the approximate dynamic models proposed are not just purely mathematical artifices, but are open to a sound physical interpretation. This physical interpretation enables one to identify the types of cascades which are likely to be well-represented by these reduced order models. Operating features which favor the use of these models are large cascades, low reflux to feed flow ratios and surprisingly, nonideal thermodynamic behavior. These conditions are fortunately often found in practice.

CONCLUSIONS AND SIGNIFICANCE

The objectives of this work have been to develop analytic reduced-order dynamic models for large equilibrium staged cascades encountered in chemical processes. The approach has been to partition the system A-matrix in a way that allows the complete spectrum of this matrix to be analytically approximated. These spectral approximations have been compared to the exact spectrum (calculated numerically) for a wide range of examples and have proven to be quite accurate. The availability of these spectral approximations has made possible the development of two different types of reduced-order models.

The dynamics of a number of equilibrium cascades have been studied ranging from single feed, ideal solution columns to more complex configurations (multiple feeds, nonideal solutions). Quantitative comparisons between the reduced-order models and their high-order counterparts have been made. In general, agreement between the two has been excellent. However, for on-line control or flowsheet simulation the use of reduced-order dynamic models has many distinct advantages.

INTRODUCTION

It is well recognized that the linear dynamics of many real chemical processes can be adequately approximated by transfer functions of the form

$$G(s) = \frac{\exp(-T_d s)}{(1 + T_1 s)(1 + T_2 s)} \tag{1}$$

Although approximate, such transfer functions find wide use in control system design (Stephanopoulos, 1984). Parameters in Eq.

1 can be obtained from fitting the approximate model to either the dynamic response of the process obtained experimentally or to the computed step response of more complicated and fundamental models of the process. The advantage of using reduced-order models similiar to Eq. 1 for large systems is that instead of using a large number of differential equations (perhaps thousands) to model process dynamics, two differential equations plus delay logic give Eq. 1. Application areas for reduced-order dynamic models in chemical engineering include control system design, dynamic flowsheeting, and operator training schemes.

In an excellent paper Kim and Friedly (1974) studied the issue of when and why an equation of the form of Eq. 1 might work for approximating the dynamics of equilibrium staged processes. That work related the phenomenological parameters of Eq. 1 to system design parameters. The authors studied the dynamics of two processes, an ideal equilibrium staged cascade similar to an ideal gas absorber model and a ten-stage distillation column. For the ideal cascade, parameters in Eq. 1 were related to the eigenvalues of the matrix describing the absorber dynamics. These eigenvalues can be obtained in closed form because of the particular form of the cascade model (uniform tridiagonal matrix structure). For the distillation column, eigenvalues of the matrix were calculated numerically. In both cases the reduced-order model of the form of Eq. 1 accurately tracked the dynamic response of the complete model or, in the case of the distillation column, the actual column response to input disturbances. In all cases, however, Kim and Friedly considered only the response of states at either end of the cascade.

Model reduction techniques have intrigued many workers in the field over the past two decades. Much of the work has been published in the electrical engineering literature where a popular approach to model reduction has been modal analysis (Gould, 1969; Mahapatra, 1978; Gopal and Mehta, 1982). A review of a mathematical perspective on the subject of spectral approximations to linear operators (which is central to our analysis) was published by Chatelin (1981). The use of model reduction techniques for chemical engineering processes was surveyed by Bosley and Lees (1972). More recently Stoever and Georgakis (1982a,b) and Benallou et al. (1982) have proposed model reduction techniques for equilibrium staged processes. Both of these approaches used a stage grouping concept. Benallou et al. approximated the dynamic behavior of a group of stages (also called a compartment) by that of a single stage having the same holdup as the compartment holdup and the composition of the so-called compartment sensitive stage. Using steady state relationships to relate various composition variables in the cascade, a set of differential equations was developed for modeling the dynamics of the cascade. The dependent variables are the sensitive stage composition variables. However, choice of the compartment size appears to be quite arbitrary. Stoever and Georgakis grouped stages and applied a modal argument to reduce the overall number of differential equations in the dynamic model by a factor m (where m is the number of groups used). They applied their analysis to an ideal gas absorber cascade modeled by a uniform tridiagonal matrix structure, for which there is an exact analytic solution available (Lapidus and Amundson, 1950). Various group sizes (both uniform and nonuniform) were examined and once again choice of tray grouping appears to be quite arbitrary. It should be remembered that the manner in which trays are grouped effects which states are "lost" in the model reduction process. The use of orthogonal collocation to derive low-order models from the partial differential equation formulation of the process model has also been proposed (Cho and Joseph, 1983) and discussed by Benallou et al.

In this paper we present concepts and an analysis which lead to analytic reduced-order dynamic models for generic models describing large equilibrium staged processes. By generic models we mean general equilibrium stage process models that accommodate multiple feed and product streams, feed conditions ranging from subcooled liquid to superheated vapor and nonuniform physical properties (if necessary) throughout the cascade. Our approach does not involve the notion of grouping trays but rather relies upon modal arguments. In spirit it develops the problem along the lines followed by Davison (1968) and Kim and Friedly (1974). However, the problem we address is considerably more complicated than that addressed in those studies. We derive explicit relationships between the phenomenological parameters of Eq. 1 and the process design parameters. Furthermore, we compare these analytic reduced-order dynamic models to results obtained by solving the complete (full-order) dynamic model by computer simulation.

GENERIC MODELS FOR STAGED SYSTEMS

To obtain general theoretical results for large staged systems we start from the idealized cascade ("gas absorber") model used by Kim and Friedly. This is a widely used linear model for the compositions of a component on each stage in a general countercurrent cascade of N equilibrium stages given by

$$\frac{dx_j}{dt} = \alpha x_{j-1} - (\alpha + \beta)x_j + \beta x_{j+1} \quad j = 1, \ldots, N \tag{2}$$

where x_j is the mole fraction of one component on the jth stage, t is time, and α and β are model parameters dependent upon tray holdups, internal liquid and vapor flows, and equilibrium ratios. For a model neglecting vapor phase holdup and assuming uniform flows, holdups and thermodynamic properties throughout the cascade, $\alpha \equiv L/H$ and $\beta \equiv K_i V/H$ where L is liquid flow rate, V vapor flow rate, K_i equilibrium ratio of component i and H holdup. This is essentially the model used by Kim and Friedly where α and β are considered constant throughout the column. In this case inlet compositions at either end of the cascade X_0 or X_{N+1} are considered as candidates for disturbances. A similar model applies to distillation columns where holdups in the reboiler and condenser are significantly larger than internal tray holdups which is often the case.

In vector notation Eq. 2 can be written

$$\frac{dx}{dt} = Ax + Bu \tag{3}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}, \quad B = \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ \vdots & \vdots \\ 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad u = \begin{bmatrix} x_0 \\ x_{N+1} \end{bmatrix} \tag{4}$$

The system matrix is the familiar tridiagonal form

$$A = \begin{bmatrix} -(\alpha+\beta) & \beta & & & \\ \alpha & -(\alpha+\beta) & \beta & & \\ & \alpha & -(\alpha+\beta) & \beta & \\ & & \ddots & \ddots & \beta \\ & & & \alpha & -(\alpha+\beta) \end{bmatrix}$$

This model is convenient since the eigenvalues of A may be obtained in closed form. Their values are given by:

$$\lambda_j = -(\alpha + \beta) + 2\sqrt{\alpha\beta}\cos\left(\frac{\pi j}{N+1}\right) \quad j = 1,\ldots,N \qquad (5)$$

The decomposition of high-order dynamic models of the form given by Eq. 3 into a lower order model depends upon the spectrum of A (i.e., its complete set of eigenvalues). In order to ignore the fast modes it is important that the absolute value of the eigenvalues associated with these modes be much larger (all the eigenvalues of A can be shown to be real and negative) than the two smallest, e.g., the first two λ_1 and λ_2. Kim and Friedly show that this is often the case using asymptotic expressions for Eq. 5 considering large values of N. It follows from Kim and Friedly's analysis that large staged systems modeled by Eqs. 3 and 4 are characterized by eigenvalues which are real, distinct, stable, and well-separated. They tend to be dominated by the first couple of time constants. Furthermore, this tends to be more the case as the size of the cascade becomes larger, a factor which favors the use of reduced-order models where they are most needed, for large scale-systems.

