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RESPONSE MODE ANALYSIS AND CONTROL OF MULTIVARIABLE CHEMICAL PROCESSES: APPLICATION TO DISTILLATION

Robert Edward Levy
(Ph. D. Thesis)

June 1967

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RESPONSE MODE ANALYSIS AND CONTROL OF MULTIVARIABLE CHEMICAL PROCESSES: APPLICATION TO DISTILLATION

Robert Edward Levy

Inorganic Materials Research Division, Lawrence Radiation Laboratory,
and Department of Chemical Engineering,
University of California, Berkeley, California

ABSTRACT

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The natural modes of a multivariable process may serve as the framework for a feedback control scheme that hastens the response of the process, overcomes the problem of control loop interaction, and guides the selection and interconnection of measured and manipulated variables. In this work the independent modes of a simulated binary distillation column are identified, and their significance and physical basis are evaluated. This provides information necessary for the development of modal controllers.

Distillation modes are determined from three different mathematical models, the most comprehensive of which includes unsteady balances for mass, chemical species, and enthalpy. The accurate computation of modes for the large unsymmetric matrices generated by the models requires efficient numerical procedures, such as the QR algorithm for eigenvalues and an inverse iteration scheme for eigenvectors.

The dominant, or most slowly decaying, mode is found to be associated with compositions throughout the column, but not with enthalpy or mass accumulation. It is highly activated by all inputs to the column. The second slowest mode, which has a characteristic decay time 2.5 times shorter than the slowest, can be identified with the accumulator. The

effects of various design and operating conditions on the modes are evaluated. A sensitivity analysis reveals those distillation parameters whose values influence the slow modes most strongly.

The limitations of modal control caused by partial observability and partial controllability are examined. A modal controller is developed by approximate methods for the slowest mode of the column. It decreases the process response time by a factor of 2.5 and causes very little alteration of the faster modes. A feedforward controller that detects disturbance inputs and cancels the activations of the three slowest modes is also investigated. The influence of these disturbances can be reduced by an order of magnitude in this way.

I. INTRODUCTION

Conventional methods for the synthesis of automatic control systems for multivariable chemical processes are frequently unsatisfactory because of three fundamental problems. First, only a small fraction of the process variables are accessible for measurement or manipulation, and those available may not be especially helpful for detecting or overcoming disturbances. Second, there is interaction among individual variables that results in interaction among the usual single-variable control loops, and there is no simple, systematic procedure for eliminating this. Third, conventional schemes provide no guidance in the selection of suitable measured and manipulated variables (or combinations of each) that should be linked by a control function in order to provide effective control. The problems of accessibility, interaction, and linkage are formidable when the number of variables is large.

An approach to the control of multivariable processes based on the control of the slowest natural modes of the process was proposed by Rosenbrock in 1962.[53] This technique yields a set of feedback controllers that are noninteracting in the sense that each influences only one of the independent modes. Moreover, the design procedure for these modal controllers guides the selection of appropriate combinations of measured and manipulated variables, and their interconnections. The use of such a control scheme requires detailed knowledge of the process modes.

In this work the modes of a binary distillation column are analyzed and their physical basis and significance are investigated. With this background a preliminary evaluation of the feasibility of modal control is conducted for the simulated column. Controllers using only input and

output variables that are accessible in practice are developed for the slowest mode of the column.

A. Modes of a Process

The dynamic behavior of most chemical processes can be represented by a set of differential equations that are usually nonlinear. Frequently the principal dynamic effects can be represented by a linear approximation, when perturbations from a steady state condition are small. Then, for lumped parameter processes, the dynamics may be expressed by a set of linear, first-order ordinary differential equations with constant coefficients. In vector notation

$$\dot{\underline{z}} = \underline{\underline{A}}\,\underline{z} + \underline{\underline{B}}\,\underline{d} \tag{1.1}$$

where $\underline{z} = \underline{z}(\theta)$ is a vector of process variables expressed as deviations from steady state; called the state vector,

$\dot{\underline{z}} = \dot{\underline{z}}(\theta)$ is the vector of derivatives of the state variables with respect to time, θ,

$\underline{\underline{A}}$ is the state space matrix of constant coefficients of state variables,

$\underline{d} = \underline{d}(\theta)$ is a vector of process inputs, and

$\underline{\underline{B}}$ is the input matrix of constant coefficients that give the effect of inputs on the rates of change of the state variables.

The state space formulation, given by Eq. (1.1), has been developed extensively by Zadeh and Desoer.[66]

The modes of a process are directions in the state space determined by the right eigenvectors, $\underline{u}^{(i)}$, of the matrix $\underline{\underline{A}}$. When the eigenvalues, λ_i, of $\underline{\underline{A}}$ are all distinct, these vectors represent the independent basis vectors of the state space. Consequently the response of any

stable process that has distinct eigenvalues may be represented as a superposition of contributions from each of the independent modes. Furthermore, each contribution decays as a single exponential with a time constant determined by the eigenvalue for that mode. The extent of the contribution from a mode is known as its activation. Typical processes have a spectrum of time constants associated with their modes, and it is only the few most slowly responding modes that are important in determining the process dynamics, the faster modes dying away very rapidly. Thus it is the slow modes to which a modal control scheme is applied in order to speed up the process recovery from disturbances. The time constant associated with a mode can be reduced by a choice of combinations of manipulated variables that drives the state vector parallel to the mode toward the origin. The controller drives the state variables an amount proportional to the activation of the mode being controlled. In addition to reducing the time constants of the slowest, or dominant, modes, ideal modal controllers do not interact with modes other than the one on which they operate. Also, the nature of the modes guides the choice of combinations of measured and manipulated variables. However, it is usually not possible to design an ideal modal controller, because only a few of the variables of a real process can be manipulated. Furthermore, activations of the modes cannot be determined perfectly, because relatively few variables are accessible for measurement.

B. Prior Work

While the concept of modes is an old one, Rosenbrock[53] seems to have been the first to propose a control scheme that takes advantage of their properties. He also presented some ideas for coping with

the problems of limited accessibility for measurement and manipulation, and gave some qualitative discussion of the application of the method to distillation control. Gordon-Clark[21] investigated the modal control procedure with a simulated five-plate distillation column, but his mathematical model was too simple to be realistic. He furthermore assumed every state variable to be measurable and manipulable. Davison[12,13] also has studied modal control of a distillation column (eight plates), using a model that is more complete than that of Gordon-Clark. Nevertheless, Davison's model does not thoroughly account for hydraulic and thermal phenomena. His work demonstrates the mechanics of a method for designing approximate controllers with only a few measured and manipulated variables. Application of modal control to a boiler was investigated by Ellis and White,[16] who designed an approximate single-loop controller for the eight-variable model using realistic measured and manipulated variables.

There have been some investigations of modal control of distributed parameter processes. Gould[22] and Murray-Lasso[23,41] have discussed the general approach and illustrated it with control of a heated rod. Schlaepfer[55] has applied the scheme to control of an ammonia synthesis reactor.

In this prior work there has been essentially no examination of the physical bases of the modes. As a consequence, there is at present little appreciation of the possible sources of difficulty in the application of the modal control concepts to chemical processes. In addition, the mathematical models used for modal control studies of distillation have not been sufficiently detailed to assess many practical aspects of the procedure. Finally, not enough attention has been given

to the selection of realistic variables for measurement and manipulation, and to the problems of designing effective controllers when the state vector is only partially observable and partially controllable.

In this work mathematical models that involve as few artificial restrictions as possible are developed for a distillation column. The problem of measurement and manipulation is acknowledged by the use of realistic input and output variables.

C. Mathematical Model

A binary stagewise distillation column was chosen for analysis because its dynamics may, under some conditions, be represented by a state space formulation and because its dynamic behavior has been studied experimentally by prior investigators. The specific unit that has been modeled is the ten-plate bubble-cap column studied by J. A. Gerster and his co-workers at the University of Delaware.[2,3,6,19,33,56]

A variety of mathematical models of this process have been investigated here because there is conflicting evidence regarding the most suitable formulation.[29,32,48] The evaluation of distillation models was a parallel objective of this work, but the problem has not been resolved.

