Dynamic Compartmental Models for Separation Processes

A low-order modeling technique for separation processes is developed by considering a staged column as a compartmental system in which a number of stages are lumped to form an equivalent stage. This method leads to low-order models of separation processes directly and without linearization. Moreover, the resulting models have state variables and parameters that are physically significant. In contrast to alternative model reduction methods, compartmental analysis guarantees preservation of both material balances and steady states for arbitrary changes in the input variables.

A comparison of compartmental analysis to a recently proposed technique based on orthogonal collocation, both methods incorporating an equimolal overflow assumption, shows the efficiency and robustness of the compartmental method.

A. Benallou, D. E. Seborg, and D. A. Mellichamp
Department of Chemical and Nuclear Engineering
University of California
Santa Barbara, CA 93106

SCOPE

Low-order, dynamic models of separation processes are desirable for a number of reasons including the evaluation of alternative control strategies, the development of on-line applications of advanced control schemes, and the training of plant personnel.

Most of the available methods for building low-order models of separation processes are deficient because they are so abstract and complicated, require linearization of the system equations, or yield models with parameters or state variables having no physical significance.

The most recent of these methods uses orthogonal collocation to derive reduced models (Wong and Luus, 1980; Cho and Joseph, 1980, 1983; Stewart et al., 1981). This approach introduces mathematical complications and leads to state variables that may not necessarily correspond to tray locations.

Another approach, linearization techniques combined with model reduction, can lead to low-order models in a state space or transfer function form (Mockzek et al., 1965; Wahl and Harriott, 1970; Weigand et al., 1972; Waller, 1972, 1979; Crockett, 1978). This class of methods offers a simpler alternative, but leads to models in which the parameters have no physical significance.

By considering a separation column as a compartmented system, it is possible to derive low-order models that avoid these deficiencies. At the same time, steady state characteristics of high- and low-order models can be matched exactly, and transient characteristics of the low-order models can closely approximate the high-order system dynamics.

Moreover, the model parameters retain their physical significance, permitting broad use of the model, especially when operating conditions change. In this development of the basic theory, several simplifying assumptions are made, including equimolal overflow, in order to compare results with those from collocation methods. Benallou (1982) presents extensions of the method to more realistic systems.

CONCLUSIONS AND SIGNIFICANCE

Compartmental modeling techniques are based on the physical characteristics of separation processes. They are suitable for developing low-order models for simulation or control purposes that are valid, with no further complications, for any process operating conditions.

The formulation of the compartment separation functions using shortcut relationships yields a dynamic low-order model whose steady state version is identical to the complete model equations in which the "nonsensitive" stage compositions and their corresponding equations are eliminated using the shortcut expressions. This feature guarantees exact steady state agreement between the compartmental and complete models; it also ensures that all material balances are satisfied exactly. Numerical comparisons of the compartmental modeling technique with existing collocation methods show the efficiency and robustness of the compartmental method. In particular, the compartmental model provided better steady state agreement than a collocation model of higher order. The compartmental model matched the initial and final steady states of the high-order model exactly, thus yielding identical process gains. For the transient response, the collocation model yielded a slightly better match during the initial responses of several of the runs.

Unlike modal methods for model reduction, the compartmental method does not require that a high-order version of the system model be developed first nor that system equations be linearized. Unlike available collocation methods for developing low-order nonlinear models of separation processes, it does not use any mathematical artifice to reduce the model order. The compartmental method offers a physical alternative to available methods. Its simplicity and its similarities with stage-by-stage modeling concepts make direct extension to complex nonlinear multicomponent columns possible.

Introduction

Since Marshall and Pigford (1947) first introduced a differential equation formulation of the dynamics of separation processes, several models of these processes have been proposed in the literature (Tolliver and Waggoner, 1980). These models can be classified in two categories, high-order models and low-order models. The term high-order models refers to dynamic models that are obtained by writing material and energy balances for each stage; they are usually highly nonlinear. This type of model can yield accurate representations of the physical process. On the other hand, low-order representations of separation processes are desirable for operator training, screening of control strategies, or use in on-line control schemes. Models of the low-order type are proposed either in transfer function or state-space form and are usually obtained by linearization and reduction of a model of the high-order type. They also may be obtained by postulating a transfer function form and then finding parameters through theoretical relationships or empirically, by fitting the response for a specific change in input.

The major criticisms that have been addressed to available models relate to the large dimensionality of high-order models, and to a limited, sometimes nonexistent, physical interpretation of the parameters or the state variables of low-order models. These two criticisms are a consequence of the fact that the relations between the model and its potential utilization (Waller, 1979), and the model parameters and those of the physical process it represents, are very often overlooked. The deficiencies of many available models become most apparent when the model is considered in the context of its utilization. When a model is designed for on-line control, it is clear that large dimensionality can become a hindrance (e.g., the number of scalar equations obtained from the system matrix Riccati equation is $n(n+1)/2$ where n is the system order). For a typical multicomponent process, a complete dynamic model may consist of several hundreds of differential equations, leading to computing times that make it impractical to use this type of model for on-line control. For the available models of low-order type, the hindrance lies in the fact that the model parameters often cannot be adjusted easily if process conditions change.

In this paper we briefly review the available low-order modeling methods for separation processes, underlining the need for new methods; then we utilize and develop a new approach, compartmental analysis. In this concept the reduction of the model order is carried out on physical grounds rather than mathematically.

Critical Review of Available Low-Order Modeling Methods

Figure 1 provides a summary of the available low-order modeling techniques for separation processes. These techniques can be classified according to the type of lower-order model they yield:

(a) Linear low-order models
(b) Bilinear low-order models
(c) Nonlinear low-order models

Among methods of type (a), the most commonly used are those based on model reduction (Bonvin and Mellichamp, 1982) of a linear state-space model, or on a transfer function approach. In recent work (Georgakis and Stoever, 1982; Stoever and Georgakis, 1982), a compartmental approach has been used to reduce the complete model. The method yields error bounds and utilizes physically meaningful variables in the reduced model. However, it also requires that a linearized, tridiagonal form of the complete model be developed; and it produces a linear, low-order model that does not match the original high-order model's steady states.

Another method of reducing the order of the system of linearized equations is based on the concept that the composition can be approximated as a continuous function of the distance along the column. Discretization is then carried out using a "net mass transfer coefficient" for a column section (Osborne et al., 1965), or the method of orthogonal collocation. The latter technique was recently used in order to derive low-order lumped models (Wong and Luus, 1980). Orthogonal collocation can be used

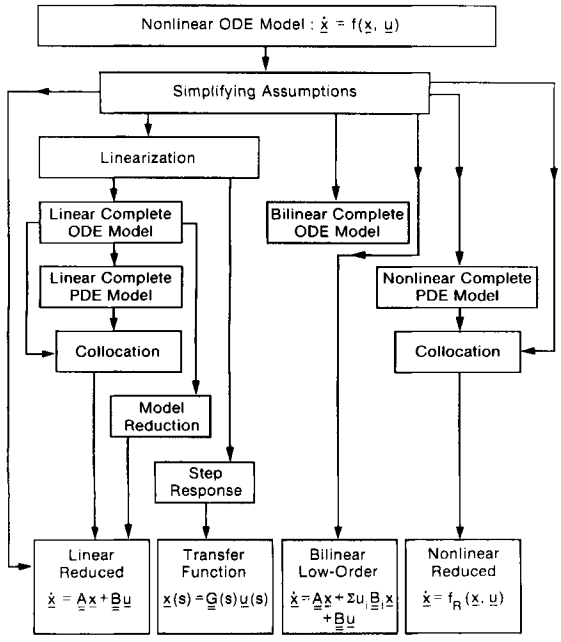

Figure 1. Available low-order modeling techniques.