Effect of Feed and Product Streams

The effect of feed and/or product streams at intermediate stages in the cascade is to alter the structure of the matrix A. For every entering feed a "switching" occurs which affects the values of the terms in the matrix but not the tridiagonal structure of the matrix itself. Switching occurs because the effect of a feed stream is to change internal liquid and vapor flows on either side of the feed tray. A single saturated liquid feed in a distillation column for example causes the internal liquid flow rate in the stripping section to be the sum of the liquid flow in the rectifying section plus the feed flow rate. Switching can also occur because of nonuniformity in physical property values (more will be said about this later on). For a single liquid feed and uniform physical properties the resultant A matrix of the model equations has a structure similar to Eq. 6 given by

$$A = \left[\begin{array}{ccc|ccc} -(\alpha+\beta) & \beta & & & & \\ \alpha & -(\alpha+\beta) & \beta & & & \\ & & \beta & & & \\ & \alpha & -(\alpha+\beta) & \beta & & \\ \hline & & \alpha & -(\gamma+\delta) & \delta & \\ & & & \gamma & & \delta \\ & & & & \gamma & -(\gamma+\delta) \end{array}\right] \begin{matrix} \\ \\ \\ \\ \\ \\ \end{matrix} \begin{matrix} \} m \\ \\ \\ \\ \} n \\ \\ \end{matrix} \qquad (6)$$

The switch occurs after the mth tray in the cascade, the feed entering on the $(m+1)$th tray. The parameters γ and δ are defined similarly to α and β defined previously, $\gamma \equiv L'/H'$, $\delta \equiv KV'/H'$. Here L', V' and H' refer to liquid flows, vapor flows, and holdups in the stripping section. It should be realized that the matrix of Eq. 6 applies to a general equilibrium staged process with a single feed at an intermediate stage in the cascade where internal flows, holdups, and thermodynamic properties are considered uniform on either side of the feed stage. These are generally good assumptions (which also make our analysis analytically tractable) for absorber and distillation column models with relatively nonideal thermodynamic solutions. The dynamics of Eq. 3 with the A matrix given by Eq. 6 is obviously dependent upon the spectrum of A. By using a sequence of similarity transformations (Lapidus and Amundson, 1950), A in Eq. 6 can be transformed to the following symmetric matrix

$$A = \left[\begin{array}{ccc|ccc} -(\alpha+\beta) & \sqrt{\alpha\beta} & & & & \\ \sqrt{\alpha\beta} & -(\alpha+\beta) & \sqrt{\alpha\beta} & & & \\ & \sqrt{\alpha\beta} & -(\alpha+\beta) & \sqrt{\alpha\beta} & & \\ \hline & & \sqrt{\alpha\beta} & -(\gamma+\delta) & \sqrt{\gamma\delta} & \\ & & & \sqrt{\gamma\delta} & & \sqrt{\gamma\delta} \\ & & & & \sqrt{\gamma\delta} & -(\gamma+\delta) \end{array}\right] \begin{matrix} \\ \\ T_1 \\ \\ \\ T_2 \end{matrix} \qquad (7)$$

The matrix A in Eq. 7 can be decomposed into two matrices, one of rank $(m+n)$ plus a symmetric rank two perturbation matrix (Parlett, 1980).

$$A = \left[\begin{array}{c|c} T_1 & 0 \\ \hline 0 & T_2 \end{array}\right] + \left[\begin{array}{c|c} 0 & \sqrt{\alpha\beta} \\ \hline \sqrt{\alpha\beta} & 0 \end{array}\right] \qquad (8)$$

The approximation to the spectrum of A is given by the eigenvalues

$$\hat{\lambda}_i = -(\alpha+\beta) + 2\sqrt{\alpha\beta}\cos\left(\frac{\pi i}{m+1}\right) \quad i = 1,\ldots,m \qquad (9a)$$

$$\hat{\lambda}_j = -(\gamma+\delta) + 2\sqrt{\gamma\delta}\cos\left(\frac{\pi j}{n+1}\right) \quad j = 1,\ldots,n \qquad (9b)$$

where the $\hat{}$ refers to approximate eigenvalues. While there is some theoretical guidance as to the validity of these approximations (Wilkinson, 1965) we interpret them from a physical standpoint. It then becomes clearer as to when these approximations are likely to work well and vice-versa. From a physical perspective the approximations imply that we have decoupled the sections of the cascade on either side of the feed from one another. We would then expect that they should become increasingly accurate as the respective time scales of response of each section of the cascade become more widely separated. Many situations give rise to this circumstance, for example when the ratio of internal flows in either section of the cascade is large and/or when the ratio of the number of stages (m/n in Eq. 6) in either section is large. Typically, reflux flow rates in distillation columns are of the same order as feed flow rates. In these cases a saturated liquid feed, for example, will lead to internal liquid flow rates in the stripping section greater by a factor of 2 or more than flow rates in the rectifying section. In such situations our approximations will be extremely accurate, a topic we explore further on in this paper.

Multiple Feeds

The situation corresponding to multiple feed and product streams involves a straightforward extension of previous results. The system A matrix can now be partitioned into a block diagonal matrix plus the sum of symmetric rank two perturbation matrices (one for each feed or product stream) leading to the following forms

$$A = C + D \qquad (10)$$

where

$$C = \left[\begin{array}{c|c|c|c} T_1 & & & \\ \hline & T_2 & & \\ \hline & & T_i & \\ \hline & & & T_{i+1} \\ \hline & & & \\ & & & T_f \end{array}\right] \begin{matrix} \\ \\ \} l \\ \\ \} q \end{matrix} \qquad (11)$$

$$D = \sum_{i=1}^{f-1} P_i \tag{12}$$

where $(f-1)$ is the number of entering feed streams and P_i is the rank two perturbation matrix (symmetric) corresponding to the ith feed stream. The spectrum of C can be obtained analytically and may be used as a first approximation to the spectrum of A as described previously.

DYNAMIC MODELS FOR CASCADES WITH SWITCHING

Here we derive a number of results which lead to dynamic models for large equilibrium staged cascades. First, exact results are obtained for these dynamic models in terms of the spectrum of the system A matrix. We are then in a position to develop various reduced-order dynamic models using our spectral approximations. We have chosen to focus upon distillation column models although the analysis is general enough to encompass other staged processes. Furthermore we present results which allow us to develop reduced-order dynamic models for any state variable in the system.

Single Feed Case

The dynamic system equations for this situation correspond to Eq. 3 with the A matrix given by Eq. 6 and B by

$$B = \begin{bmatrix} 0 \\ \vdots \\ \theta Z_0 \\ \vdots \\ 0 \end{bmatrix} \begin{matrix} \} m \\ \\ \} n \end{matrix} \tag{13}$$

where θ is a physical parameter corresponding to feed flow rate divided by holdup on the feed tray, etc. Taking the Laplace transform of Eq. 3 leads to

$$sI\bar{x}(s) - A\bar{x}(s) = \begin{bmatrix} 0 \\ \vdots \\ \theta \bar{Z}_0(s) \\ \vdots \\ 0 \end{bmatrix} \tag{14}$$

or

$$(sI - A)\bar{x}(s) = \begin{bmatrix} 0 \\ \vdots \\ \theta \bar{Z}_0(s) \\ \vdots \\ 0 \end{bmatrix} \tag{15}$$

where I is the $(m+n) \times (m+n)$ identity matrix.

The solution of Eq. 15 can be developed using Cramer's rule. If we are interested in tracking the jth state variable (composition on the jth stage) in response to a disturbance in feed composition Z_0, Cramer's rule leads to the following expression for $x_j(s)$

$$x_j(s) = \frac{\Delta^{(j)}}{\Delta} \tag{16}$$

where Δ is the determinant of the matrix $(sI - A)$ and $\Delta^{(j)}$ is the determinant of $(sI - A)$ with the jth column of $(sI - A)$ replaced by B in Eq. 13. If we are interested in tracking say x_1, then the value of the determinant $\Delta^{(1)}$ is required, given by the determinant of the following matrix $\tilde{A}$

$$\tilde{A} = \begin{bmatrix} 0 & -\beta & & & & & \\ 0 & s+(\alpha+\beta) & -\beta & & & & \\ 0 & -\alpha & s+(\alpha+\beta) & -\beta & & & \\ \vdots & & \ddots & \ddots & \ddots & & \\ & & & -\alpha & s+(\alpha+\beta) & -\beta & \\ \theta\bar{Z}_0(s) & & & & -\alpha & s+(\gamma+\delta) & -\delta \\ \vdots & & & & & \ddots & \ddots \\ 0 & & & & & -\gamma & s+(\gamma+\delta) \end{bmatrix} \begin{matrix} \\ \\ \} m \\ \\ \\ \\ \} n \end{matrix} \tag{17}$$