Three models, ranging from simple to detailed, are used here to describe binary stagewise distillation in general, and the experimental column of Gerster in particular. The most detailed model, which was used for most of the calculations of this study, includes many phenomena that are normally omitted from dynamic calculations. At every plate unsteady balances on total mass, enthalpy, and chemical species are taken into account. Expressions for vapor flow rate as a function of pressure drop, for liquid flow as a function of liquid height on the

plate, vapor-liquid equilibria for nonideal mixtures, and Murphree efficiencies are used. In addition care has been taken to describe the reboiler and condenser systems accurately so that all common process inputs can be included.

In state space form the detailed distillation model yields 34 differential equations. Numerical methods for the modal decomposition are required. The computation of eigenvalues and eigenvectors of large matrices requires sophisticated numerical methods, and adequate algorithms have been found for this purpose. The QR procedure* determines eigenvalues by orthogonal transformation of the matrix $\underline{\underline{A}}$; an inverse iteration scheme yields accurate eigenvectors.[65]

While the modes and the modal control of a specific simulated, binary, stagewise distillation column are examined here, much of this work has considerably broader applicability. A discussion of the problems of designing modal controllers when there are few measured and manipulated variables, which is included in the presentation of theoretical background in Chapter II, is pertinent for any modal control application. However some of these basic problems in modal control have not been attacked here, and there are certainly others that have not yet been recognized. The computational procedures assembled here and described in Chapter III are not original, but are highly successful for modal decomposition of a variety of matrices. Even the mathematical

---

* See Wilkinson[65]

models (developed in Chapter IV) can be adapted easily to nearly any stagewise distillation process because of their generality. It is hoped that this work will not be viewed merely as another scheme for controlling a distillation column. Rather, this is a critical examination of a novel approach to multivariable process control that uses distillation as a testing ground.

II. THEORETICAL BASIS FOR MODAL DECOMPOSITION AND MODAL CONTROL

A. State Space Formulation

The calculation of process modes requires a state space formulation, which is based on the concept of the process state and is defined rigorously by Zadeh and Desoer.[66] The set of n variables that completely defines the state of a process at any instant constitutes the state vector. The state vector lies in the n-dimensional state space and can be calculated from knowledge of initial conditions, process input functions and the dynamic relationships among the state variables. These relationships are derived from the mathematical description of the physical and chemical phenomena that comprise the process.

In this work consideration is restricted to lumped parameter processes (no dependence on a distance variable) and to processes having no pure time delays. Furthermore, the differential equations describing the process dynamics must be linear, or more commonly, must be linearized about a steady state operating condition. In the latter case the predicted dynamic behavior is valid only for small excursions from the steady state, and the variables are usually expressed as deviations from steady state. With a constant steady state as a basis the process is stationary, and therefore the coefficients of the differential equations are constant. Thus the state space formulation used here consists of a set of linear, first-order, ordinary differential equations with constant coefficients. These may be written in vector notation as

$$\dot{\underline{z}} = \underline{\underline{A}}\,\underline{z} + \underline{\underline{B}}\,\underline{d} \qquad (2.1)$$

where $\underline{z} = \underline{z}(\theta)$ is the state vector, consisting of n state variables, and defines a point in the state space that represents the state of the process at any time,

$\dot{\underline{z}} = \dot{\underline{z}}(\theta)$ is the vector of derivatives of the state variables with respect to time, θ,

$\underline{\underline{A}}$ is the nxn state matrix of constant coefficients of the state variables,

$\underline{d} = \underline{d}(\theta)$ is the m-dimensional vector of inputs ($m \leq n$), and

$\underline{\underline{B}}$ is the nxm input matrix of constant coefficients giving the effect of inputs on the rates of change of the state variables.

The input vector, $\underline{d}$, may be subdivided into q distrubance inputs, $\hat{\underline{d}}$, and p manipulable inputs, $\underline{g}$, as follows

$$\underline{\underline{B}}\,\underline{d} = \left[\begin{array}{c|c} & \\ \underline{\underline{C}} & \underline{\underline{D}} \\ & \end{array}\right]\left[\begin{array}{c} \underline{g} \\ \hline \hat{\underline{d}} \end{array}\right] = \underline{\underline{C}}\,\underline{g} + \underline{\underline{D}}\,\hat{\underline{d}} \qquad (2.2)$$

where $\underline{\underline{C}}$ is the nxp input matrix for manipulated variables, and $\underline{\underline{D}}$ is the nxq input matrix for disturbance variables.

The process is represented schematically by the portion of Fig. 2.1 marked "Process." As shown in the figure, measurements $\underline{\xi}$ of the state variables are made according to the rxn matrix $\underline{\underline{H}}$ so that

$$\underline{\xi} = \underline{\underline{H}}\,\underline{z} \qquad (2.3)$$

For the present the controller shown in Fig. 2.1 may be ignored.

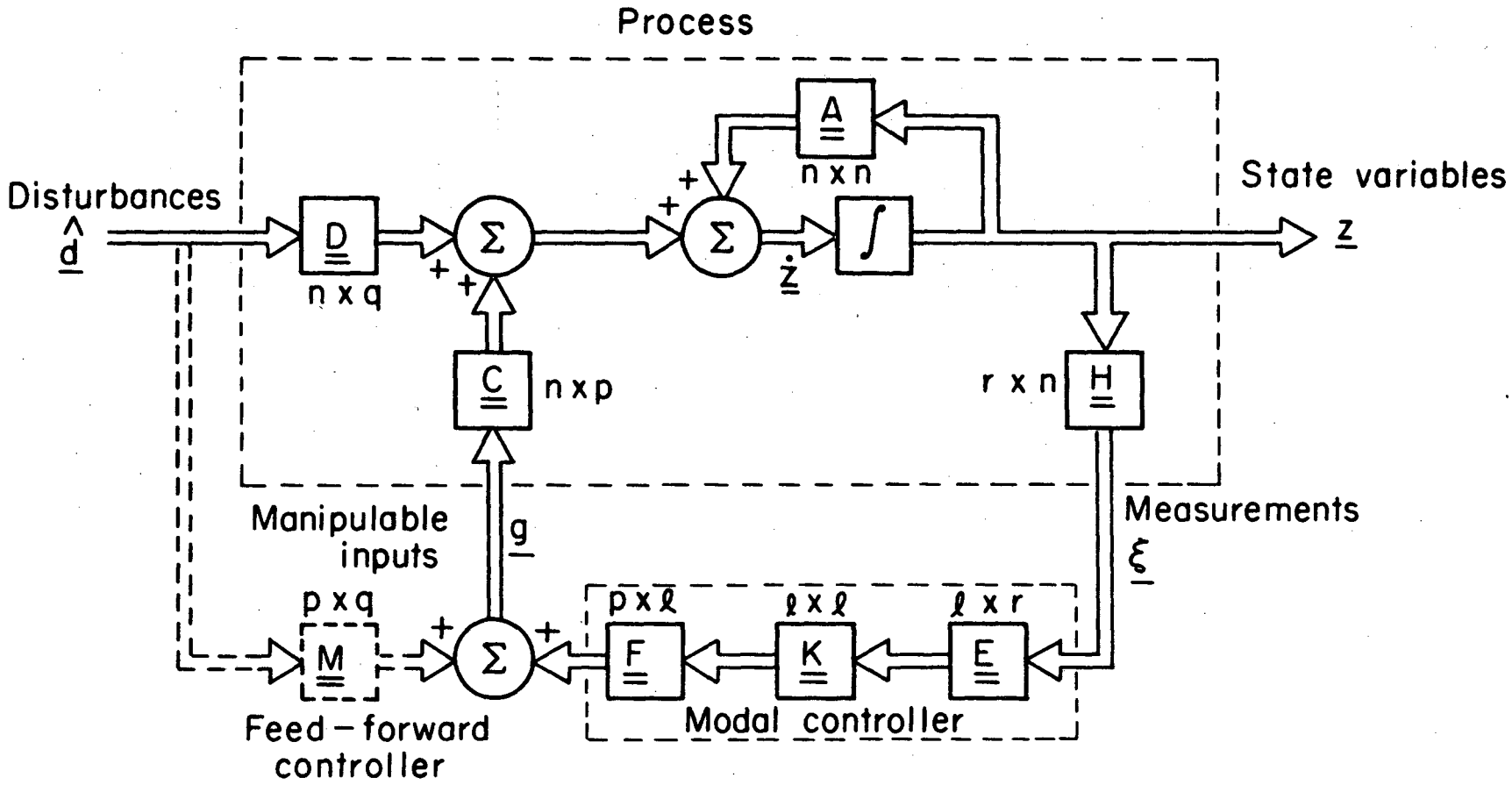

Fig. 2.1 Signal flow diagram.