either directly on the linearized system equations or on their partial differential equation formulation (Cho and Joseph, 1980). Besides the mathematical complications introduced by orthogonal collocation (e.g., finding the roots of the collocation polynomials for which a closed-form solution is possible only when their degree is not larger than 4 [Hermite, 1905], interpolation, curve fitting of initial conditions), these models yield a set of fictitious state variables (compositions at the collocation points, i.e., the roots of the polynomials). Given that the collocation points seldom correspond to actual tray locations, the reduced-order model state variables must inevitably be interpolated in order to yield stage compositions. This difficulty leads to a common and important disadvantage of these methods: a discrepancy between the states of the reduced and complete models at steady state.

The third class of methods of type (a) leads to transfer function models. These models are usually obtained from a step, or an impulse response of the complete model or the process itself. Extensive investigations of the physical interpretation of the parameters in these models has led to some empirical and theoretical relationships between the model parameters and process characteristics/operating conditions (Moczek et al., 1965; Wahl and Harriot, 1970; Weigand et al., 1972; Waller, 1972, 1979; Crockett, 1978). However, these relationships often are quite approximate and the empirical transfer function model form requires that an observer be used to eliminate internal state variables in the model for any on-line control applications.

In principle, type (b) or bilinear models provide a more accurate representation of the dynamic behavior of distillation columns than linear models since they retain the basic structure of the process; however, to our knowledge only one method of this type is discussed in the literature (España and Landau, 1978, 1979). Unfortunately, the approach leads to a low-order model in which only one of the three state variables, and none of the model parameters, has physical significance.

The last category, method (c), is used when a low-order, nonlinear representation of the process is sought. In one method, the reduction step is carried out by orthogonal collocation (Cho and Joseph, 1981; Stewart et al., 1981). Consequently this approach inherits all of the collocation-induced problems discussed earlier. An alternative compartmental approach for model reduction utilizes steady state material balance relationships for the individual stages to eliminate some of the stage compositions from the transient model, exactly as in shortcut (steady state) design methods. Such an approach thus yields a nonlinear, low-order model that can match the steady states of the original model. Dahlqvist (1979) used this approach to develop a low-order model of a binary distillation column for adaptive control studies. He made no attempt to formalize the method nor to extend it more generally; nevertheless it does offer a number of conceptual advantages.

This brief review shows that most of the available methods achieve model reduction by using some mathematical artifice that tends to blur the physical picture; consequently the physical significance of the resulting model parameters, and sometimes even the state variables, becomes lost and the relationship between the model and physical process becomes obscure. These observations lead us to define a set of requirements that a low-order model designed for control purposes should possess:

- The model should retain the physical structure of the process.
- The state variables should have physical significance.
- The model parameters must be related to process parameters and should be easily obtainable from steady state plant data.

It is seen that none of the available low-order modeling methods satisfies all of these requirements with the possible exception of the compartmental approach that utilizes steady state stage relationships to eliminate superfluous concentration variables. In the next section this method is developed and elaborated to yield a general technique for the generation of separation process models that are inherently low-order and yet that retain the physical characteristics of the original processes.

Compartmental Analysis

It is common practice in engineering analysis to represent the behavior of an ensemble of elements composing a system by an equivalent single element having similar dynamic and/or steady state characteristics. Electrical engineers use this idea to represent R-C or L-R-C networks. The same concept is also the basis for aggregation methods. In structural analysis, the method of finite elements (Hinton and Owen, 1977) is used to represent a continuous medium (whose description would require an infinite number of equations) by elements physically connected at a finite number of nodal points. In biological system modeling, complex phenomena are usually represented by a small number of compartments separated by "anatomical boundaries" through which mass transfer occurs (Jacquez, 1972).

Finally, in modeling chemical reaction kinetics for complex systems, lumping parallel reactions has proved to be a successful simplification of an otherwise intractable problem (Jacob et al., 1976). More recently, models in which several units of a given process (e.g., reactor plus separator) are replaced by a single equivalent unit have been developed. For separation processes, the models proposed by Kuznik and Kzyzanowski (1975, 1977), Osborne et al. (1965), España and Landau (1978), Rademaker et al. (1975), and the collocation models discussed above, all replace a number of the system equations by a single one.

The Compartmental Method for Separation Processes

The following analysis is presented for a binary distillation column, but the development is valid for all staged separation processes. Equimolal overflow and piecewise linear equilibrium assumptions are made in order to make comparisons with existing models based on the same assumptions (Wong and Luus, 1980; Stewart et al., 1981). Extensions of the compartmental approach to constant relative volatility equilibrium are given in the Appendix; extensions to complex multicomponent columns have been reported by Benallou (1982). With the assumptions stated above, the conventional component balances for the column shown in Figure 2 are:

$$M_1\dot{x}_1 = V_R y_2 - L_R x_1 - (V_R - L_R)y_1 \tag{1}$$

$$M_i\dot{x}_i = L_R(x_{i-1} - x_i) + V_R(y_{i+1} - y_i); \quad 2 \le i \le Nf - 1 \tag{2}$$

$$M_{Nf}\dot{x}_{Nf} = L_R x_{Nf-1} - L_S x_{Nf} + V_S y_{Nf+1} - V_R y_{Nf} + F z_F \tag{3}$$

$$M_i\dot{x}_i = L_S(x_{i-1} - x_i) + V_S(y_{i+1} - y_i); \quad Nf + 1 \le i \le N - 1 \tag{4}$$

$$M_N\dot{x}_N = L_S x_{N-1} - V_S y_N - (L_S - V_S)x_N \tag{5}$$

where

$$y_1 = x_1 \qquad \text{for a total condenser} \tag{6}$$

$$y_1 = K_1 x_1 \qquad \text{for a partial condenser} \tag{7}$$

$$y_i = K_i x_i; \quad 2 \le i \le N \tag{8}$$

Using the compartmental concept, the column is considered to be made of a number of compartments (Figure 2), each compartment containing a number of stages. The different compartments are connected by liquid and vapor flows such that the vapor leaving the compartment is the same as the vapor leaving its first (top) stage, and the liquid leaving the compartment corresponds to the liquid from its last (bottom) stage. A typical compartment is shown in Figure 3. The basic idea in this new compartmental approach is to associate the dynamic behavior of a given compartment with that of one of its stages, the sensitive stage. The choice of the sensitive stage for a compartment can be based on physical considerations as discussed by Tolliver and McCune (1978) (e.g., the tray that most closely represents the average conditions prevailing within the entire compartment or that is most sensitive to external disturbances), or it may simply be dictated by instrumentation considerations (e.g., the tray for which a temperature or composition measurement is available, etc.). We propose to represent the dynamic behavior of a compartment by that of a single stage whose inlet and outlet flows and compositions match the flows and compositions of the compartment it represents, as in Figure 4. This representation is based on the following compartmentation assumption:

> The dynamic behavior of a section of stages, or a compartment, can be represented by that of a single stage having the same holdup as the total compartment holdup and the composition of the compartment sensitive stage.