The determinant of $\tilde{A}$ can be shown to have the following form

$$\Delta(\tilde{A}) = (-1)^{1+m+1}\theta\bar{Z}_0(-\beta)^m \begin{vmatrix} \overbrace{s+(\gamma+\delta) & -\delta & & \\ -\gamma & s+(\gamma+\delta) & -\delta & \\ & \ddots & \ddots & \ddots \\ & & -\gamma & s+(\gamma+\delta) \end{vmatrix}}^{E} \tag{18}$$

where the last determinant is of order $(n-1)$ and more importantly may be found analytically to have the following form

$$\Delta(E) = \prod_{i=1}^{n-1} (s - \mu_i) \tag{19}$$

where the μ_i are the eigenvalues of an $(n-1) \times (n-1)$ tridiagonal matrix E given by

$$E = \begin{bmatrix} -(\alpha+\delta) & \delta & & \\ \gamma & -(\gamma+\delta) & \delta & \\ & \ddots & \ddots & \ddots \\ & & \gamma & -(\gamma+\delta) \end{bmatrix} \tag{20}$$

The μ_i are therefore given by

$$\mu_i = -(\gamma+\delta) + 2\sqrt{\gamma\delta}\cos\left(\frac{\pi i}{n}\right), \quad i = 1, \ldots, n-1 \tag{21}$$

Now

$$\Delta(\tilde{A}) = (-1)^{2m+2}\theta\bar{Z}_0 \prod_{i=1}^{n-1} (s - \mu_i) \cdot \beta^m \tag{22}$$

or

$$\Delta(\tilde{A}) = \theta\bar{Z}_0 \prod_{i=1}^{n-1} (s - \mu_i) \cdot \beta^m \tag{23}$$

Therefore, from Eq. 16

$$\bar{x}_1(s) = \frac{\theta \bar{Z}_0 \prod_{i=1}^{n-1} (s - \mu_i) \cdot \beta^m}{\prod_{i=1}^{m+n} (s - \lambda_i)} \tag{24}$$

Equation 24 is exact if the various sets of eigenvalues are known precisely. The λ_i's are the eigenvalues of the $(m + n)$ order matrix given by Eq. 6.

Intermediate States

In the previous section we derived exact results for states at the extreme ends of the cascade (i.e., top or bottom stages). Here we present results for intermediate states where the required determinants become a little different (and more complex) to determine.

The problem here is to determine the transfer function relating the jth state to a disturbance in feed composition in a cascade with the feed stream entering on the ith stage. From Eq. 16 the main difficulty lies in finding the determinant $\Delta^{(j)}$. After some manipulation $\Delta^{(j)}$ can be formulated in the following terms.

$$\Delta^{(j)} = (-1)^{i+j}\theta\bar{Z}_0 \begin{vmatrix} (j-1)\left\{\begin{matrix} s+(\alpha+\beta) & -\beta \\ -\alpha & s+(\alpha+\beta) \end{matrix}\right. & -\beta & 0 \\ m-(j-1)\left\{\begin{matrix} -\alpha & \\ 0 & \end{matrix}\right. & \begin{matrix} -\beta \\ s+(\alpha+\beta) \\ -\alpha \end{matrix} & \begin{matrix} -\beta \\ -\beta \\ s+(\alpha+\beta) \end{matrix} \\ & \begin{matrix} -\alpha & s+(\alpha+\beta) & -\beta \end{matrix} & \begin{matrix} 0 \\ -\delta \\ s+(\gamma+\delta) \end{matrix} \\ (n-1)\left\{\begin{matrix} & \\ & \end{matrix}\right. & \begin{matrix} -\gamma \\ -\gamma \end{matrix} & \begin{matrix} s+(\gamma+\delta) & -\delta \\ -\gamma & s+(\gamma+\delta) \end{matrix} \end{vmatrix} \tag{25}$$

Using the properties of determinants (Wilkinson, 1965) $\Delta^{(j)}$ can be shown to be of the form

$$\Delta^{(j)} = \prod_{i=1}^{j-1} (s - \xi_i) \cdot L \cdot \prod_{i=1}^{n-1} (s - \mu_i) \tag{26}$$

where the ξ_i, $i = 1 \ldots j - 1$ are eigenvalues of the following matrix of order $(j - 1)$

$$\begin{bmatrix} -(\alpha+\beta) & \beta & & \\ & \ddots & \ddots & \\ & \alpha & -(\alpha+\beta) & \beta \\ & & \ddots & \ddots \end{bmatrix} \tag{27}$$

and the μ_i are eigenvalues of an $(n - 1) \times (n - 1)$ matrix of the form given by Eq. 20. L is the determinant of the $m - (j - 1)$ order lower tridiagonal matrix sandwiched between the extremes in Eq. 25. It follows simply that

$$L = (-\beta)^{m-j+1}$$

Putting all this together leads to the following exact result for $x_j(s)$.

$$x_j(s) = \frac{(-1)^{i+j}\theta\bar{Z}_0(-\beta)^{m-j+1} \prod_{i=1}^{j-1} (s - \xi_i) \prod_{i=1}^{n-1} (s - \mu_i)}{\prod_{i=1}^{m+n} (s - \lambda_i)} \tag{28}$$

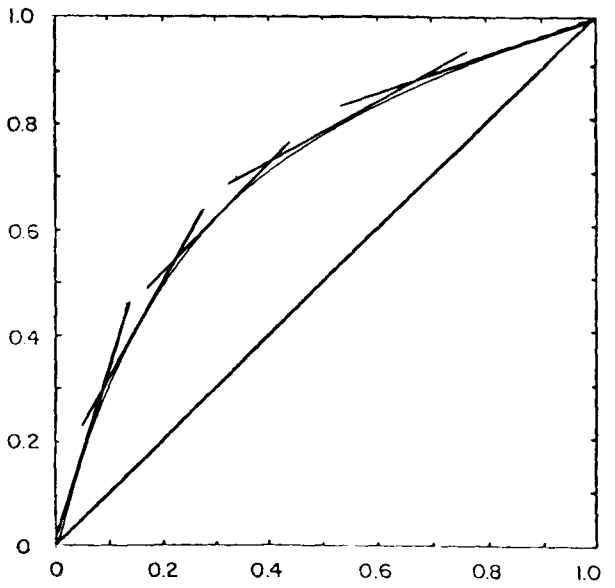


Figure 1. Tangent planes to the phase envelope for thermodynamic property calculations.

Generalization to Multiple Feeds and/or Product Streams

Generalization of the previous analysis to multiple-feed and/or product stream cases is reasonably straightforward. Interestingly enough it sets up a recursive problem whereby a problem with f streams (i.e., f switches) requires the determinant of matrices with less than f switches. We refer to Eqs. 10, 11 and 12, which define the system A matrix and its decomposition. For a disturbance in the feed stream after the ith block tridiagonal matrix T_i (Eq. 11) the transfer function relating, say, the composition at the top of the column to a disturbance in the ith feed stream concentration is given exactly by Eq. 24. However, now the set of μ_i's and λ_i's in Eq. 24 are the eigenvalues of more complicated matrices. The set of λ_i's are the eigenvalues of the entire matrix given by Eq. 10. The μ_i's are the eigenvalues of the block tridiagonal matrix consisting of the *blocks below the feed point* $\{T_{i+1}| \ldots |T_f\}$. Once again we propose to approximate these eigenvalues using the spectrum of C and various of its subsets (Eq. 11) which may be obtained analytically.

To illustrate the multiple-feed case, consider a saturated liquid two-feed column with corresponding A matrix given by

$$A = \left[\begin{array}{ccc|c|c}
-(\alpha+\beta) & \beta & & & \\
\alpha & -(\alpha+\beta) & \beta & & \\
 & \alpha & -(\alpha+\beta) \quad \beta & & \\
\hline
 & & \alpha \quad -(\gamma+\delta) \quad \delta & & \\
 & & \gamma \quad -(\gamma+\delta) & \delta & \\
\hline
 & & & \alpha \quad -(\eta+\psi) \quad \psi & \\
 & & & \eta \quad -(\eta+\psi) &
\end{array}\right] \begin{array}{l} \} m \\ \text{feed 1} \\ \} P \\ \text{feed 2} \\ \} n \end{array} \qquad (29a)$$

If for example the dynamics of the top tray composition variable in response to a change in composition in feed stream 2 is of interest, then a similar analysis to that leading to Eq. 24 applies. The following equation applies

$$\bar{x}_1(s) = \frac{\theta \bar{Z}_0 \beta^m \delta^P \prod_{i=1}^{n-1} (s-\mu_i)}{\prod_{i=1}^{m+n+P} (s-\lambda_i)} \qquad (29b)$$

The set of λ_i's is given by the entire spectrum of A which we propose to approximate using Eqs. 10, 11 and 12. The μ_i's are given by the spectrum of the bottom block tridiagonal matrix (defined in terms of η and ψ in Eq. 29a), which can be found exactly.