B. Modes of a Linear System

The modes of a dynamic system are directions in the state space that correspond to the right eigenvectors, $\underline{u}^{(i)}$, of the state matrix $\underline{\underline{A}}$. These eigenvectors are defined by

$$\underline{\underline{A}}\ \underline{u}^{(i)} = \lambda_i\ \underline{u}^{(i)} \tag{2.4}$$

where λ_i is an eigenvalue of $\underline{\underline{A}}$ corresponding to $\underline{u}^{(i)}$. Each eigenvalue satisfies the relationship

$$\det\ (\underline{\underline{A}} - \lambda_i\ \underline{\underline{I}}) = 0 \tag{2.5}$$

The mode representation is applicable whenever there are n linearly independent eigenvectors, which then span the variable space and form a basis for the state variables. The state vector may be represented in state space as a superposition of independent, or noninteracting, contributions from each of the modes. For a stable autonomous process, the contribution of each mode is a pure exponential decay along the direction determined by the right eigenvector, with a time constant determined by the real part of the corresponding eigenvalue.

In general the modes may be complex, although complex modes occur only as conjugate pairs, because the matrix $\underline{\underline{A}}$ is real. The time constant, τ, associated with a mode is the negative reciprocal of the real part of the eigenvalue

$$\tau = -\frac{1}{\lambda_i'} \tag{2.6}$$

where a complex eigenvalue is represented

$$\lambda_i = \lambda_i' + j\ \lambda_i'', \quad j = \sqrt{-1} \tag{2.7}$$

For a stable process the real parts of all eigenvalues are negative.

The magnitude of the contribution to the state vector made by each mode is called the activation and depends upon the initial condition $\underline{z}(0)$ and the input vector $\underline{d}(\theta)$. For the initial condition $\underline{z}(0)$, the activation $\hat{w}_i$ is given by[14]

$$\hat{w}_i = \underline{v}^{(i)^T} \underline{z}(0) \tag{2.8}$$

and for the input $\underline{d}(\theta)$, the activation w_i is given by[14]

$$w_i = \underline{v}^{(i)^T} \underline{\underline{B}}\, \underline{d}(\theta) \tag{2.9}$$

The vector $\underline{v}^{(i)^T}$ used to determine the activation is a left eigenvector of the matrix $\underline{\underline{A}}$ and is defined by

$$\underline{v}^{(i)^T} \underline{\underline{A}} = \underline{v}^{(i)^T} \lambda_i \tag{2.10}$$

The left and right eigenvectors form a biorthogonal set, which has the property

$$\underline{v}^{(j)^T} \underline{u}^{(i)} \begin{cases} = 0, & i \neq j \\ \neq 0, & i = j \end{cases} \tag{2.11}$$

Thus the j'th left eigenvector is orthogonal to every right eigenvector except the j'th. As a result, when the state vector is aligned along $\underline{u}^{(j)}$, the scalar product of all left eigenvectors except the j'th with $\underline{z}$ is zero, which shows that only mode j is activated. If all the modes are real, the process response may be written as

$$\underline{z}(\theta) = \sum_{i=1}^{n} \hat{w}_i \, \underline{u}^{(i)} \, e^{\lambda_i \theta} + \int_{\theta_o}^{\theta} \sum_{i=1}^{n} w_i(t) \, \underline{u}^{(i)} \, e^{\lambda_i (\theta - t)} \, dt \quad (2.12)$$

where the first term is the response due to the nonzero initial condition, and the second is that caused by the input vector $\underline{d}(t)$. The second term can be simplified if only step changes in inputs to the process are considered. Then

$$\underline{d}(\theta) = \begin{cases} \underline{0}, & \theta < \theta_o \\ \underline{d} = \text{constant}, & \theta \geq \theta_o \end{cases} \quad (2.13)$$

and Eq. (2.12) becomes

$$\underline{z}(\theta) = \sum_{i=1}^{n} \hat{w}_i \, \underline{u}^{(i)} \, e^{\lambda_i \theta} + \sum_{i=1}^{n} - \frac{w_i}{\lambda_i} \, \underline{u}^{(i)} \left(1 - e^{\lambda_i (\theta - \theta_o)} \right) \quad (2.14)$$

If some of the modes are complex the response has a form similar to Eq. (2.14) but somewhat more complicated. It is demonstrated in Appendix A.1 that a complex conjugate pair contribute to the response as if they were real modes equal to the sum and difference of the complex ones. They also contribute sinusoidal oscillation at a frequency governed by the imaginary part of the eigenvalue. Desoer[14] gives a discussion of the mode representation of process dynamics. Additional eigensystem relationships may be found in Wilkinson[64] or Faddeeva.[17]

As has been indicated, the mode representation is not applicable when the set of eigenvectors does not span the space. This results when there are identical eigenvalues and the matrix, in Wilkinson's terminology,[64] has a nonlinear elementary divisor, or is deficient. Such a matrix can

arise, for instance, from the model of a cascade of identical stages in which the flow is in one direction only so that a stage is not influenced by any of those beyond it. The equations then are of the form (stages are numbered from the downstream end)

$$\dot{z}_i = a\, z_{i+1} - a\, z_i \tag{2.15}$$

giving a state matrix

$$\underline{\underline{A}} = \begin{bmatrix} -a & a & & & \\ & -a & a & & \\ & & \ddots & \ddots & \\ & & & \ddots & a \\ & & & & -a \end{bmatrix} \tag{2.16}$$

The eigenvalues are all -a (with multiplicity n) and the response of state variable z_n takes the form

$$z_n = \left[\alpha_1 + \alpha_2\theta + \alpha_3\theta^2 + \ldots + \alpha_n\theta^{n-1}\right] e^{-a\theta} \tag{2.17}$$

Equation (2.17) shows that there is only one exponential and the coefficients are time dependent. As the limiting case of identical stages is approached, the modal representation begins to fail, as shown in Appendix A.2. For such a case, the response is determined by modes with almost identical time constants and directions, and they are very highly activated in such a way that they nearly cancel each other when summed. In what follows, the existence of modes will be assumed.

C. Eigenvalue Sensitivities

Sensitivity analysis of a simulated process can mean sensitivity of the state vector or trajectory to changes in parameter values,[11,60]

or sensitivity of the eigenvalues to changes in values of parameters.[39,40,49,54,61] The latter calculation can be made for any parameter affecting $\underline{\underline{A}}$, using right and left eigenvectors,[61] as shown in Appendix A.4. A relative sensitivity S of eigenvalue λ_i to a parameter α is given by

$$S = \frac{\alpha}{\lambda_i} \frac{\partial \lambda_i}{\partial \alpha} = \frac{\alpha}{\lambda_i} \left[\frac{\partial \underline{\underline{A}}}{\partial \alpha} \underline{u}^{(i)} \right]^T \underline{v}^{(i)} \qquad (2.18)$$

where it is assumed that the right and left eigenvectors are normalized such that

$$\underline{u}^{(i)^T} \underline{v}^{(j)} = \delta_{ij} \text{ (Kronecker delta)} \qquad (2.19)$$

Sensitivities may be used to aid in the identification of the physical basis for a mode. Also, the dominant modes are particularly sensitive to the values of only certain parameters, and therefore it is these parameters, identified through the sensitivities, that must be known accurately, while the values of others used in the mathematical model are less important.

D. Modal Control

The object of modal control is to speed the response of the slowest modes so that the process recovers from disturbances more quickly. The principles of the method have been presented by Rosenbrock[53] and others,[12,13,16,21,22,57] but they are re-examined here from a slightly different viewpoint.

An ideal modal controller can always be designed if it is assumed that every state variable is both measurable and manipulable. The controller must operate on combinations of the manipulable inputs such

that the state vector is driven in directions in state space that are opposite to the directions of activations of the slowest modes. The modes are thus forced to return to steady state (the origin) more rapidly by the control action. To assure that the slow modes are driven precisely to the origin it is necessary to measure their activations at every instant and to adjust the magnitude of the control actions. When every state variable is measurable, the activations are determined by combinations of these measurements that are made according to the elements of the left eigenvectors of the slow modes as described previously (see Eq. (2.11)).