Note that this assumption is considerably more general than that of Dahlqvist, who assumed that the entire compartment would be characterized by the concentration of the last (bottom) stage in the compartment.

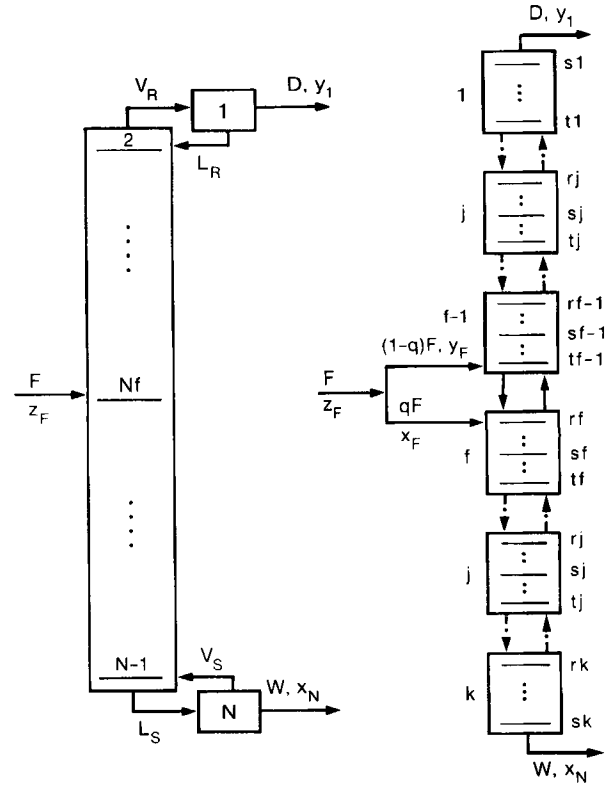

Figure 2. General compartmental representation of a distillation column.

For a compartment containing stages r through t, the total compartment holdup is given by:

$$M_c = \sum_{i=r}^{t} M_i \tag{9}$$

Using the compartmentation assumption, it is possible to represent the dynamic behavior of a compartment by a single differential equation obtained from a dynamic material balance. The compartmental model then is the set of the dynamic equations obtained for all the compartments. In order to illustrate the development of the compartmental equations in more detail, we

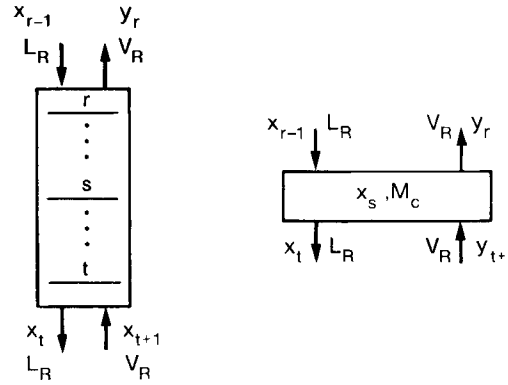

Figure 3. Sensitive stage representation of a compartment.

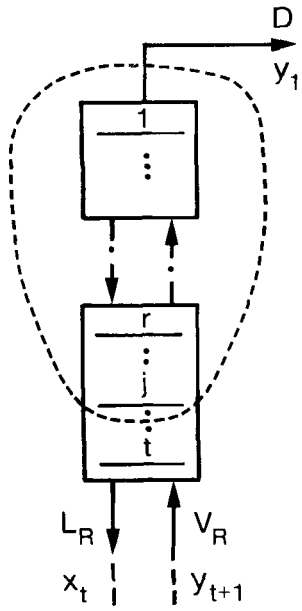

Figure 4. Material balance envelope for tray *j*.

write a component balance for the compartment represented in Figure 3. (For a more general development, see Benallou, 1982). Using the compartmentation assumption, a material balance around the compartment yields:

$$M_c\dot{x}_s = L_R x_{r-1} + V_R y_{t+1} - L_R x_t - V_R y_r \tag{10}$$

Next, approximate expressions for the compartment outlet streams, x_t and y_r will be derived in terms of the compartment sensitive stage composition, x_s, and the distillate composition, x_D or y_1. These expressions are developed using shortcut calculation methods (Smoker, 1938; Garber and Lerman, 1943; Tiller and Tour, 1944; Edmister, 1957; Ramalho and Tiller, 1962) in such a way that the steady state material balances are preserved.

Consider a steady state component balance around the envelope shown in Figure 4:

$$V_R y_{j+1} = L_R x_j + D y_1 \tag{11}$$

Assuming piecewise linear equilibrium,

$$y_j = K_j x_j, \quad j = 1, \ldots, N \tag{12}$$

Eq. 12 becomes:

$$L_R x_{j+1} = A_{j+1}(L_R x_j + DK_1 x_1) \tag{13}$$

where A_j is the absorption factor for stage j, defined by Edmister (1957):

$$A_j \equiv \frac{L_R}{V_R K_j} \quad \text{for } 2 \le j \le Nf \tag{14}$$

$$A_1 \equiv \frac{L_R}{DK_1} \tag{15}$$

Note that $D = V_R - L_R$ and $K_1 = 1$ for a total condenser.

Equation 13 is a first-order difference equation that can be solved easily by successive substitutions to yield the steady state solution for x_t in terms of the sensitive stage and first stage compositions:

$$L_R x_t = DK_1 x_1(A_t + A_t A_{t-1} + \cdots + A_t A_{t-1} \cdots A_{s+1}) + A_t A_{t-1} \cdots A_{s+1} \cdot L_R x_s \tag{16}$$

or

$$x_t = \left(\frac{V_R}{L_R} - 1\right) K_1 x_1 \sum_s^t{}_A + x_s \prod_s^t{}_A \tag{17}$$

where $\sum_s^t{}_A$ and $\prod_s^t{}_A$ are extensions of the notation used by Edmister for the sums and products of the absorption factors. $\sum_s^t{}_A$ and $\prod_s^t{}_A$ are defined by:

$$\sum_s^t{}_A = A_t + A_t A_{t-1} + \cdots + A_t A_{t-1} \cdots A_{s+1} \tag{18}$$

$$\prod_s^t{}_A = A_t A_{t-1} \cdots A_{s+1} \tag{19}$$

Equation 17 relates the steady state composition of the liquid leaving the compartment to the distillate and sensitive stage compositions. We propose to use the steady state relation as an approximate relation for transient conditions.