VARIATION OF THERMODYNAMIC PROPERTIES THROUGHOUT THE CASCADE

The models used here assume uniform internal flows in each section of the cascade. This is a widely used assumption whose accuracy has been examined in previous studies on the dynamics of distillation processes (Sourisseau, 1978; Chimowitz et al., 1985). Equilibrium ratios can, however, vary considerably throughout the cascade even for relatively ideal systems. Consider Eq. 6, which shows the A matrix for a column with a single feed stream (with uniform flows and thermodynamic properties on either side of the feed).

The parameters β and δ in the matrix contain equilibrium ratios. Specifically $\beta \equiv (K_i V/H)r$ and $\delta \equiv (K_i V/H)s$ where r and s refer to the rectifying and stripping sections, respectively. These quantities are available from the steady state operating conditions of the column. The equilibrium ratios in each section of the cascade are obtained by constructing a tangent line to the phase envelope diagram covering that section of the cascade (Figure 1 illustrates this idea in a binary system). The value of K_i in the model is the gradient of this tangent line. For highly nonideal systems where equilibrium ratios may vary greatly from one end of the cascade to the other, many such tangent lines may be required. This leads to switches within sections of the cascade and the system A matrix takes on a finer block tridiagonal structure. This approach (termed piecewise linear equilibrium ratios) has formed the basis for handling thermodynamic properties in many previous studies (Benallou et al., 1982).

From the point of view of this study our foregoing analysis applies in its entirety. Whether switching occurs because of feed/product streams or varying thermodynamic properties, the cascade is still modeled by equations of the form given by Eqs. 10 and 11.

TABLE 1. COMPARISON OF EXACT EIGENVALUES WITH ANALYTIC APPROXIMATIONS IN A (10 × 10) SYSTEM

$\alpha = 1.0, \beta = 0.5, \delta = 1.5, \gamma = 1.0$

Exact λ's	Approx λ's	|S|*
$m = 5, n = 5$		
4.64	4.62	0.0043
3.79	3.72	0.018
2.79	2.72	0.0250
2.587	2.50	0.0340
2.13	2.21	0.0375
1.56	1.50	0.0384
1.187	1.27	0.069
0.722	0.793	0.0983
0.371	0.378	0.0189
0.208	0.275	0.322
$m = 6, n = 4$		
4.508	4.48	0.0062
3.378	3.26	0.035
2.765	2.77	0.0018
2.395	2.38	0.0063
1.9841	1.81	0.0877
1.906	1.74	0.0834
1.108	1.18	0.065
0.6551	0.618	0.0566
0.4078	0.518	0.270
0.1907	0.226	0.185
$m = 7, n = 3$		
4.283	4.23	0.0124
2.8686	2.81	0.0204
2.7168	2.51	0.076
2.4082	2.51	0.042
1.9686	2.04	0.036
1.4723	1.50	0.0188
1.014	0.958	0.0552
0.6861	0.768	0.1193
0.4076	0.500	0.226
0.1735	0.193	0.112
$m = 8, n = 2$		
3.848	3.72	0.033
2.826	2.83	0.0014
2.581	2.58	0.00038
2.2241	2.21	0.0063
1.8178	1.75	0.0373
1.4260	1.28	0.1023
1.0558	1.25	0.1839
0.6886	0.793	0.152
0.3715	0.417	0.122
0.1598	0.171	0.0700

* $S = \dfrac{\lambda_{exact} - \lambda_{approx}}{\lambda_{exact}}$

TABLE 2. COMPARISON OF EXACT EIGENVALUES WITH ANALYTIC APPROXIMATIONS IN A (10 × 10) SYSTEM

$\alpha = 1.0, \beta = 0.5, \delta = 2.5, \gamma = 1.0$

Exact λ's	Approx λ's	|S|*
$m = 5, n = 5$		
6.248	6.23	0.0028
5.118	5.08	0.0074
3.59	3.50	0.0251
2.717	2.72	0.001
2.263	2.21	0.0234
1.926	1.92	0.00311
1.403	1.50	0.0691
0.8489	0.793	0.0658
0.634	0.761	0.200
0.249	0.275	0.104
$m = 6, n = 4$		
6.0744	6.06	0.0024
4.541	4.47	0.0156
2.825	2.78	0.0159
2.657	2.52	0.05156
2.295	2.38	0.037
1.7558	1.81	0.031
1.2013	1.119	0.068
0.8914	0.942	0.0567
0.5477	0.618	0.128
0.2102	0.226	0.076
$m = 7, n = 3$		
5.767	5.73	0.0064
3.633	3.50	0.0367
2.798	2.80	0.0007
2.480	2.50	0.0081
2.032	2.04	0.0039
1.563	1.50	0.040
1.2201	1.26	0.033
0.856	0.959	0.120
0.459	0.500	0.089
0.183	0.193	0.053
$m = 8, n = 2$		
5.154	5.08	0.0144
2.834	2.82	0.0049
2.6136	2.58	0.0128
2.3175	2.21	0.046
2.0015	1.92	0.041
1.6130	1.75	0.0850
1.168	1.25	0.070
0.7411	0.793	0.0700
0.392	0.416	0.0612
0.1647	0.171	0.038

* $S = \frac{\lambda_{exact} - \lambda_{approx}}{\lambda_{exact}}$

REDUCED-ORDER DYNAMIC MODELS

Results in previous sections (Eqs. 16–28) led to exact dynamic models for the cascades we are studying. The model reduction procedure we use rests upon two distinct types of approximations. The first utilizes ideas similar to those studied by Kim and Friedly. Their objective was to approximate high-order transfer function models by simpler transfer functions similar to that given in Eq. 1. In the development of their reduced-order models though, Kim and Friedly required the entire spectrum of various matrices which they obtained numerically (except for the gas absorber model with no switching, where the spectrum is available in closed form). We propose analytic forms for the various spectra required similar to those given in Eqs. 9a and 9b. This then is the second type of approximation we are proposing. The net result of these concepts is the development of reduced-order dynamic models for complex cascades where parameters in these models are available analytically and depend upon the fundamental physical parameters of the cascade: flows, holdups, and thermodynamic properties. These parameters are available from the steady state operating conditions of the cascade.

Model Reduction

We illustrate the ideas using as our starting point the exact transfer function model given by Eq. 24:

$$\frac{\bar{x}_1(s)}{\theta \bar{Z}_0(s)} = \frac{\prod_{i=1}^{n-1}(s-\mu_i)}{\prod_{i=1}^{m+n}(s-\lambda_i)} = \frac{P(s)}{Q(s)} \tag{24}$$

Kim and Friedly proposed a rationale for approximating Eq. 24 in the following manner

$$Q(s) \approx \frac{(s-\lambda_1)(s-\lambda_2)}{\exp(-T_d s)} \tag{30}$$

Here $|\lambda_1|$ and $|\lambda_2|$ are the two smallest eigenvalues of the system A matrix (corresponding to the two slowest modes). The delay time for the system is given by

$$T_d = \sum_{j=3}^{m+n}\left(-\frac{1}{\lambda_j}\right) \tag{31}$$

Similarly $P(s)$ is approximated by a lower order approximation which from physical arguments must be of lower order than $Q(s)$ given in Eq. 30

$$P(s) \approx \frac{(s-\mu_1)}{\exp(-T_v s)} \tag{32}$$

where $|\mu_1|$ is the smallest eigenvalue of the tridiagonal matrix below the feed (see Eqs. 20, 21)

and

$$T_v = \sum_{j=2}^{n-1}\left(-\frac{1}{\mu_j}\right) \tag{33}$$

Therefore, Eq. 24 becomes

$$\frac{\bar{x}_1(s)}{\theta \bar{Z}_0(s)} = \frac{(s-\mu_1)}{(s-\lambda_1)(s-\lambda_2)} \exp[-(T_d - T_v)s] \tag{34}$$

Equation 34 correctly reflects the time delay between the disturbance in the feed and the state variable of interest here (composition at the top of the column). This is the dead time for the entire cascade minus the dead time for the stage *below* the disturbance. We now propose to use analytic approximation given by Eqs. 9a and 9b to calculate λ_1, λ_2 and T_d. The values for μ_1 and T_v can be found exactly, using Eq. 21. A similar analysis can be applied to more complex cascades modeled by Eqs. 22–28 leading to reduced-order dynamic models where once again the parameters can be obtained analytically. We examine models for complex cascades later on.