The mathematical relationships for ideal modal controllers can be developed by reference to the signal flow diagram (Fig. 2.1). For the present the feedforward controller shown in the figure will be ignored. The modal controller uses the measurements, $\underline{\xi}$, and manipulates inputs, $\underline{g}$. There is no vector of set points or desired values indicated because it is assumed that this is merely the null vector. In other words, the desired operating point is the steady state condition. The matrices $\underline{\underline{C}}$ and $\underline{\underline{H}}$ are part of the process and considered to be fixed. However the controller matrices $\underline{\underline{F}}$, $\underline{\underline{K}}$, and $\underline{\underline{E}}$ have elements that may be chosen in any desired way.

The relationships for the process and for the measurements that are shown by the diagram are expressed by Eqs. (2.1-2.3). The modal controller relates the manipulated variables to the measurements by

$$\underline{g} = \underline{\underline{F}}\,\underline{\underline{K}}\,\underline{\underline{E}}\,\underline{\xi}$$

Assume that there are n measurements (r=n) and n manipulable inputs (p=n) such that the process is both controllable and observable.

Columns of the controller matrix $\underline{\underline{F}}$ specify linear combinations of manipulable inputs, while rows of controller matrix $\underline{\underline{E}}$ specify linear combinations of measurements. If the i'th column of $\underline{\underline{F}}$ is $\underline{f}^{(i)}$, the ideal controller for mode i must satisfy

$$\underline{\underline{C}}\,\underline{f}^{(i)} = \underline{u}^{(i)} \tag{2.20}$$

and the n elements of $\underline{f}^{(i)}$ are determined by solutions of these n simultaneous equations. Similarly, if the i'th row of $\underline{\underline{E}}$ is $\underline{e}^{(i)T}$, the ideal controller for mode i must also satisfy

$$\underline{e}^{(i)T}\,\underline{\underline{H}} = \underline{v}^{(i)T} \tag{2.21}$$

and the n elements of $\underline{e}^{(i)T}$ are determined by these n equations.

If all n modes are controlled then the relationships for the controller matrices are

$$\underline{\underline{E}}\,\underline{\underline{H}} = \underline{\underline{V}}^{T} \tag{2.22}$$

and

$$\underline{\underline{C}}\,\underline{\underline{F}} = \underline{\underline{U}} \tag{2.23}$$

where $\underline{\underline{V}}^{T}$ has rows that are the left eigenvectors

$$\underline{\underline{V}}^{T} = \begin{bmatrix} \underline{v}^{(1)T} \\ \vdots \\ \underline{v}^{(i)T} \\ \vdots \\ \underline{v}^{(n)T} \end{bmatrix} \tag{2.24}$$

and $\underline{\underline{U}}$ has columns that are the right eigenvectors

$$\underline{\underline{U}} = \left[\underline{u}^{(1)} \; . \; . \; . \; \underline{u}^{(i)} \; . \; . \; . \; \underline{u}^{(n)} \right] \tag{2.25}$$

The differential equations describing the process plus modal controller are

$$\dot{\underline{z}} = (\underline{\underline{A}} + \underline{\underline{C}}\,\underline{\underline{F}}\,\underline{\underline{K}}\,\underline{\underline{E}}\,\underline{\underline{H}})\underline{z} + \underline{\underline{D}}\,\hat{\underline{d}} \tag{2.26}$$

The modes of the controlled process are no longer derived from $\underline{\underline{A}}$, but rather from the matrix $(\underline{\underline{A}} + \underline{\underline{C}}\,\underline{\underline{F}}\,\underline{\underline{K}}\,\underline{\underline{E}}\,\underline{\underline{H}})$. When the ideal modal controllers for all n modes are applied

$$\dot{\underline{z}} = (\underline{\underline{A}} + \underline{\underline{U}}\,\underline{\underline{K}}\,\underline{\underline{V}}^{T})\underline{z} + \underline{\underline{D}}\,\hat{\underline{d}} \tag{2.27}$$

The state matrix $\underline{\underline{A}}$ can be expressed in terms of $\underline{\underline{U}}$ and $\underline{\underline{V}}^{T}$ by

$$\underline{\underline{A}} = \underline{\underline{U}}\,\underline{\underline{\Lambda}}\,\underline{\underline{V}}^{T} \tag{2.28}$$

where $\underline{\underline{\Lambda}}$ is the diagonal matrix of eigenvalues

$$\underline{\underline{\Lambda}} = \begin{bmatrix} \lambda_1 & & & \\ & \ddots & & \\ & & \lambda_i & \\ & & & \ddots \\ & & & & \lambda_n \end{bmatrix} \tag{2.29}$$

Thus Eq. (2.27) becomes

$$\dot{\underline{z}} = \underline{\underline{U}}(\underline{\underline{\Lambda}} + \underline{\underline{K}})\underline{\underline{V}}^{T} + \underline{\underline{D}}\,\hat{\underline{d}} \tag{2.30}$$

The controller matrix $\underline{\underline{K}}$ is chosen to be a diagonal matrix of negative proportionality factors, k_i; one for each mode being controlled. In the previous discussion it was assumed that all n modes are controlled so that

$$\underline{\underline{K}} = \begin{bmatrix} -k_1 & & & & \\ & \ddots & & & \\ & & -k_i & & \\ & & & \ddots & \\ & & & & -k_n \end{bmatrix} \tag{2.31}$$

A proportional linkage between activation and manipulation is chosen so that control action is zero when the activation is zero.

The consequence of the relationship expressed by Eq. (2.30) is that the eigenvalues of the controlled process are no longer λ_i, but rather are $\lambda_i - k_i$. Normally only ℓ modes ($\ell < n$) are controlled, in which case the eigenvalues are $(\lambda_1 - k_1)$, $(\lambda_2 - k_2)$, ..., $(\lambda_\ell - k_\ell)$, $\lambda_{\ell+1}$, ..., λ_n. By appropriate choice of the k_i each of the time constants associated with the ℓ controlled modes can be made as small as desired. Moreover, for inputs that drive the process away from steady state, the modal controller decreases the magnitude of the contributions of the ℓ controlled modes. This can be seen by the response expression for a step change of inputs at time zero

$$\underline{z}(\theta) = \sum_{i=1}^{\ell} - \frac{w_i}{\lambda_i - k_i} \underline{u}^{(i)} \left(1 - e^{(\lambda_i - k_i)\theta} \right)$$

$$+ \sum_{i=\ell+1}^{n} - \frac{w_i}{\lambda_i} \underline{u}^{(i)} \left(1 - e^{\lambda_i \theta} \right) \tag{2.32}$$

The factors $\left(\frac{1}{\lambda_i - k_i} \right)$ in the first summation reduce the activation considerably when k_i is large. The controllers are noninteracting

in the sense that each operates only on one mode. Furthermore, the choice of combinations of measured and manipulated variables and their interconnection has been specified by Eqs. (2.20) and (2.21).

When only ℓ modes ($\ell < n$) are to be controlled then ℓ columns of $\underline{\underline{F}}$ are chosen so that the first ℓ columns of $\underline{\underline{C}}\,\underline{\underline{F}}$ are the ℓ right eigenvectors, and ℓ rows of $\underline{\underline{E}}$ are chosen so that the first ℓ rows of $\underline{\underline{E}}\,\underline{\underline{H}}$ are the left eigenvectors.

The design of controllers for real processes typically must be based on only a few measurements ($r << n$) and only a few manipulable inputs ($p << n$). When there are fewer than n measured or manipulated variables it is impossible, in general, to satisfy Eqs. (2.20) and (2.21) exactly because there are n equations in only p unknowns or r unknowns. As a result there is no assurance that the activation of a single mode can be detected or that the state vector can be driven opposite to the direction of activation of that mode. In terms of the ideas developed by Kalman[31] and Gilbert,[20] the process may not be completely controllable or completely observable. Rosenbrock[53] shows that an approximate modal controller results in alteration of modes other than the one being controlled. However, if the controller succeeds in reducing the time constants of the slow modes and interaction does not create any new slow modes, then the control scheme may be worthwhile. Rosenbrock's discussion[53] of systematic procedures for the design of approximate controllers is inadequate and the problems are re-examined here.