Using Eq. 17, we define the compartment separation function as the relationship between the composition of the liquid stream leaving the compartment, the terminal (distillate or bottoms) composition, and the sensitive tray composition:

$$g(x_1, x_s) = \left(\frac{V_R}{L_R} - 1\right) K_1 x_1 \sum_s^t{}_A + x_s \prod_s^t{}_A \tag{20}$$

Similarly, the compartment separation function for the vapor stream leaving the compartment (stage r) is obtained from:

$$y_r = K_r\left[x_s - \left(\frac{V_R}{L_R} - 1\right) K_1 x_1 \sum_r^s{}_A\right] \Big/ \prod_r^s{}_A \tag{21}$$

namely,

$$f(x_1, x_s) = K_r\left[x_s - \left(\frac{V_R}{L_R} - 1\right) K_1 x_1 \sum_r^s{}_A\right] \Big/ \prod_r^s{}_A \tag{22}$$

Substitution of Eqs. 20 and 22 into Eq. 10 yields the final model for the compartment:

$$M_c\dot{x}_s = L_R x_{r-1} + V_R y_{t+1} - L_R g(x_1, x_s) - V_R f(x_1, x_s) \tag{23}$$

Full compartmental model

For the column represented in Figure 2, the compartmental model is obtained by writing Eq. 23 for each compartment to

obtain:

$$M_{ci}\dot{x}_{si} = L_{i-1}g_{i-1}(x_{se}, x_{si-1}) + V_{i+1}f_{i+1}(x_{se}, x_{si+1}) - L_i g_i(x_{se}, x_{si}) - V_i f_i(x_{se}, x_{si}) + \delta_{if}qFx_F + \delta_{i(f-1)}(1-q)Fy_F; \quad 1 \le i \le k \quad (24)$$

where δ represents the Kronecker delta, and f_i and g_i are generalizations of the compartment separation functions given by Eqs. 20 and 22 for the first and last stages of compartment i (see Appendix):

$$f_i(x_1, x_{si}) = K_{ri}\left[x_{si} - \left(\frac{V_R}{L_R} - 1\right)K_1 x_1 \sum_{ri}^{si} \Sigma_A\right] \Big/ \prod_{ri}^{si} \Pi_A; \quad 1 \le i \le f-1 \quad (25)$$

$$f_i(x_N, x_{si}) = \left(\frac{L_S}{V_S} - 1\right)x_N \sum_{ri}^{si} \Sigma_S + K_{si}x_{si}\prod_{ri}^{si}\Pi_S; \quad f \le i \le k \quad (26)$$

$$g_i(x_1, x_{si}) = \left(\frac{V_R}{L_R} - 1\right)K_1 x_1 \sum_{si}^{ti} \Sigma_A + x_{si}\prod_{si}^{ti}\Pi_A; \quad 1 \le i \le f-1 \quad (27)$$

$$g_i(x_N, x_{si}) = \left[K_{si}x_{si} - \left(\frac{L_S}{V_S} - 1\right)x_N \sum_{si}^{ti}\Sigma_S\right] \Big/ \left(K_{ti}\prod_{si}^{ti}\Pi_S\right); \quad f \le i \le k \quad (28)$$

Σ_S and Π_S can be obtained from Eqs. 18 and 19 by replacing the absorption factors A_j by the stripping factors $S_j = K_j V_S/L_S$. The subscript se denotes the appropriate terminal concentration

$$se = s1 = 1, \quad \text{for the rectification compartments} \quad (29)$$

$$se = sk = N, \quad \text{for the stripping compartments} \quad (30)$$

Also,

$$\begin{aligned} L_o &= 0 \\ L_i &= L_R \quad \text{for } 1 \le i \le f-1 \\ L_i &= L_S \quad \text{for } f \le i \le k-1 \\ L_k &= L_S - V_S \end{aligned} \quad (31)$$

$$\begin{aligned} V_1 &= V_R - L_R \\ V_i &= V_R \quad \text{for } 2 \le i \le f-1 \\ V_i &= V_S \quad \text{for } f \le i \le k \\ V_{k+1} &= 0. \end{aligned} \quad (32)$$

Remarks

1. Equations 24–32 represent a compartmental model for a simple distillation column where the retained stage concentrations (state variables) and the compartmental configuration can be chosen independently and arbitrarily. Elaborating on the ideas presented in this section, a similar type of dynamic model can be obtained for other separation processes and for more complex columns where variable holdup, energy balances, stage efficiencies, multiple feed trays, and side streams are considered. These types of models have been considered by Benallou (1982).

2. The order of the compartmental model is k, the number of compartments, which will normally be much less than N. The compartmental model also includes the four algebraic equations consisting of the compartment separation functions in Eqs. 25–28. Notice that these functions are expressed analytically in terms of the process parameters. This type of formulation is particularly useful if the process conditions change since the same model is still valid.

3. In contrast to existing low-order modeling techniques, use of compartmental analysis does not require that the complete high-order model be available. Rather, the low-order material balances are written out directly using compartmental functions.

4. In the model given by Eqs. 24–32, we have imposed the condition that the sensitive stages of the first and last compartments be the condenser and reboiler stages, respectively. This assumption is not necessary, but it permits the top and bottom compositions to be retained as state variables.

5. Because of the nature of the compartment separation functions, steady state agreement between the complete and compartmental models will be guaranteed, i.e., the compartmental model will predict the correct steady state for an arbitrary change in any of the input variables. In fact, at steady state, the compartmental model is identical to the complete model in which the "nonsensitive" compositions and their corresponding equations are eliminated using shortcut expressions. No more than two compartments are required to obtain an approximate dynamic model that matches distillate and bottoms compositions exactly. Among the available low-order modeling techniques, steady state agreement can be achieved only in the linear case (Marshall, 1966; Litz, 1981). For nonlinear models with constant relative volatility, some of the methods based on orthogonal collocation yield models that satisfy material balances; however these methods do not guarantee steady state agreement between the collocation and complete models.

Application to Distillation

In order to illustrate the compartmental approach, we consider the 20-stage distillation column example used by Stewart et al. (1981). Constant molal overflow and constant relative volatility of $\alpha = 1.6$ are assumed. Figure 5 shows the extent of the column nonlinearities for ±40% step changes in feed flow rate.

For comparison with the sixth-order collocation model developed by Stewart et al. (1981), a six-compartment model was constructed. The compartmental model configuration is shown in Figure 6. The model equations were obtained from Eqs. 24 and 29–32 using the separation functions developed in the Appendix and the parameters given in Table 1. Note that the sensitive trays for the first and last compartments were taken to be the condenser and reboiler stages, respectively. For the feed compartment, the sensitive tray was taken at the feed location; for the remaining compartments, sensitive trays were taken midway between the first and last stages in the compartment. This configuration is somewhat arbitrary; other configurations lead to comparable results.

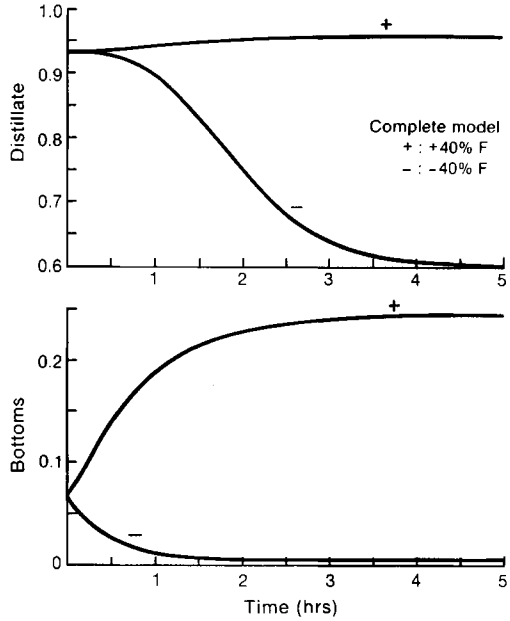

Figure 5. Nonlinearity test: distillate and bottoms composition responses to +40% and −40% step changes in feed flow rate.