The normalized time domain form of Eq. 34 is found by inverting from the Laplace domain and given by

$$x_1(t) = u(t-\tau_D) + \frac{\lambda_2(\mu_1-\lambda_1)}{\mu_1(\lambda_1-\lambda_2)} e^{\lambda_1(t-\tau_D)} u(t-\tau_D)$$

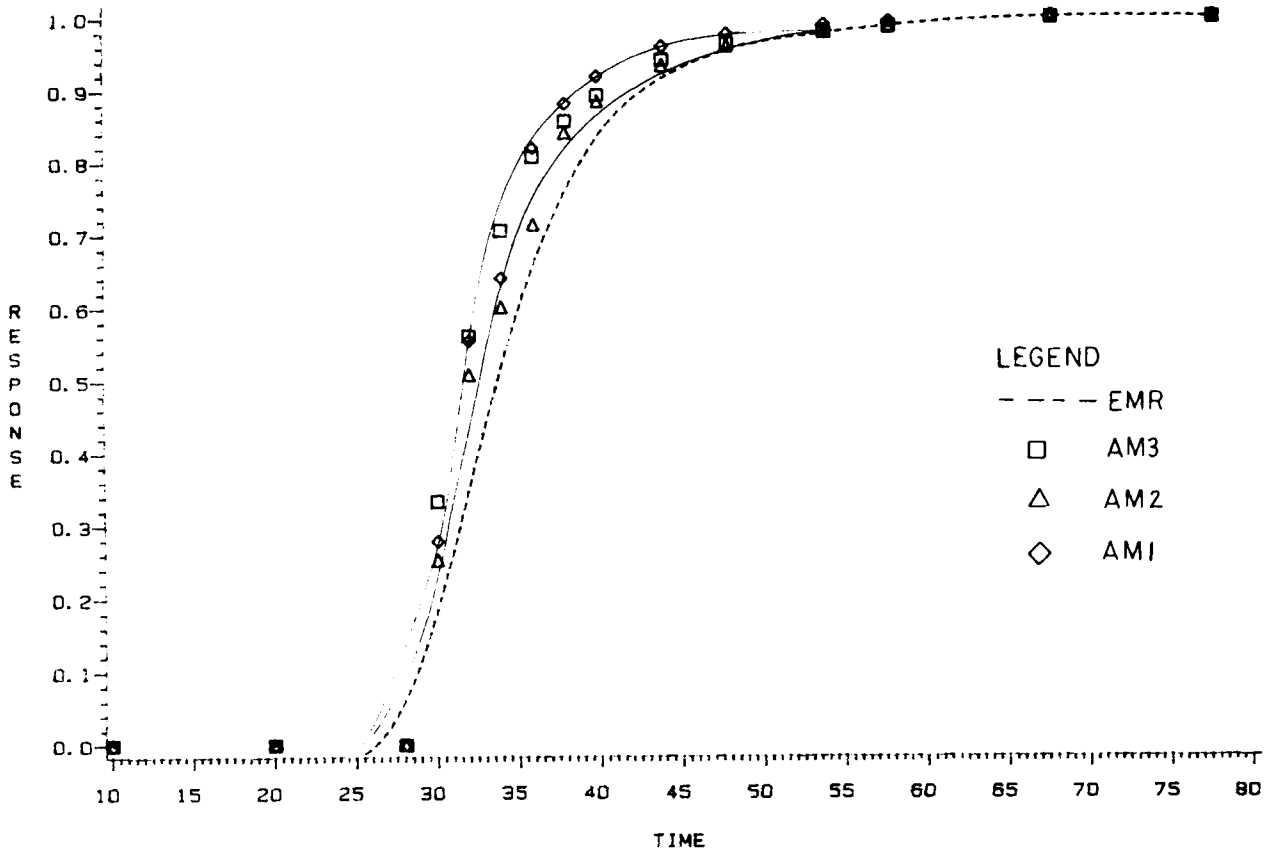


Figure 2. Comparison of exact model and approximate model transient responses in a 40-stage cascade (top stage composition).

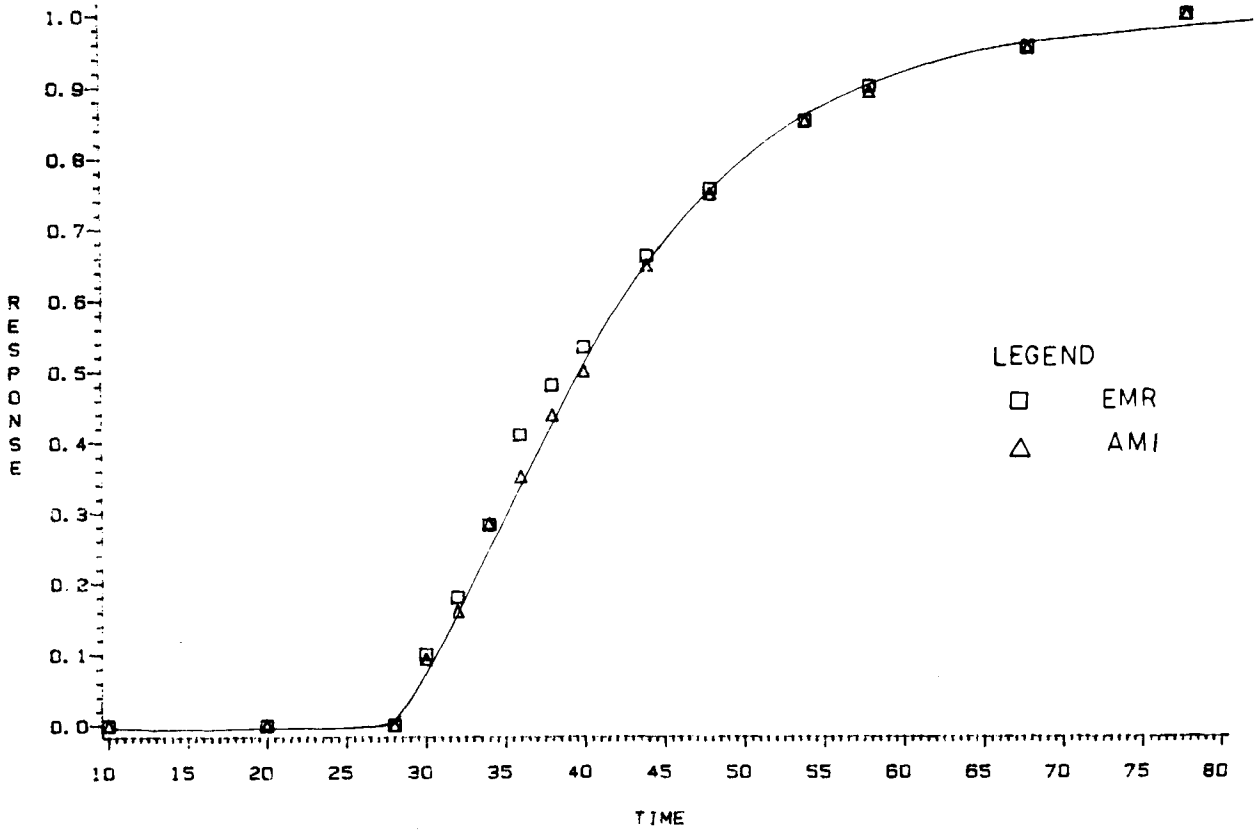


Figure 3. Comparison of exact model and approximate model transient responses in a 40-stage cascade (bottom stage composition).