The manipulation problem can be viewed in another way by consideration of the mapping of the input vector $\underline{g}$ by matrix $\underline{\underline{C}}$ into the n-dimensional state space. The possible directions attainable in the space are con-

fined to the subspace defined by the p vectors that result from the p individual inputs g_1, g_2, ..., g_p, each mapped into the n-space. In other words, the possible directions in which the state vector may be driven are determined by combinations of

$$\underline{\underline{C}} \begin{bmatrix} g_1 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \quad \underline{\underline{C}} \begin{bmatrix} 0 \\ g_2 \\ 0 \\ \cdot \\ \cdot \\ 0 \end{bmatrix}, \ldots, \underline{\underline{C}} \begin{bmatrix} 0 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 0 \\ g_p \end{bmatrix} .$$

Some or all of the modes may not have major components that lie in the subspace defined by these p vectors, and, consequently, the state vector cannot be driven in a direction that is even approximately parallel to such modes; there is no way to oppose their activation. If any modes are actually orthogonal to all p of the $\underline{\underline{C}}\,\underline{g}$ basis vectors, these modes are said to be uncontrollable.

The detection of the activation of a single mode is readily accomplished in the full state space by the corresponding left eigenvector, because of the biorthogonality relationship, Eq. (2.11). However, when only r measurements are made, all n of the n-dimensional modes must be viewed from their mappings by the matrix $\underline{\underline{H}}$ into the r-dimensional measurement space. Likewise, all that can be known of the position of the state vector must be judged from the measurement vector, $\underline{\xi}$, which is its mapping into the r-space. Thus, it is impossible to detect the activations of the modes by measurements in this reduced space except in the special case when one or more of the modes lies in this space. Such measurements could, at best, detect the activation of the mappings

of the modes in r-space. This is equivalent to the decomposition of the mapping $\underline{\xi}$ of the state vector into the mapping $\underline{\underline{H}}\,\underline{u}^{(i)}$ of each mode.

Unfortunately, the activation of a mode in the state space cannot, in general, be estimated by the activation of the mapping of the mode in the reduced space. The activation of the mapping is significant only if the components of the mode that are orthogonal to the measurement space are small in magnitude compared to the mode itself. If any mode is orthogonal to the measurement space it maps as a null vector, and is completely unobservable. Therefore, the measurement space must be chosen, if possible, so that the criterion of small orthogonal components is satisfied for the mode whose activation is to be detected.

Even if the activation of the mapping of a mode is a useful measure of the activation of the mode itself, there is usually no way to detect it unambiguously. The rows of $\underline{\underline{E}}$, $\underline{e}^{(i)^T}$, (which are linear combinations of measurements) serve to detect the activations of the mappings of the modes in r-space. This can be accomplished only if $\underline{e}^{(i)^T}$ is orthogonal to each of the vectors $\underline{\underline{H}}\,\underline{u}^{(j)}$ except the i'th (that is, $\underline{e}^{(i)^T}\,\underline{\underline{H}}\,\underline{u}^{(j)} = \delta_{ij}$). However, it is possible to make $\underline{e}^{(i)^T}$ orthogonal to the mappings of only $(r - 1)$ of the n modes. Thus $\underline{\xi}$ cannot be resolved unambiguously into the mappings of the modes, and none of their activations can be determined uniquely. If other vectors $\underline{\underline{H}}\,\underline{u}^{(j)}$ are nearly coincident with $\underline{\underline{H}}\,\underline{u}^{(i)}$ then no choice of $\underline{e}^{(i)^T}$ can determine even an approximate activation for the i'th mode. The selection of a "best" direction for $\underline{e}^{(i)^T}$ depends on the directions of the vectors $\underline{\underline{H}}\,\underline{u}^{(j)}$ and of $\underline{\underline{H}}\,\underline{u}^{(i)}$, but it may not be desirable to consider them with equal weight. Factors that should influence the choice of $\underline{e}^{(i)^T}$ are the time constants associated

with each mode and, if known by prior calculations, the activations caused by typical inputs.

It is clear that the problem of detection of activations becomes quite complex when the measurement space is restricted to a few dimensions. There are many subtleties involved in the selection of appropriate $\underline{e}^{(i)^T}$. Likewise, the best choice of manipulable inputs is not easily determined. However, it is not within the scope of this work to develop systematic procedures to cope with these complications. In Chapter VI approximate modal controllers are designed by rather crude and partially intuitive methods in order to demonstrate the usefulness and shortcomings of this type of control scheme.

E. Feedforward Control

Knowledge of the modes of a process can be used to design a feedforward controller that tends to eliminate the effect of disturbances, but this scheme can be applied only when disturbances are measurable before they enter the process. If the disturbances $\hat{\underline{d}}$ are known, then the activation of the slow modes can be calculated and the manipulated inputs can be changed so as to exactly cancel these activations for some of the modes. The objectives of this feedforward controller are not the usual ones, namely to hold one or more output variables constant.[4,5,7] Instead only selected modes are eliminated by the controller.

The feedforward controller is indicated by (pxq) matrix $\underline{\underline{M}}$ in the signal flow diagram (Fig. 2.1). The process with feedforward controller and modal controller is described by

$$\dot{\underline{z}} = (\underline{\underline{A}} + \underline{\underline{C}}\,\underline{\underline{F}}\,\underline{\underline{K}}\,\underline{\underline{E}}\,\underline{\underline{H}})\underline{z} + (\underline{\underline{D}} + \underline{\underline{C}}\,\underline{\underline{M}})\hat{\underline{d}} \qquad (2.33)$$

The objective is to pick p-dimensional columns (q columns) of $\underline{\underline{M}}$ ($\underline{m}^{(i)}$) so that $\underline{\underline{C}}\ \underline{m}^{(i)}\ \hat{d}^{(i)}$ generates activations that exactly cancel those caused by the i'th disturbance acting through $\underline{\underline{D}}$ alone.

A unit change in the j'th manipulable input results in a set of activations for the modes represented by vector $\underline{w}_g^{(j)}$, and there are p of these vectors that may be grouped in an (nxp) matrix $\underline{\underline{W}}$

$$\underline{\underline{W}} = \left[\underline{w}_g^{(1)} \cdots \underline{w}_g^{(p)} \right] \tag{2.34}$$

Also a unit change in the i'th disturbance input causes a vector of activations $\underline{w}_{\hat{d}}^{(i)}$. Thus it is desired that the i'th column of $\underline{\underline{M}}$ satisfy

$$\underline{\underline{W}}\ \underline{m}^{(i)} + \underline{w}_{\hat{d}}^{(i)} = \underline{0} \tag{2.35}$$

In order for Eq. (2.35) to be meaningful, $\underline{w}_{\hat{d}}^{(i)}$ must be restricted to p elements. As a consequence it is possible to cancel the activations of only p modes. The modes chosen would normally be the slowest ones, but could include some faster ones that tend to be highly activated. There is the possible difficulty that the feedforward controller will activate some of the uncontrolled modes strongly while cancelling activations of others. Consequently there is no assurance that this type of controller will always be effective.

III. COMPUTATIONAL ASPECTS OF MODAL ANALYSIS

When the number of state variables is large, the computation required for a complete analysis of process modes and response is formidable. Considerable effort has been devoted to the search for and evaluation of the numerical procedures discussed in this chapter. The accuracy and time requirements of the computer programs that perform the calculations are also discussed.

A. Computational Methods

The analysis of the modes of a process may be subdivided into procedures for the calculation of:

1. steady state conditions
2. state matrix coefficients
3. eigenvalues
4. right and left eigenvectors
5. sensitivities of eigenvalues to values of parameters
6. process responses to step changes of inputs

Although all of the computations tend to be lengthy, only the procedures for eigenvalues and eigenvectors present severe numerical difficulties.

There are a multitude of algorithms for calculating eigenvalues of large, unsymmetric matrices, but the so-called QR algorithm[18,30,43,44,64] appears unquestionably to be the best. The method is applied after the original matrix is transformed to Hessenberg form, which is upper triangular except for one subdiagonal. This QR method operates on the Hessenberg form with orthogonal transformations. When the eigenvalues are real the subdiagonal elements become zero, but for every complex conjugate pair a 2×2 submatrix centered on the main diagonal is the result. The real eigenvalues are the main diagonal elements and the complex eigenvalues

are eigenvalues of the 2×2 submatrices.

For equivalent accuracy the QR procedure is at least an order of magnitude more rapid than any other scheme investigated. Eigenvalue calculations based on the generation of a characteristic polynomial with subsequent root-seeking can yield accurate results. However, the susceptibility of these methods to accumulation of errors requires the use of special devices (such as reorthogonalization and high precision arithmetic) in order to make them accurate. As a consequence they are normally much slower than the QR procedure.