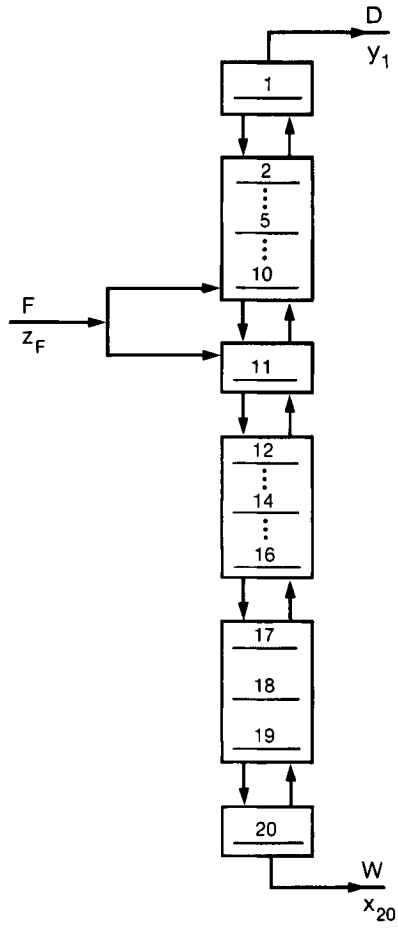

Figure 6. Distillation column compartmentation, six compartments.

Table 1. Compartmentation Parameters (Six-Compartment Model)

k = 6	$r1 = 1$	$s1 = 1$	$t1 = 1$	$f = 3$
	$r2 = 2$	$s2 = 5$	$t2 = 10$	
	$r3 = 11$	$s3 = 11$	$t3 = 11$	
	$r4 = 12$	$s4 = 14$	$t4 = 16$	
	$r5 = 17$	$s5 = 18$	$t5 = 19$	
	$r6 = 20$	$s6 = 20$	$t6 = 20$	

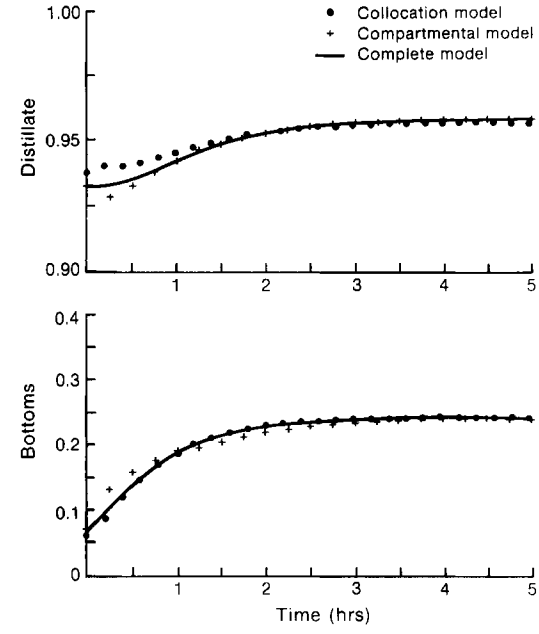

Figure 7. 20-stage distillation column: distillate and bottoms responses to a +40% step change in feed flow rate.

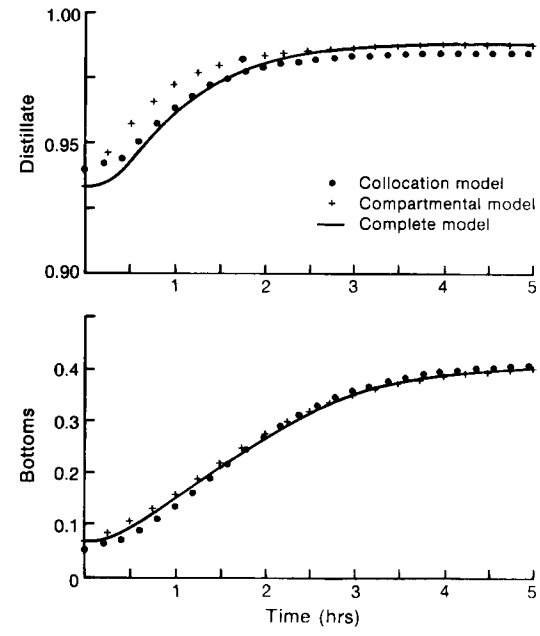

Figure 8. 20-stage distillation column: distillate and bottoms composition responses to a +40% step change in feed composition.

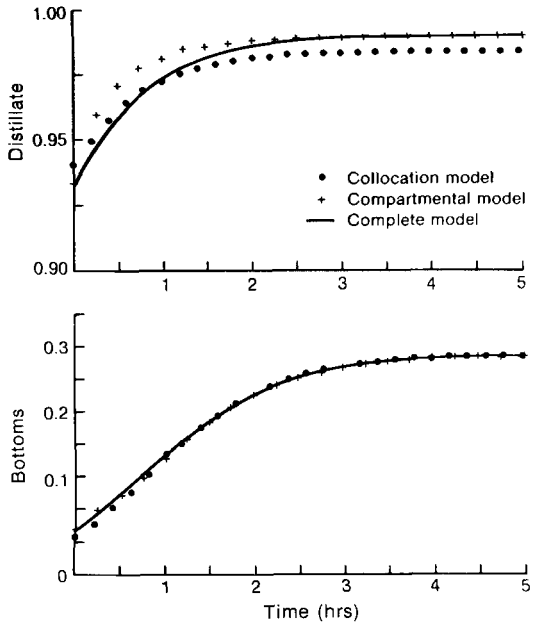

Figure 9. 20-stage distillation column: distillate and bottoms composition responses to a −10% step change in vapor flow rate.

For different input forcings, typical responses of the complete, collocation, and compartmental models are shown in Figures 7 through 10. For a change in the feed flow (Figure 7), the collocation model exhibits initial and final steady state errors. By contrast, the compartmental model response shows a reasonably close representation of the dynamics and, as expected, exact initial and final steady state agreement. However, this response shows an initial inverse response that does not appear in the complete model response. The inverse response characteristics are attributed to the fact that the compartmental model uses steady state relationships in its development.

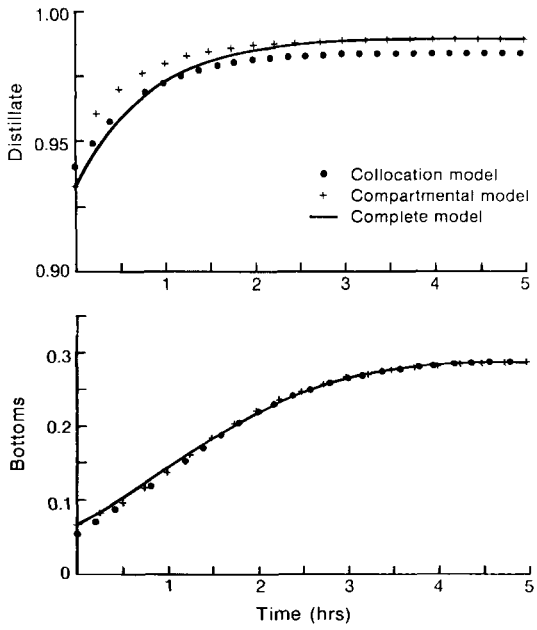

Figure 10. 20-stage distillation column: distillate and bottoms composition responses to a +10% step change in reflux flow rate.