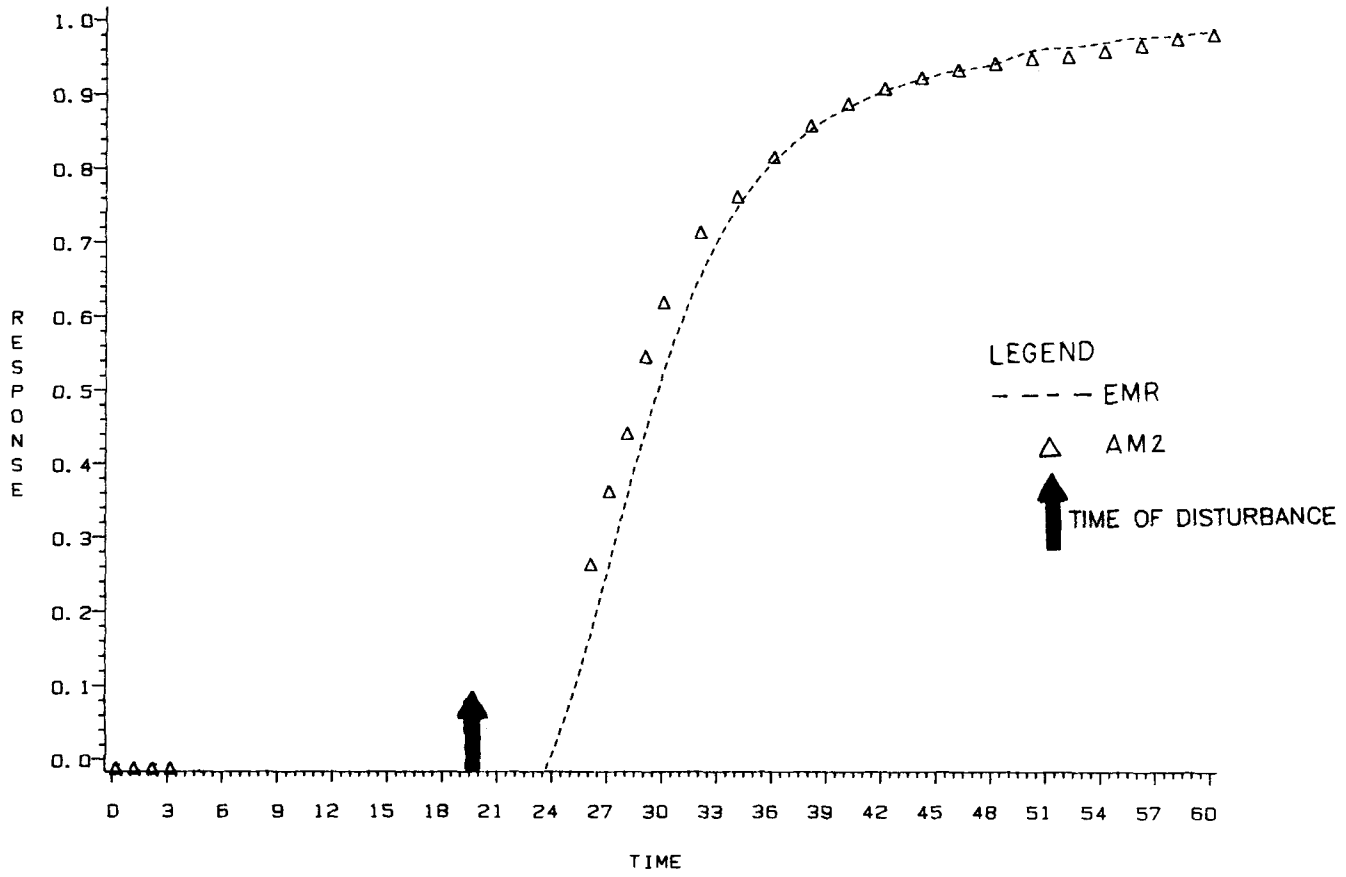


Figure 4. Comparison of exact model and approximate model transient responses for an intermediate state in a 40-stage cascade (tray ten composition).

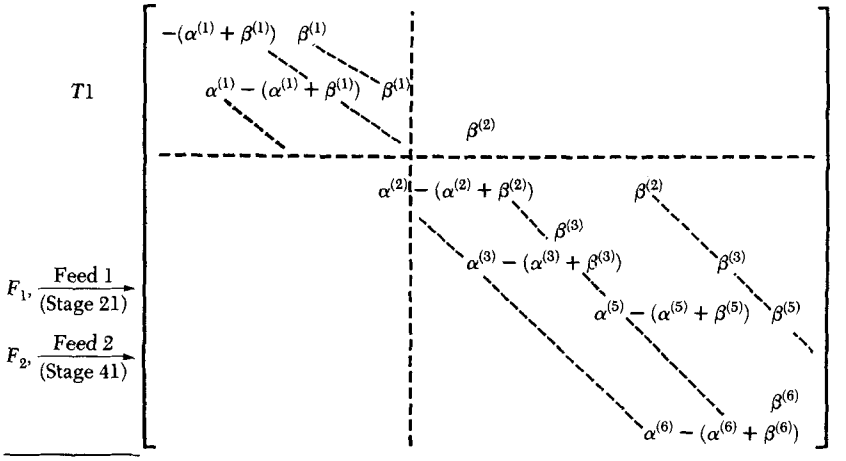
$$+\frac{\lambda_1(\lambda_2-\mu_1)}{\mu_1(\lambda_1-\lambda_2)}e^{\lambda_2(t-\tau_D)}u(t-\tau_D) \quad (35)$$

where $\tau_D = T_d - T_v$ and $u(t-\tau_D)$ is the unit step function. We refer to the type of reduced-order model given by Eq. 35 as approximate model 1 (AM1).

Alternative Reduced-Order Model Concepts

Since our spectral approximations furnish the entire spectrum of the necessary matrices, other kinds of reduced order models can be developed. The normalized eigenfunction solution to Eq. 24 (with a step disturbance) can be expressed as

TABLE 3. SYSTEM MATRIX FOR TWO FEEDS AND NONUNIFORM THERMODYNAMIC PROPERTIES



$\alpha^{(1)} = 1.0;\ \alpha^{(2)} = 1.0,\ \alpha^{(3)} = 3.0,\ \alpha^{(4)} = 3.0,\ \alpha^{(5)} = 5.0,\ \alpha^{(6)} = 5.0$

$\beta^{(1)} = 2.5,\ \beta^{(2)} = 6.25,\ \beta^{(3)} = 10.0,\ \beta^{(4)} = 13.75,\ \beta^{(5)} = 17.50,\ \beta^{(6)} = 21.25$

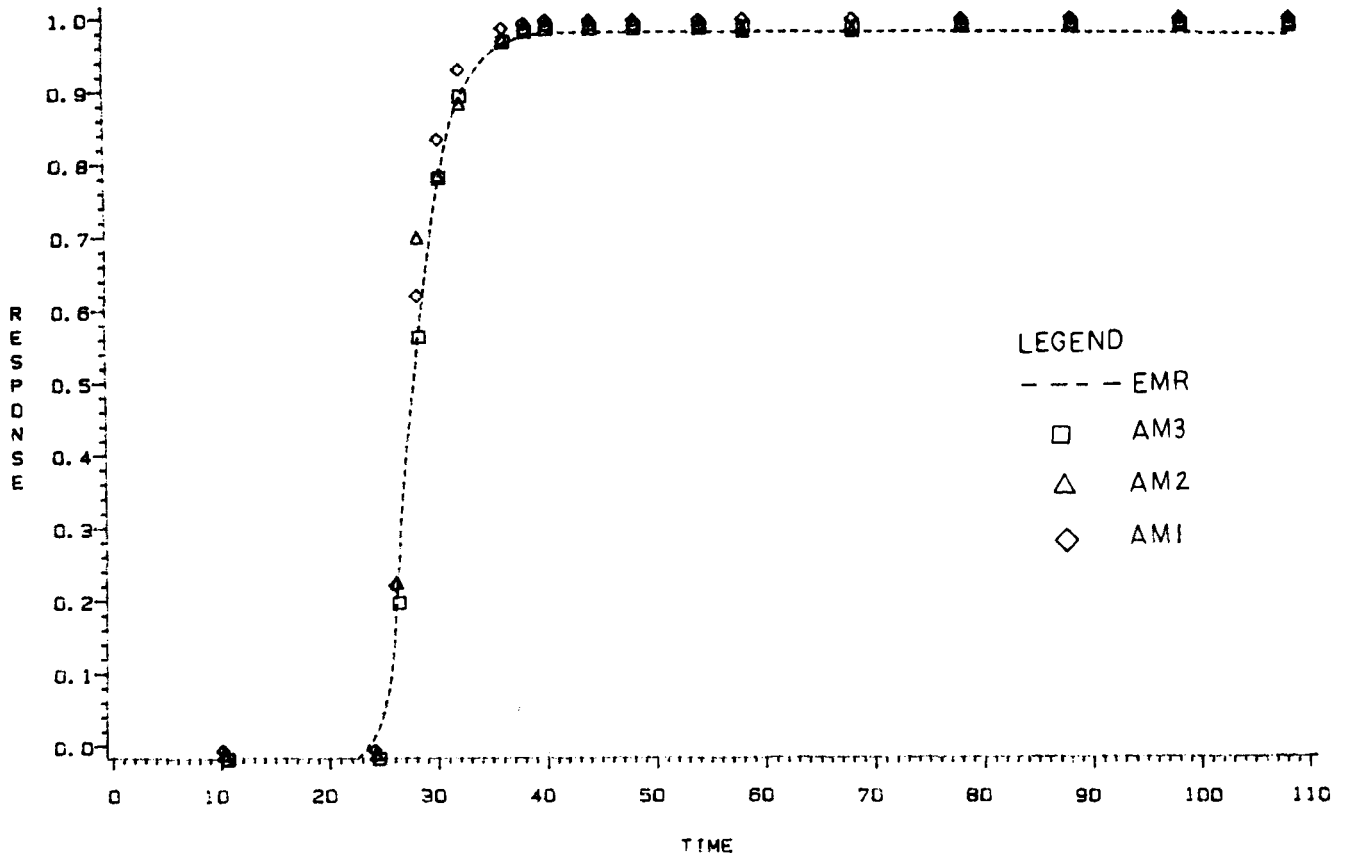


Figure 5. Comparison of exact model and approximate model transient responses in a 60-stage, two-feed cascade with varying thermodynamic properties (top stage composition).

$$x_1(t) = 1 - \sum_{i=1}^{m+n} a_i e^{\lambda_i t} \tag{36}$$

The set of constants $\{a_i: i = 1, \ldots, m+n\}$ can be calculated using our spectral approximations for the $\{\lambda_i: i = 1, \ldots, m+n\}$ from Eqs. 9a, 9b, and the set $\{\mu_i: i = 1, \ldots, n-1\}$ which we get exactly from Eq. 21. This is tantamount to a partial fraction expansion of Eq. 24. We propose a new and alternative second-order reduced model given by a form similar to Eq. 36, where terms with $i > 3$ contribute to the dead time (which we can calculate analytically) and beyond the dead time a second-order form of Eq. 36 applies. Mathematically this model is given in normalized form by

$$\begin{aligned} x_1(t) &= 0, \quad t < \tau_D \\ x_1(t) &= 1 - a_1 e^{\lambda_1 t} - a_2 e^{\lambda_2 t}, \quad t \geq \tau_D \end{aligned} \tag{37}$$

We refer to this as approximate model 2 (AM2). This model has the important feature that it can match final steady state values for the state variable of interest. (AM1, in contrast, can represent only the normalized trajectory of the state variable of interest.)