Eigenvectors of unsymmetric matrices are notoriously difficult to calculate with accuracy. The definition of an eigenvector

$$(\underline{\underline{A}} - \lambda_i \underline{\underline{I}})\, \underline{u}^{(i)} = \underline{0} \tag{3.1}$$

gives n equations, of which n-1 are independent. If one element of the vector is chosen arbitrarily and the rest are found by triangularization of the matrix of Eqs. (3.1) and recursive back substitution, rounding errors often cause inaccurate eigenvectors to result. However, if the matrix is sufficiently well conditioned an efficient procedure based on simple back substitution has been suggested by J. E. Van Ness and co-workers.[62] Their scheme finds both right and left eigenvectors in the same computation.

A method that has been satisfactory for finding the eigenvectors of any matrix encountered in this work is the inverse iteration procedure described by Wilkinson[64,65] and outlined in Appendix C. While this algorithm has been employed for the calculations to be presented, it is slow and somewhat unwieldy. There is a faster and more efficient eigenvector scheme based on the QR procedure that has been developed only

recently.[44] If all of the QR transformations are recorded, the eigenvectors of the triangular matrix, which are easily calculated, may be transformed back to the original vector space. This method is rapid and accurate, and it is to be highly recommended for the calculations in work of this nature. Preliminary calculations suggest that it is more than five times faster than the inverse iteration procedure.

The rest of the computational procedures are relatively straightforward. The steady state conditions and the state matrix coefficients depend on the process and the mathematical model used. Calculations in this work are based on distillation column models that are discussed in Chapter IV. The distillation steady state computation, which solves the nonlinear component, mass, and heat balances, is basically due to Hanson, et al.[24] with an improved temperature correction scheme by Newman.[42]

Responses to step changes of inputs are calculated by summation of the contributions of each mode at selected times. Real modes are calculated with Eq. (2.14) and complex modes with Eq. (A.1.9)(Appendix A).

In many cases it is sufficient to calculate only the eigenvectors of those few slowest modes that are important in determining process response. However, the contribution of the rapidly decaying modes to the final steady state may be significant. This contribution can be determined for step inputs without calculating the eigenvectors by use of a second steady state calculation with the input variables at their final values. The contribution of the slow modes to the final steady state levels of the state variables can be calculated and subtracted from the total change in level. This difference is then treated as a bias. It is a step response due to all of the fast modes that have not been evaluated. In

this work the procedure just described has not been used because all modes that make a significant contribution are included in the calculations.

Eigenvalue sensitivities are determined according to Eq. (2.18). The derivative of the state matrix with respect to a parameter is the same as a matrix of derivatives. For most of the parameters these derivatives can be calculated analytically, but the amount of algebra involved is prohibitive if many parameters are to be considered. Consequently the derivative of the state matrix with respect to a parameter is found numerically by finite difference approximation using a one percent change in the parameter of interest.

Modal control calculations are made by modification of the $\underline{\underline{A}}$ matrix so that it applies to the process plus controller rather than the process alone. The modification normally involves relatively few of the matrix coefficients.

B. Accuracy of the Numerical Procedures

There is an inherent limitation to the accuracy with which an eigenvalue and eigenvector may be calculated that depends on the "condition" of the matrix. Wilkinson[64] has defined a gauge for this accuracy, called a condition number; it is calculated as the reciprocal of the scalar product of the normalized right and left eigenvectors. Thus there is a condition number associated with each eigenvalue. When the matrix is symmetric the eigenvectors form an orthogonal set; the left and right eigenvectors are coincident and all the condition numbers are unity. Therefore symmetric matrices are always well-conditioned, and their eigenvalues and eigenvectors can be calculated to working accuracy. When the right and left eigenvectors corresponding to any eigenvalue

become more nearly orthogonal the condition number is large. This "ill-conditioning" means that it is impossible to calculate a highly accurate eigenvalue or eigenvector when the number of significant figures available with a digital computer is used. One extreme example of ill-conditioning occurs when a matrix has nearly identical eigenvalues. (This case was mentioned in Chapter II and is illustrated in Appendix A.2.) In the limit the right and left eigenvectors are orthogonal and the condition number is infinite.

The condition number is an eigenvalue sensitivity, but is determined by all matrix elements rather than by specific parameters of the matrix. Typically some of the eigenvalues and eigenvectors of a matrix are well-conditioned, while others have rather large condition numbers. The range of condition numbers encountered in this work is approximately 1.0 to 20,000. Eigenvalues having the largest condition numbers have only three or four significant figures that are accurate.

Computed eigenvalues were checked by comparison of their product with the determinant of the matrix, and by comparison of their sum with the trace of the matrix. Usually the former agree to three or four significant figures and the latter to six significant figures.

The accuracy of computed eigenvectors is tested by application of several definitions. First the product $(\underline{\underline{A}} - \lambda_i \underline{\underline{I}})\ \underline{u}^{(i)}$ is tested to determine if the vector elements are sufficiently small. For important eigenvectors these are normally 10^{-3} or less. The set of right and left eigenvectors is checked by formation of the product $\underline{\underline{U}}^T\underline{\underline{V}}$, which should yield the identity matrix. The main diagonal elements are always exactly unity because of the normalizing procedure for the left eigenvectors. However the off-diagonal elements are usually 10^{-3} or less. The product

$\underline{\underline{V}}\underline{\underline{U}}^T$ should also give the identity matrix, but can only be formed if the entire set of n right and left eigenvectors is calculated. In this case the main diagonal elements provide a good indication of the biorthogonality of the vector sets. Normally these elements are unity to three significant figures or more, and the off-diagonal elements again are usually 10^{-3} or less.

C. Computer Programs and Time Requirements

The numerical procedures are coded as a set of FORTRAN IV programs implemented on an I.B.M. 7094 digital computer. Various combinations of the modal analysis calculations may be chosen. Appendix G is devoted to an extensive description of the program structure and usage. Also included in the appendix are individual subprogram descriptions, flow charts, and listings.

In their present form the programs for computing all the modes of a moderately large process require considerable time. Some examples of typical execution times for a complete calculation, including responses to step changes in six inputs, are given below.

Size of State Matrix	No. of Modes	Execution Time
13×13	13	1.4 minutes
19×19	19	3.1
34×34	26	8.2

The calculation times for various portions of the calculation may be broken down as follows. The times quoted here apply to the case of 34 state variables and are approximate.

Steady state calculation and matrix preparation	0.3 min
Eigenvalue calculation (34 eigenvalues)	0.2 min
Eigenvector calculation	0.15 min. per mode
Eigenvalue sensitivity calculation	0.1-0.2 min per parameter for 26 modes
Response calculation for one input (30 modes)	0.3 min.

The rapid increase in computation time with matrix size becomes a serious limitation to the application of modal analysis. A practical limit for the calculation of all modes with the present procedures is at about 35 state variables. However, one of the slowest portions of the program is the calculation of eigenvectors, and this bottleneck can be eliminated by use of the eigenvector calculation based on the QR algorithm and by calculation of only the dominant eigenvectors. Both of these improvements were discussed in the first section of this chapter.

IV. MATHEMATICAL MODELS OF A BINARY DISTILLATION COLUMN

A. Selection of Models

In order to calculate the modes of a stagewise distillation column a mathematical description of its dynamic behavior is needed. A general dynamic distillation model consists of a large set of nonlinear differential equations that arise from the material and enthalpy balances, and from other relationships. For the purposes of modal analysis the generality of such relationships must be restricted considerably, but the assumptions and restrictions will be justified whenever possible.

There is an extensive literature on distillation dynamics and control, in which a great variety of different models have been used, and this background might be expected to serve as a guide in selecting an appropriate formulation. However, success in predicting experimental response data has been indicated[28,29,32] for such diverse models that it seems worthwhile to explore and compare some of them from the point of view of modal analysis. In addition, it seems desirable to investigate a quite detailed model, since such models have been used rarely in actual calculations,[37,44a,48,50] or for comparison with and evaluation of simpler models.