Table 2. Compartmentation Parameters (Four-Compartment Model)

k = 4	$r1 = 1$	$s1 = 1$	$t1 = 1$	$f = 3$
	$r2 = 2$	$s2 = 5$	$t2 = 10$	
	$r3 = 11$	$s3 = 16$	$t3 = 19$	
	$r4 = 20$	$s4 = 20$	$t4 = 20$	

For a feed composition change, Figure 8, as well as for the other tests—vapor flow, Figure 9; reflux flow, Figure 10—the compartmental model gives a good representation of the dynamics and yields exact steady state agreement.

In order to test the robustness of the compartmental technique, a four-compartment model was constructed, Table 2. As shown by Benallou (1982), a reduction in the number of compartments used to represent the column does degrade the accuracy of the compartmental model slightly. However, the responses of the complete, fourth-order compartmental, and sixth-order collocation models for different input forcings show that the fourth-order compartmental model predicts the complete model steady states exactly and approximates its dynamics fairly closely.

In Figures 11 and 12 the dynamic responses of the four state variables retained in the compartmental model are shown against the complete model responses. It is seen from these figures that the dynamic behavior of the intermediate stages (stages 5 and 16) is also predicted with reasonable accuracy.

It should be noted that changing the order of the compartmental model does not involve any additional computations,

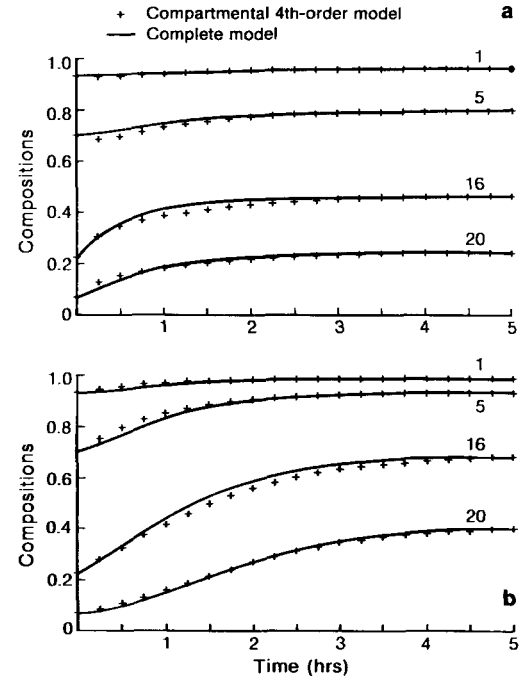

Figure 11. 20-stage distillation column: composition responses of stages 1, 5, 16, and 20 to feed changes.

(a) +40% step change in feed flow rate
(b) + 40% step change in feed composition

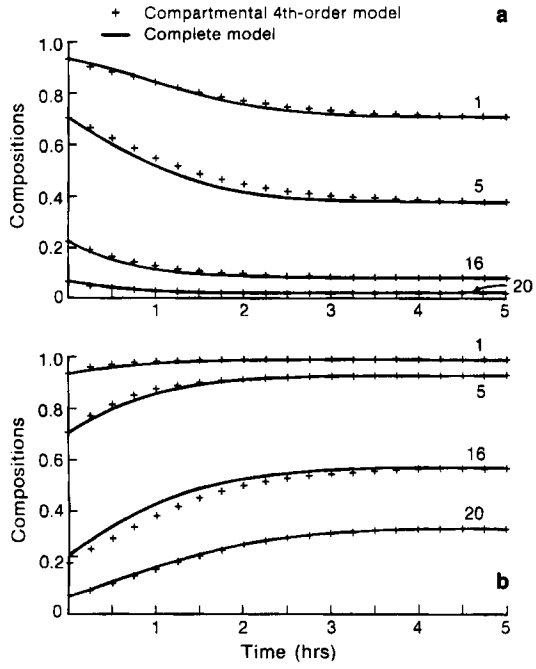

Figure 12. 20-stage distillation column: composition responses of stages 1, 5, 16, and 20 to reflux and vapor changes.

(a) – 10% step change in reflux flow rate
(b) – 10% step change in vapor flow rate

which is not the case with most methods for determining low-order models and collocation-based techniques in particular. The compartmental model is completely defined when its parameters—Table 2, for example—are specified.

Finally, this numerical comparison of compartmental and collocation-based techniques shows that the methods are somewhat complementary. Compartmental and high-order model results always match exactly at the initial and final steady states; hence gains calculated from the low-order model always will match those of the high-order model. In comparison, gains computed from collocation models exhibited significant errors in several cases. On the other hand, with the exception of the erroneous instantaneous response at $t = 0$, collocation results often matched the high-order model response better during the initial transient period. Hence, the final use of the low-order model will dictate whether the increased computational complexity of collocation-based methods is justified. In any case, a much more extensive comparison of the methods is necessary before generalizations can be made.

Acknowledgment

The authors wish to thank W.E. Stewart and K.L. Levien of the University of Wisconsin and M. Morari of Caltech for communicating results of their collocation method. These have been used in several of the comparisons in this paper. The financial support of the Agency for International Development and the Moroccan Ministry of Energy for A. Benallou is gratefully acknowledged.

Notation

A = absorption factor = L/VK
B = function, Eq A17
D = distillate flow
D_R, D_S = function, Eqs. A18 and A22
E = function of the sensitive composition, Eq. A19
F = feed flow rate
f = number of the feed compartment
f_i = separation function for the first stage of compartment i
g_i = separation function for the last stage of compartment i
K = equilibrium constant
k = order of the compartmental model = number of compartments
L = liquid flow rate
M = holdup
N = number of stages in the column
Nf = feed stage location
q = feed quality
r = number of the first stage in a compartment
ri = number of the first stage in compartment i
S = stripping factor = KV/L
s = number of the sensitive stage of a compartment
si = number of the sensitive stage of compartment i
t = number of the last stage in a compartment
ti = number of the last stage in compartment i
V = vapor flow
W = bottoms flow
x = liquid composition
y = vapor composition
z = feed composition

Greek letters

α = relative volatility
δ = Kronecker symbol
Σ_A = function of the absorption factor
Σ_S = function of the stripping factor, Eq. A6
Π_A = function of the absorption factor
Π_S = function of the stripping factor, Eq. A7

Subscripts

ci = compartment i
F = feed
f = feed compartment number
R = rectification section
r = first stage of a compartment
ri = number of the first stage in compartment i
S = stripping section
s = sensitive stage of a compartment
se = terminal (end) stage, i.e., 1 or N
si = number of the sensitive stage of compartment i
t = last stage of a compartment
ti = number of the last stage in compartment i

Appendix: Separation Functions

Since their introduction into separation processes (Tiller and Tour, 1944), finite-difference methods have been used extensively and have led to the development of shortcut calculation methods that are used to express the number of stages in a separation tower in terms of the terminal compositions (Smoker, 1938; Garber and Lerman, 1943; Tiller and Tour, 1944; Edmister, 1957; Ramalho and Tiller, 1962; Gilbert et al., 1969; Eckert and Hlavacek, 1978). In turn, shortcut methods have found considerable success in application-oriented problems (Edmister, 1957; Gilbert et al., 1969; Eckert and Hlavacek, 1978; Ohmura et al., 1979; Fleisher and Prett, 1981).