For comparative purposes we have also used a third type of reduced-order model (called AM3) which uses exact eigenvalues calculated numerically wherever necessary and corresponds to the model used by Kim and Friedly.

While here we have used a single feed cascade with top tray composition as the variable of interest to illustrate our model reduction procedures, the same approach may be used on more complex cascades (modeled by Eqs. 25–28 for example), resulting in reduced-order models for any state variable of interest in these cascades. In the following section we examine the accuracy of our reduced-order models for cascades of varying degrees of complexity.

APPLICATION OF REDUCED-ORDER MODELS

Initially we illustrate the accuracy of our spectral approximations given by Eqs. 9a and 9b. It was argued earlier that these approximations should be increasingly accurate the more widely separated the time scale of response of the cascade's sections. We examine this hypothesis for a single feed cascade with an A matrix given by Eq. 6. This corresponds to a one-switch cascade with the feed stream entering on the $(m+1)$th stage. The larger the ratios of parameters γ/α, δ/β, n/m, the more widely separated will be the time scales of the slowest modes in either section of the cascade. Tables 1 and 2 show calculations for two different sets of values for these ratios in a (10×10) system. It is evident that the approximations are better for the larger values of these ratios which confirms our expectations. Also, the larger eigenvalues (in an absolute sense) are most accurately approximated. Similar results have been observed in many other systems (Celebi, 1985).

Our next example involves a 40-stage cascade corresponding to a distillation column with a saturated liquid feed entering on tray 21 (trays numbered from top to bottom). This system is modeled by Eqs. 3 and 6, and a feed to reflux flow rate of 2:1 was used. This leads to parameter values of $\alpha = 1$, $\beta = 2.5$, $\gamma = 3.0$, $\delta = 2.5$, $m = 20$, $n = 20$.

Transients of various composition variables in response to a step change in feed composition were calculated. Three reduced-order dynamic models were used (AM1, AM2, and AM3); in

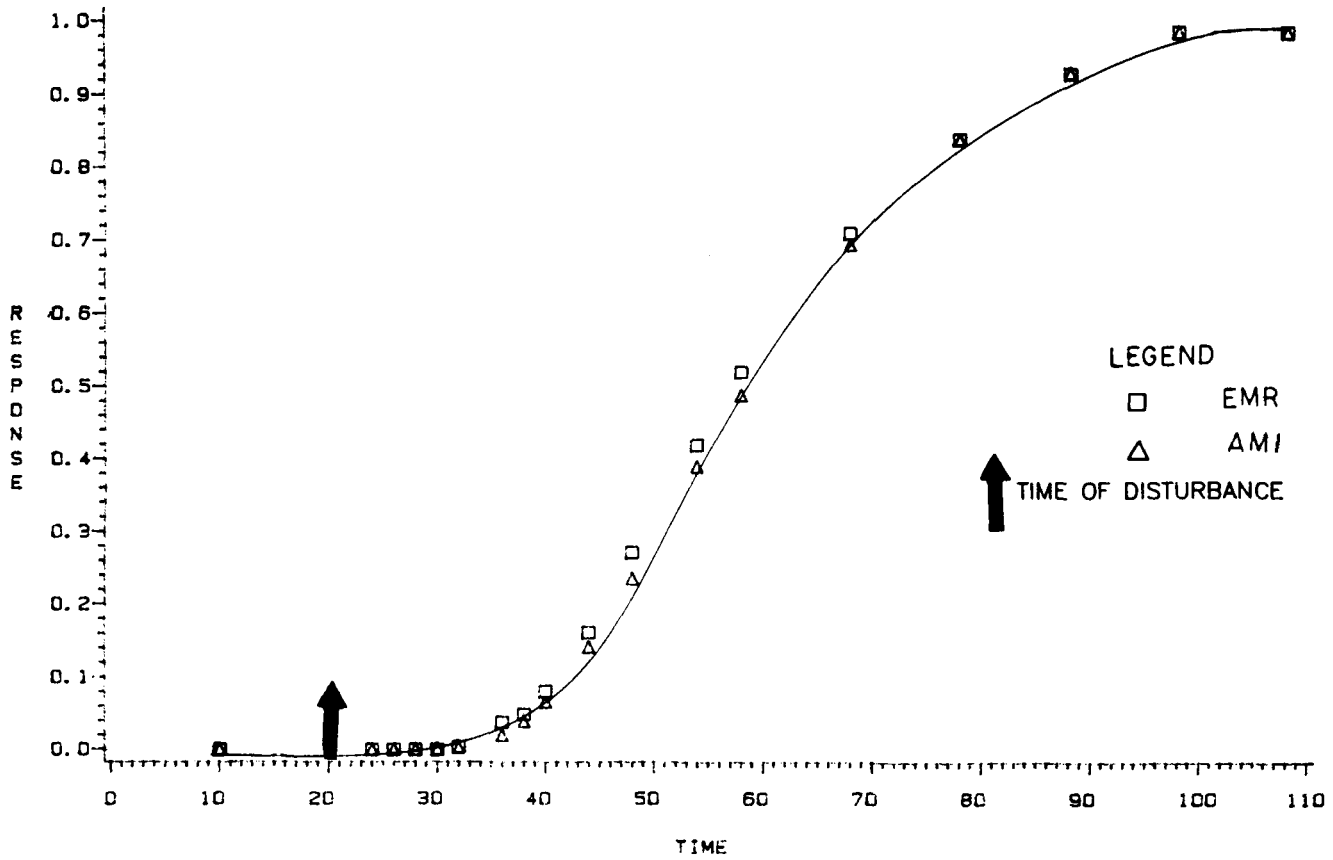


Figure 6. Comparison of exact model and approximate model transient responses in a 60-stage, two-feed cascade with varying thermodynamic properties (bottom stage composition).

addition, the exact model response (EMR) was obtained by integrating the 40 differential equations corresponding to the complete system dynamic model. Figure 2 shows a comparison of all of these models in predicting the composition transient on the top stage. Agreement between the reduced-order models and the exact model response is good, and in fact excellent for reduced-order model AM2. Surprisingly, use of the exact eigenvalues in formulating reduced-order model AM3 does not shown much improvement over AM1, which uses eigenvalues approximated by Eqs. 9a and 9b. Figure 3 shows the bottom stage concentration transient for the exact model and AM1. The reduced-order model AM1 almost exactly replicates the exact model response. The dead time predicted by AM1 is 8.69 in comparison to the value of 8.17 obtained using the exact spectrum of the system A matrix. In addition, Figure 3 confirms our expectations that the reduced-order models would better predict the dynamic response for the faster section of the cascade (since the fast and slow modes are more widely separated here). Here this corresponds to the stripping section and a comparison of the results in Figures 2 and 3 shows that this is the case.

The 40-stage cascade illustrates the use of a reduced-order model based upon Eq. 28 for predicting the transient response of intermediate states. Figure 4 shows a comparison of the exact model response with AM2; agreement between the two is excellent, showing that with these models it is possible to access any intermediate state in the system.

Our final problem tests many of the concepts presented in this paper on a 60-stage complex cascade with two intermediate feedstreams dividing the cascade into three 20-stage sections. In addition, with each of these sections, thermodynamic properties are treated as uniform within 10-stage groups, the net result being a five-switch cascade. The entering saturated liquid feeds are on stages 21 and 41, with a ratio of feed 1 flow rate to reflux rate of 2:1, and feed 2 flow rate to reflux rate of 2:1. Thermodynamic K-values varied by a factor of 10 from the top to the bottom of the cascade. This steady state design information is sufficient to specify parameters in the system A matrix shown in Table 3. It is useful to see how our reduced-order models are derived with this information; these calculations are presented in Appendix A for the top stage concentration response. Figure 5 compares the reduced-order models with the exact model response for the top tray concentration transient in response to a step change in feed composition in feed stream 1 (once again, these responses have been normalized). Agreement between the exact solution and the approximate models is excellent. The dead time predicted by AM1 is 4.9, which should be compared to the value of 5.19 given by using the exact eigenvalues in Eqs. 31 and 33. Figure 6 shows the transient response of the bottom stage concentration in response to the same disturbance in the feed composition. Once again, the reduced order model AM1 almost exactly replicates the exact model response.