In this work four representative models have been chosen to span the range from simple to complex. These models, which are to be described in more detail in the following sections, are classified by the unsteady balances they include. A formulation including unsteady balances on enthalpy, mass, and chemical species is called Model 1, and is the type of model that has been proposed by Rademaker and

Rijnsdorp,[48] and Peiser and Grover.[44a] Model 2 includes unsteady enthalpy and component balances but assumes mass holdups to be constant. It has been used by Huckaba, Franke, and May.[28,29] Model 3 incorporates unsteady mass and component balances but does not account for accumulation of enthalpy. Such models are presented by Lamb, Pigford and Rippin,[22] Armstrong and Wood,[1] Rosenbrock,[51,53] Harriott,[25] and others. The simplest model has only unsteady balances on chemical species and is referred to as Model 4. It has been used for investigations by Wilde,[63] Pigford,[46] Mah, Michaelson and Sargent,[34] and Ceaglske.[8]

Table 4.1 contains a summary of the four models and their characteristics. In this table the variables are classified as: "state variables", that that are principals in the unsteady balances, "derived variables", those that change with time as a function of the state variables, and "steady variables", those that are independent of time. The table also lists typical inputs that are included in the models, and for which the corresponding model can predict response.

There are requirements for the state space formulation and modal decomposition that are imposed on all of the models, and these restrictions are presented before the details that distinguish the models are examined. It is assumed for convenience that the process is stationary (the model parameters do not change with time). Other general assumptions are that the liquid at every stage, including the reboiler and the accumulator, is thoroughly mixed, the process contains no pure time delays that are significant, the column is adiabatic, and the vapor holdup is negligible compared to liquid holdup.

One of the most severe limitations of the modal representation is the requirement for linearity. While many nonlinear processes can be

Table 4.1 Distillation column models

Model	State variables	Derived variables	Steady variables	Input variables
1	x,H,T	L,V,P,y		$F,T_F,x_F,L_{N+1},T_s,T_{cw}$
2	x,T	L,V,y	H,P	$F,T_F,x_F,L_{N+1},T_s,T_{N+1}$
3	x,H	L,V,y	T,P	F,T_F,x_F,L_{N+1},V_0
4	x	y	L,V,H,T,P	x_F

x composition of the light component in the liquid on a plate

y composition of the light component in the vapor over a plate

H total liquid holdup on a plate

T temperature of the liquid on a plate

L flow rate of liquid from a plate

V flow rate of vapor from a plate

P pressure at a plate

F feed flow rate

T_F feed temperature

x_F feed composition

L_{N+1} reflux flow rate

T_s reboiler steam temperature

T_{cw} condenser coolant temperature

V_0 reboiler boilup rate

adequately approximated by linear differential equations if the deviations from a steady state are sufficiently small, nevertheless some nonlinear effects in distillation can be so strong that very small disturbances produce large changes in the variables. For example, if a distillation column is operated to give a very pure product a pinched region (a section of the column across which there is very little composition change) results, which introduces severe nonlinearity. Moczek, Otto, and Williams have shown that disturbances in one direction tend to increase the extent of the pinch while like disturbances of opposite sign tend to relieve the pinch effect.[38] The column has significantly different responses for these two cases, a result that cannot be predicted by a linear model. Consequently a linear model must not be used when such a pinch is present. However, the pinch at the top or bottom of the column, which is caused by a pure product requirement, must be distinguished from a pinch at the feed plate, which is caused by an improper choice of the feed point. The latter pinch does not create nonlinearities as large as those of the former, because it is usually restricted to one or two plates, and its location is shifted less by small disturbances.

When a simple binary distillation column is operated in such a way that it does not give very pure products, a linear model has been shown to be adequate.[33]

B. A Comprehensive Model

The formulation classified as Model 1 incorporates nearly all significant phenomena that can be included in a tractable set of equations. Most of the features of the model are applicable to any binary, stage-wise distillation column. However, a specific column is modeled here which has a few special characteristics that will be noted during the

development. This column is the one studied experimentally by J. A. Gerster and his coworkers at the University of Delaware.[2,3,33,56] Here, the concepts in the development of this model are discussed, while the mathematical details are given in Appendix B.1. The diagram of a typical bubble-cap plate, Fig. 4.1, may be referred to during the discussion of the relationships for a plate which follows.

The dynamic behavior of a plate is assumed to hinge on three important quantities for which the liquid on the plate provides a capacity: mass, enthalpy, and chemical species. Balances with accumulation terms are written for these. The thermal capacity of the plate and column material, and the mass capacity of the vapor phase are neglected. As a consequence of the latter, vapor flow changes are transmitted instantly to the plate above.

In addition to the unsteady balances, which express conservation of mass, enthalpy, and species at each plate, phenomenological relationships exist among the process variables. The amount of liquid held on a plate determines the rate of flow over the outlet weir and is influenced by the vapor flow rate. The vapor flow between plates depends on the pressure drop through the bubble-cap slots, as expressed by an orifice-type relationship.[44a] The equilibria between compositions in the vapor and the liquid are described by relationships that depend on temperature, pressure, and liquid activity coefficients. The latter are determined by a Van Laar correlation.

On a real plate the liquid develops a horizontal concentration gradient during flow from inlet weir to outlet weir, and the rate of mass transfer at each point is proportional to the local driving force and a mass transfer coefficient. The description used here does not account for the finite rate of mass transfer. Instead, the model,

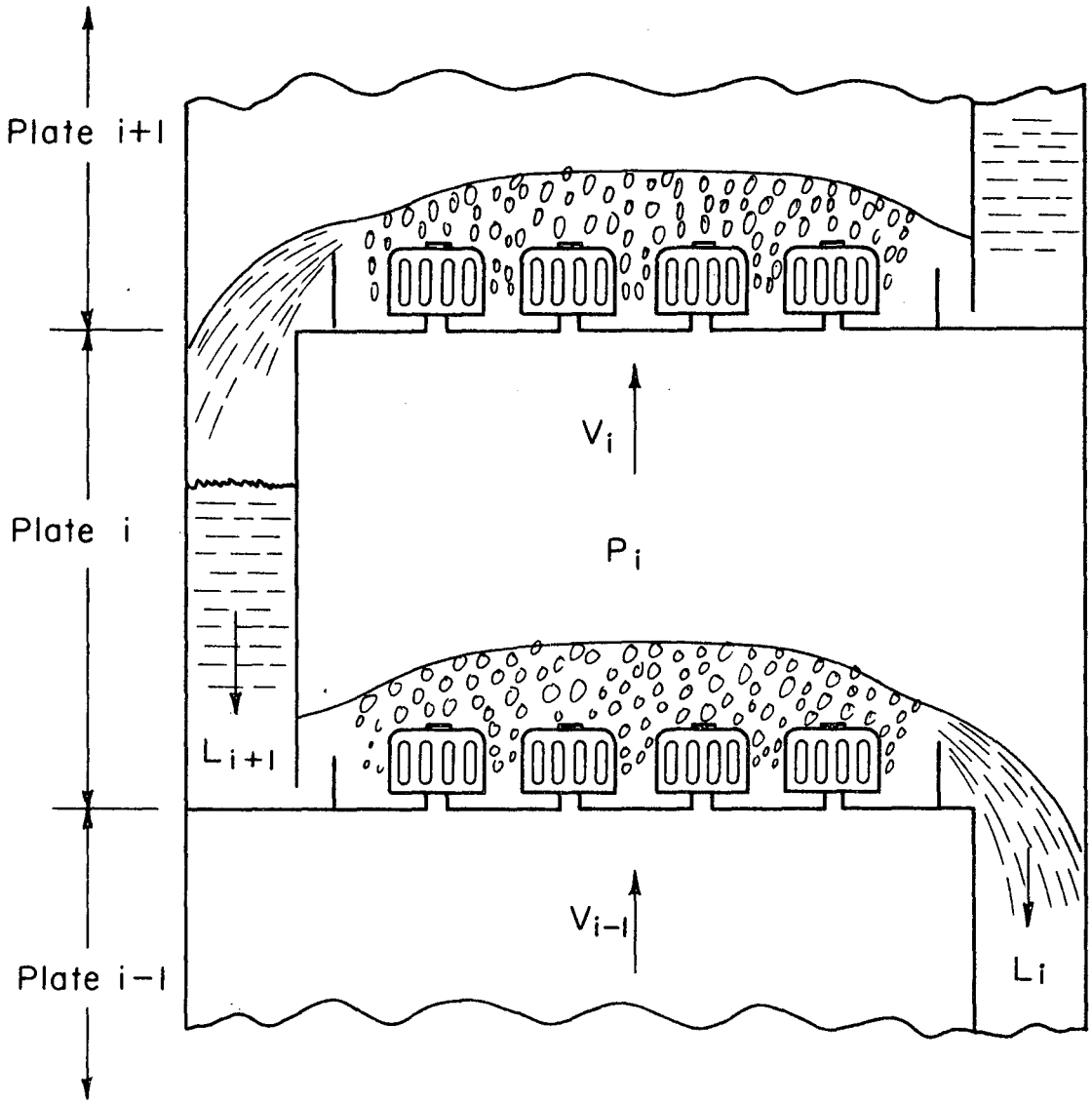

Fig. 4.1 A bubble-cap plate

which assumes complete mixing of the liquid and instantaneous transfer of mass between liquid and vapor, matches the performance of the real plate by applying an overall Murphree plate efficiency. A Murphree efficiency based on liquid phase (rather than vapor phase) compositions is used for convenience in developing the model.