In this development, finite-difference calculus is used in a similar way to shortcut methods in order to develop expressions for the compartment separation functions. The following development is for a distillation column, making the equimolal overflow assumption. For absorption, the development is similar. Compartmental separation functions are obtained from material balances around the stages of the stripping or rectification section, figures A1 and A2.

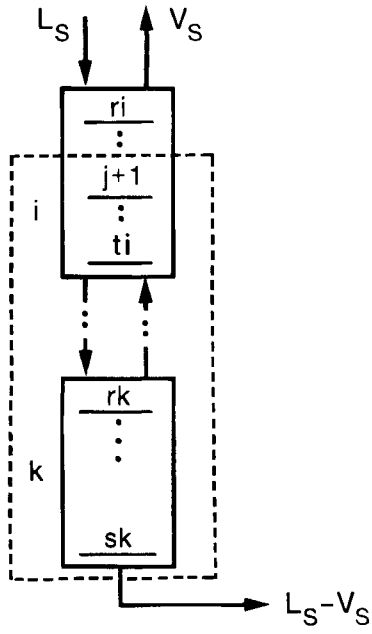

Figure A1. Material balance envelope for tray $j+1$ of compartment i.

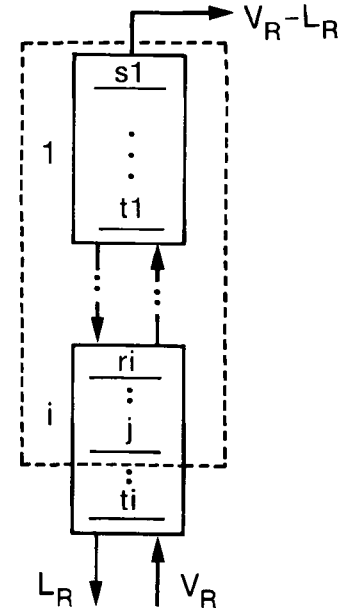

Figure A2. Material balance envelope for a rectification stage.

Consider a component balance around the envelope shown in Figure A1:

$$L_S x_j = V_S y_{j+1} + (L_S - V_S)x_{sk} \tag{A1}$$

Assuming piecewise linear equilibrium, Eq. A1 becomes:

$$V_S y_j = S_j(V_S y_{j+1} + W x_{sk}) \tag{A2}$$

where

$$S_j = \frac{K_j V_S}{L_S} \quad Nf + 1 \le j \le N - 1$$

$$S_N = \frac{K_N V_S}{W} \tag{A3}$$

and

$$W = L_S - V_S \tag{A4}$$

Solving Eq. A1 by back-substitution yields:

$$y_{ri} = \left(\frac{L_S}{V_S} - 1\right) x_{sk} \overset{si}{\underset{ri}{\Sigma}}_S + K_{si} x_{si} \overset{si}{\underset{ri}{\Pi}}_S \tag{A5}$$

where,

$$\overset{si}{\underset{ri}{\Sigma}}_S = S_{ri} + S_{ri} S_{ri+1} + \cdots + S_{ri} S_{ri+1} \cdots S_{si-1} \tag{A6}$$

and

$$\overset{si}{\underset{ri}{\Pi}}_S = S_{ri} S_{ri+1} \cdots S_{si-1} \tag{A7}$$

Hence, the separation function for the first stage of compartment i of the stripping section is:

$$f_i(x_{sk}, x_{si}) = \left(\frac{L_S}{V_S} - 1\right) x_{sk} \overset{si}{\underset{ri}{\Sigma}}_S + K_{si} x_{si} \overset{si}{\underset{ri}{\Pi}}_S \tag{A8}$$

Using a similar development, the composition of the liquid leaving the last tray of compartment i is given by:

$$x_{ti} = \left[K_{si} x_{si} - \left(\frac{L_S}{V_S} - 1\right) x_{sk} \overset{ti}{\underset{si}{\Sigma}}_S\right] \Big/ \left(K_{ti} \overset{ti}{\underset{si}{\Pi}}_S\right) \tag{A9}$$

Thus, the separation function for the last tray of compartment i is given by:

$$g_i(x_{sk}, x_{si}) = \left[K_{si} x_{si} - \left(\frac{L_S}{V_S} - 1\right) x_{sk} \overset{ti}{\underset{si}{\Sigma}}_S\right] \Big/ \left(K_{ti} \overset{ti}{\underset{si}{\Pi}}_S\right) \tag{A10}$$

For the rectification section stages, the separation functions given by Eqs. 20 and 22 can be written in their general form as follows:

For the last stage of compartment i:

$$g_i(x_{sl}, x_{si}) = \left(\frac{V_R}{L_R} - 1\right) K_{sl} x_{sl} \overset{ti}{\underset{si}{\Sigma}}_A + x_{si} \overset{ti}{\underset{si}{\Pi}}_A \tag{A11}$$

For the first stage of compartment i:

$$f_i(x_{sl}, x_{si}) = K_{ri}\left[x_{si} - \left(\frac{V_R}{L_R} - 1\right) K_{sl} x_{sl} \overset{si}{\underset{ri}{\Sigma}}_A\right] \Big/ \overset{si}{\underset{ri}{\Pi}}_A \tag{A12}$$

Remark

For the case of constant relative volatility, a similar development leads to the following separation functions (Benallou, 1982):

Rectification Section Stages

First stage of compartment i:

$$f_i(x_{s1}, x_{si}) = \frac{\alpha x_{ri}}{1 + (\alpha - 1)x_{ri}} \tag{A13}$$

where:

$$x_{ri} = E_R + \left[\left(\frac{1}{x_{si} - E_R} - \frac{1}{A_R - B_R - 2E_R}\right)\left(\frac{A_R - E_R}{B_R - E_R}\right)^{\text{ri-si}} + \frac{1}{A_R - B_R - 2E_R}\right]^{-1} \tag{A14}$$

Last stage of compartment i:

$$g_i(x_{s1}, x_{si}) = E_R + \left[\left(\frac{1}{x_{si} - E_R} - \frac{1}{A_R - B_R - 2E_R}\right) \cdot \left(\frac{A_R - E_R}{B_R + E_R}\right)^{\text{ti-si}} + \frac{1}{A_R - B_R - 2E_R}\right]^{-1} \tag{A15}$$

where:

$$A_R = \frac{V_R}{(\alpha - 1)L_R} \cdot \left[\alpha - (\alpha - 1)\left(1 - \frac{L_R}{V_R}\right)\frac{\alpha x_{s1}}{1 + (\alpha - 1)x_{s1}}\right] \tag{A16}$$

$$B_R = \frac{1}{\alpha - 1} \tag{A17}$$

$$D_R = \frac{-1}{\alpha - 1}\left(\frac{V_R}{L_R} - 1\right)\frac{\alpha x_{s1}}{1 + (\alpha - 1)x_{s1}} \tag{A18}$$

$$E_R = \frac{A_R - B_R}{2} + \frac{1}{2}[(A_R - B_R)^2 + 4D_R]^{1/2} \tag{A19}$$

Stripping Section Stages:

Separation functions are obtained from Eqs. A14 and A15 by substituting A_S, B_S, D_S, and E_S for A_R, B_R, D_R, and E_R, where:

$$A_S = \frac{V_S}{(\alpha - 1)L_S}\left[\alpha - (\alpha - 1)\left(1 - \frac{L_S}{V_S}\right)x_{sk}\right], \tag{A20}$$

$$B_S = B_R \tag{A21}$$

$$D_S = -\frac{1}{\alpha - 1}\left(\frac{V_S}{L_S} - 1\right)x_{sk} \tag{A22}$$

and E_S is obtained using A_S, B_S, and D_S in Eq. A19.