These calculations were repeated for lower feed-to-reflux ratios of 1.5:1. The ratios $\alpha^{(1)}/\alpha^{(3)}$, $\alpha^{(3)}/\alpha^{(5)}$ (see Table 3) become smaller, and from our earlier analysis the spectral approximations are expected to be less accurate, resulting in a degradation of the reduced-order models' performance. The dynamic response of the top tray concentration transient to a step change in feed composition in feed stream 1 is shown in Figure 7. Even at these unfavorable conditions, agreement between the reduced-order models and the exact model solution is reasonable. The exact dead time was calculated to be 8.0, which should be compared to a value of 9.01 predicted by AM1. It should be reiterated that the

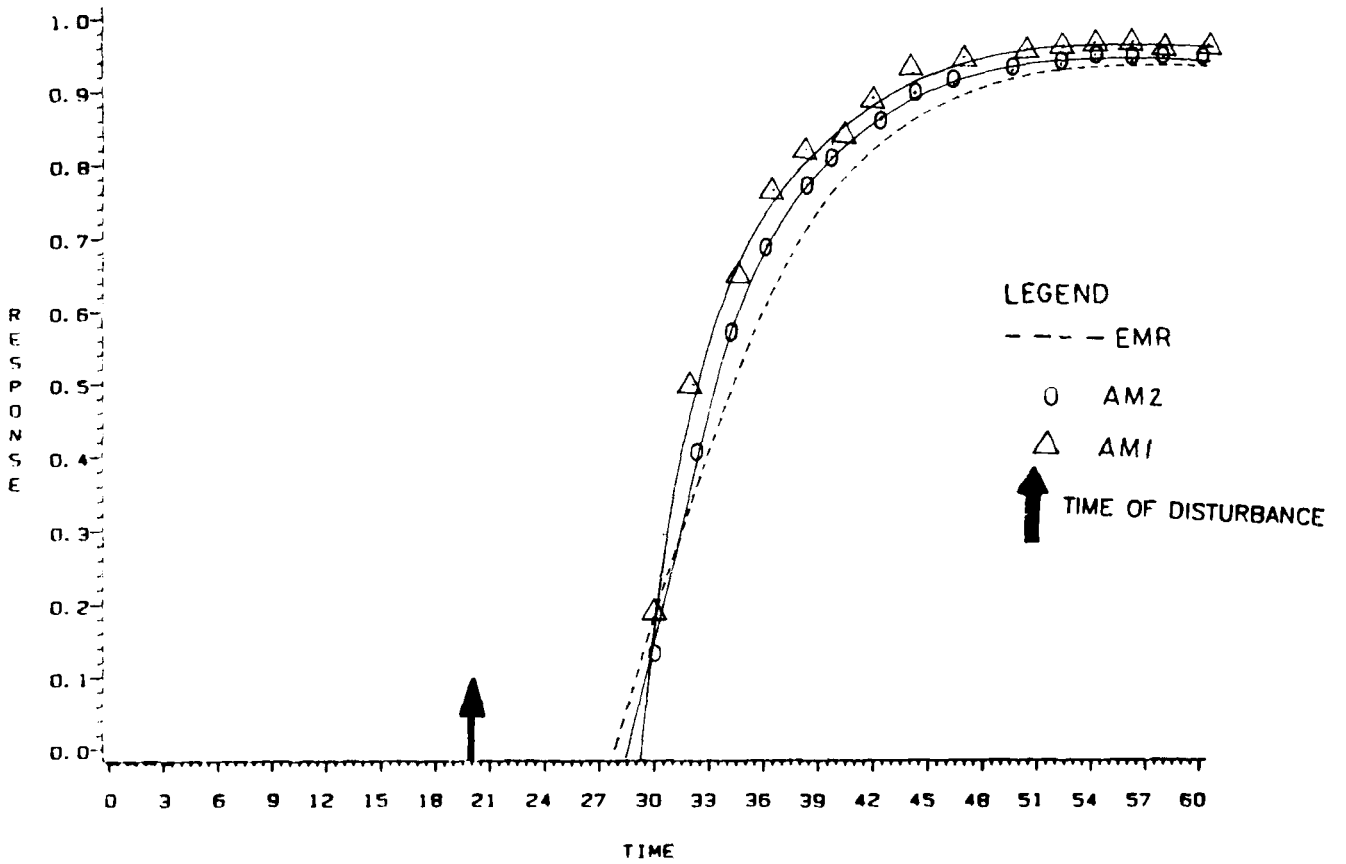


Figure 7. Comparison of exact model and approximate model transient responses in a 60-stage, two-feed cascade (top stage composition).

likely operating conditions of an energy efficient column (low reflux-to-feed ratios, large number of stages) lead to high ratios for parameters between sections of the cascade (i.e., $\alpha^{(1)}/\alpha^{(3)}$), hence to better spectral approximations and reduced-order models.

CONCLUSIONS

We have presented a new approach for developing reduced-order dynamic models in large, complex equilibrium staged processes. The basis for our analysis rests upon spectral approximations for various matrices that model the process dynamics. These approximations depend in a very clear manner upon the fundamental process design variables: flow, thermodynamic properties, and holdups. Parameters in the reduced-order models can in turn be calculated using the complete set of these spectral approximations. Two different types of reduced-order models were developed, one type (AM1) based upon mode separation arguments, the other (AM2) based upon an eigenfunction solution to the governing differential equations. While both types were in excellent agreement with the exact model dynamic response on a variety of problems, AM2 was quantitatively superior. Model AM3 was developed using the exact eigenvalues (calculated numerically). Considering the increased computation required to calculate these eigenvalues, and the fact that the increase in accuracy with AM3 was insignificant, its use is not warranted on the types of problems studied here.

One of the main reasons for developing reduced-order dynamic models is their potential use for control system design. The models proposed here are particularly attractive in an adaptive control environment since parameters in the models are clearly related to process parameters which can be measured. As these parameters change, the models can be forced to adapt to the new process conditions. Current research is focusing upon this problem.

ACKNOWLEDGMENT

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APPENDIX A

Development of Model AM1 for 60-Stage Cascade

The system A matrix is given in Table 3. Assume that we are interested in developing AM1 for top tray composition dynamics in response to a change in feed concentration in stream F_1.

Partition the A matrix into six matrices $T_1, T_2, \ldots, T_6$, since we have five switches in this cascade. (See Table 3 for T_1; T_2, etc. follow similarly.) For model AM1 given by Eqs. 30–34, we require the following parameters μ_1, λ_1, λ_2, T_d, and T_v. μ_1 and T_v are approximated using the union of the spectra of $T_3, \ldots, T_6$ which may be obtained analytically. These calculations give $\mu_1 = -2.5813$ and $T_v = 2.864$. λ_1, λ_2, and T_d are approximated using the union of the spectra of $T_1, \ldots, T_6$ which once again may be obtained analytically. These calculations give $\lambda_1 = -0.46513$, $\lambda_2 = -0.83941$ and $T_d = 7.775$.

NOTATION

A = system matrix

$\tilde{A}$ = system matrix given in Eq. 17
B = matrix given in Eq. 3
C = approximation matrix
D = perturbation matrix
E = matrix given in Eq. 18
F = feed flow rate
G = process transfer function
H = liquid holdup
I = identity matrix
K_i = slope of tangent to equilibrium surface (component i)
L = liquid flow rate
m = number of stages above the feed
n = number of stages including the feed and stages below the feed
N = total number of stages in the cascade
$P(s)$ = transfer function given in Eq. 24
$Q(s)$ = transfer function given in Eq. 24
s = Laplace transform parameter
t = absolute time
T_d = total dead time measured at the top of the cascade for a given disturbance at the bottom
T_i = submatrices of the system matrix A
T_v = dead time due to stages below the feed stage
u = vector of disturbances
u_s = unit step function
v = vapor flow rate
Z_0 = feed composition

Greek Letters

α = model parameter, L/H
β = model parameter, K_iV/H
δ = model parameter, K_iV/H
γ = model parameter, L/H
θ = model parameter, F/H
Δ = determinant of a matrix
$\Delta^{(i)}$ = determinant of a matrix with ith column replaced by another vector
λ_i = eigenvalues of a matrix
μ_i = eigenvalues of a matrix
ξ_i = eigenvalues of a matrix

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