Literature Cited

Benallou, A., "Dynamic Modeling and Bilinear Control Strategies for Distillation Columns," Doctoral Thesis, Univ. California, Santa Barbara (1982).

Bonvin, D., and D. A. Mellichamp, "A Unified Derivation and Critical Review of Modal Approaches to Model Reduction," *Int. J. Control*, **35**, 829 (1982).

Cho, Y. S., and B. Joseph, "The Development of Simple Dynamic Models for Separation Processes," *Paper 2d, 73rd Ann. AIChE Meet.*, Chicago (1980).

———, "Reduced Order Steady State and Dynamic Models for Separation Processes. II: Application to Nonlinear Multicomponent Systems," *AIChE J.*, **29**, 270 (1983).

Crockett, W. E., "Approximate Distillation Dynamics from Steady State Data," *Proc. JACC*, **1**, 223 (1978).

Dahlqvist, S. A., "Control of the Top and Bottom Compositions in a Pilot Distillation Column," *ICE Symp. Ser.*, **56**, 2.6/25 (1979).

Eckert, E., and V. Hlavacek, "Calculation of Multicomponent Distillation of Nonideal Mixtures by a Shortcut Method," *Chem. Eng. Sci.*, **33**, 77 (1978).

Edmister, W. G., "Absorption and Stripping-Factor Functions for Distillation Calculation by Manual- and Digital-Computer Methods," *AIChE J.*, **3**, 165 (1957).

España, M., and I. D. Landau, "Reduced-Order Bilinear Models for Distillation Columns," *Automatica*, **14**, 345 (1978).

———, "Distillation Columns—A Class of Systems with Multiplicative Inputs," *Trans. ASME J. Dyn. Meas. Contr.*, **101**, 58 (1979).

Fleischer, M. T., and D. M. Prett, "Simplified Techniques for Simulating Complex Columns," *Chem. Eng. Prog.* **77**, 72 (1981).

Garber, H. J., and F. Lerman, "Principles of Stripping Operations: Particularly Steam Distillation," *Trans. AIChE*, **39**, 113 (1943).

Georgakis, C., and M. A. Stoever, "Time Domain Order Reduction of Tridiagonal Dynamics of Staged Processes. I: Uniform Lumping," *Chem. Eng. Sci.*, **37**, 687 (1982).

Gilbert, R. J. H., G. J. Wanless, and R. D. Wilsdon, "Assessment of Fractionator Performance: Shortcut Methods," *Inst. Chem. Eng. Symp. Ser.*, **32**, 34 (1969).

Hermite, C., "Considerations sur la résolution algébrique de l'équation du Cinquième degré," in *Oeuvres de Charles Hermite*, E. Picard, ed., Gauthier-Villars, Paris (1905).

Hinton, E., and D. R. J. Owen, *Finite Element Programming*, Academic Press, New York (1977).

Jacob, S. M., et al., "A Lumping and Reaction Scheme for Catalytic Cracking," *AIChE J.*, **22**, 701 (1976).

Jacquez, J. A., *Compartmental Analysis in Biology and Medicine*, Elsevier, New York, 1972.

Kuznik, J., and R. Kzyzanowski, "Calculated Designations of the Dynamic Properties of Simplified Models of Distillation Columns," *Int. Chem. Eng.*, **15**, 553 (1975).

———, "Numerical Determination of the Dynamic Properties of a Distillation Column and a Measurement Verification Test of the Column Model," *Int. Chem. Eng.*, **17**, 360 (1977).

Litz, L., "Order Reduction of Linear State Space Models via Optimal Approximation of the Dominant Modes," *Large-Scale Syst. Theor. App.*, **2**, 171 (1981).

Marshall, W. R., and R. L. Pigford, *The Application of Differential Equations to Chemical Engineering Problems*, Univ. Delaware Press, Newark, DE (1947).

Marshall, S. A., "An Approximate Method for Reducing the Order of a Linear System," *Control*, **10**, 642 (1966).

Moczek, J. S., R. E. Otto, and T. J. Williams, "Approximation Models for the Dynamic Response of Large Distillation Columns," *CEP Symp. Ser.*, **61**, 136 (1965).

Ohmura, S., M. Hirata, and S. Kashara, "New Distillation Calculation Method Utilizing Salient Features of Both Shortcut and Tray-by-Tray Methods," *ICE Symp. Ser.*, **56**, 51 (1979).

Osborne, W. G., Jr., et al., "A Simplified Model for the Transient Behavior of Distillation Columns," *AIChE—ICE Symp. Ser.*, **1**, 84 (1965).

Rademaker, O., J. E. Rijnsdorp, and A. Maarleveld, *Dynamics and Control of Continuous Distillation Units*, Elsevier, New York (1975).

Ramalho, R. S., and F. M. Tiller, "Single Formula for Replacing Smoker Equations in Binary Distillation," *AIChE J.*, **8**, 559 (1962).

Smoker, E. H., "Analytic Determination of Plates in Fractionating Columns," *Trans. AIChE*, **34**, 165 (1938).
Stewart, W. E., K. L. Levien, and M. Morari, "A New Model Reduction Technique for Staged Separation Operations," *Paper 55c, 74th Ann. AIChE Meet.*, New Orleans (1981).
Stoever, M. A., and C. Georgakis, "Time Domain Order Reduction of Tridiagonal Dynamics of Staged Processes. II: Nonuniform Lumping," *Chem. Eng. Sci.*, **37**, 699 (1982).
Tiller, F. M., and R. S. Tour, "Stagewise Operations: Applications of the Calculus of Finite Differences to Chemical Engineering," *Trans. AIChE*, **40**, 317 (1944).
Tolliver, T. L., and L. C. McCune, "Distillation Control Design Based on Steady State Simulation," *ISA Trans.*, **17**, 3 (1978).
Tolliver, T. L., and R. C. Waggoner, "Distillation Column Control. A Review and Perspective from the C.P.I.," *Advances in Instrumentation*, **35**, 83 (1980).
Wahl, E. F., and P. Harriott, "Understanding and Prediction of the Dynamic Behavior of Distillation Columns," *IEC Proc. Des. Dev.*, **9**, 396 (1970).
Waller, K. V., "On the Dynamics and Control of Continuous Plate Distillation Columns," Doctoral Thesis, Åbo Akademi, Finland (1972).
Waller, K. V., "Simple Models for Distillation Dynamics," *86th Natl. AICHE Meet.*, Houston (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**, 1,243 (1972).
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 (1980).

Manuscript received Jan. 27, 1983, and revision received May 15, 1985.