The three differential equations for each plate determine the dynamic behavior of that plate. The number of variables that define the state of the process at any time (state variables) must be exactly the same as the number of differential equations, and therefore, from the total of seven variables (L, V, P, T, x, y, H) associated with each plate, any three may be chosen as the state variables. Then the remaining four are related to the state variables by linear algebraic relationships. In this work the holdup, liquid composition, and temperature are chosen to be the state variables.

The state variables on plate i normally depend on liquid compositions and temperatures on the adjacent plates above and below, (i + 1) and (i - 1), because of the structure of the countercurrent, stagewise process. However, when the liquid phase Murphree efficiency, E_i, is employed and is not equal to unity, the variables on plate i depend in addition on the variables on plate (i + 2). This occurs because the vapor flow rate from plate i depends on pressure at plate (i + 1), which is determined by the vapor-liquid equilibrium relations for that plate. The definition of the Murphree efficiency is substituted into the equilibrium expression to eliminate the equilibrium liquid composition as follows

$$x^*_{i+1} = \frac{x_{i+1}}{E_{i+1}} + x_{i+2}\left(1 - \frac{1}{E_{i+1}}\right)$$

Thus dependence on plate i + 2 is introduced when $E_{i+1} \neq 1$. Hydraulic disturbances are only transmitted down the column, and, therefore, the state variables on a plate do not depend on the holdup of the plate above.

A complete mathematical formulation of distillation column dynamics requires a description of the reboiling and condensing portions of the process (see Fig. 4.2). These accessories to the distillation column seldom have been modeled with sufficient care, and sometimes have been ignored altogether.[8,46] The liquid holdup in the reboiler and accumulator, which is usually at least an order of magnitude larger than the holdup of a single plate, can be expected to account for significant lags. The unsteady enthalpy and component balances for the liquid held in the accumulator and in the reboiler (which is treated as a kettle type) result in two state variables for each, composition and temperature. The mass of liquid in these units is assumed to be held constant by an ideal level control device as indicated in Fig. 4.2, and therefore these holdups are not state variables. As a consequence of these constant holdups, flow rate disturbances in the vapor overhead and the bottom plate liquid are transmitted directly to the overhead product stream and bottom product stream respectively. Such flow disturbances are not transmitted back into the column. Finally, the large mass of metal in the condenser and reboiler might be expected to contribute significant lags to the thermal response of these units, but the simple calculations given in Appendix B.5 show that this is not the case.

The experimental column is somewhat atypical in that it produces reflux that is appreciably subcooled. A model for this situation is constructed by postulation of a total condenser that produces saturated

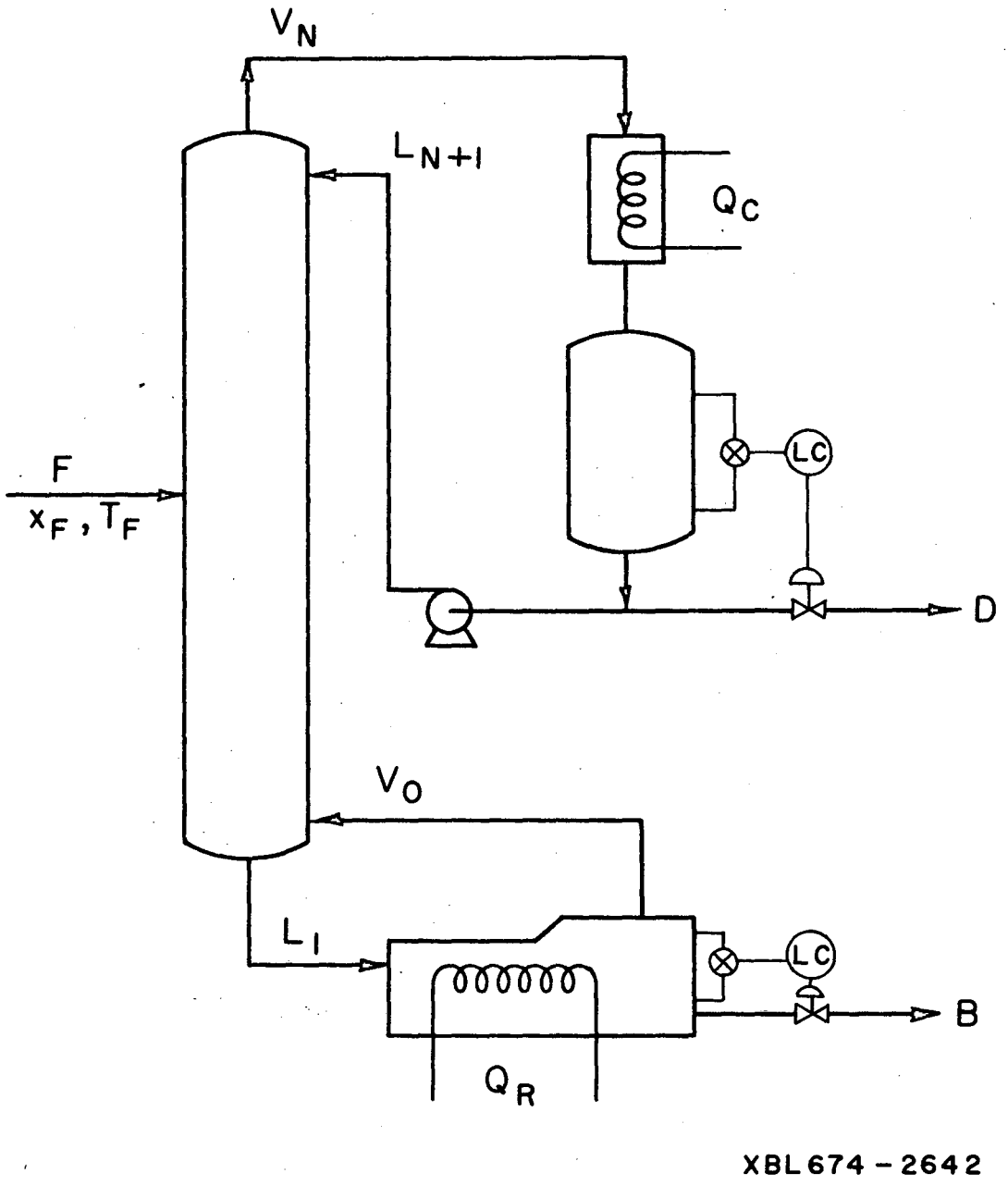

Fig. 4.2 Schematic diagram of the distillation column

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A complete mathematical formulation of distillation column dynamics requires a description of the reboiling and condensing portions of the process (see Fig. 4.2). These accessories to the distillation column seldom have been modeled with sufficient care, and sometimes have been ignored altogether.[8,46] The liquid holdup in the reboiler and accumulator, which is usually at least an order of magnitude larger than the holdup of a single plate, can be expected to account for significant lags. The unsteady enthalpy and component balances for the liquid held in the accumulator and in the reboiler (which is treated as a kettle type) result in two state variables for each, composition and temperature. The mass of liquid in these units is assumed to be held constant by an ideal level control device as indicated in Fig. 4.2, and therefore these holdups are not state variables. As a consequence of these constant holdups, flow rate disturbances in the vapor overhead and the bottom plate liquid are transmitted directly to the overhead product stream and bottom product stream respectively. Such flow disturbances are not transmitted back into the column. Finally, the large mass of metal in the condenser and reboiler might be expected to contribute significant lags to the thermal response of these units, but the simple calculations given in Appendix B.5 show that this is not the case.

The experimental column is somewhat atypical in that it produces reflux that is appreciably subcooled. A model for this situation is constructed by postulation of a total condenser that produces saturated

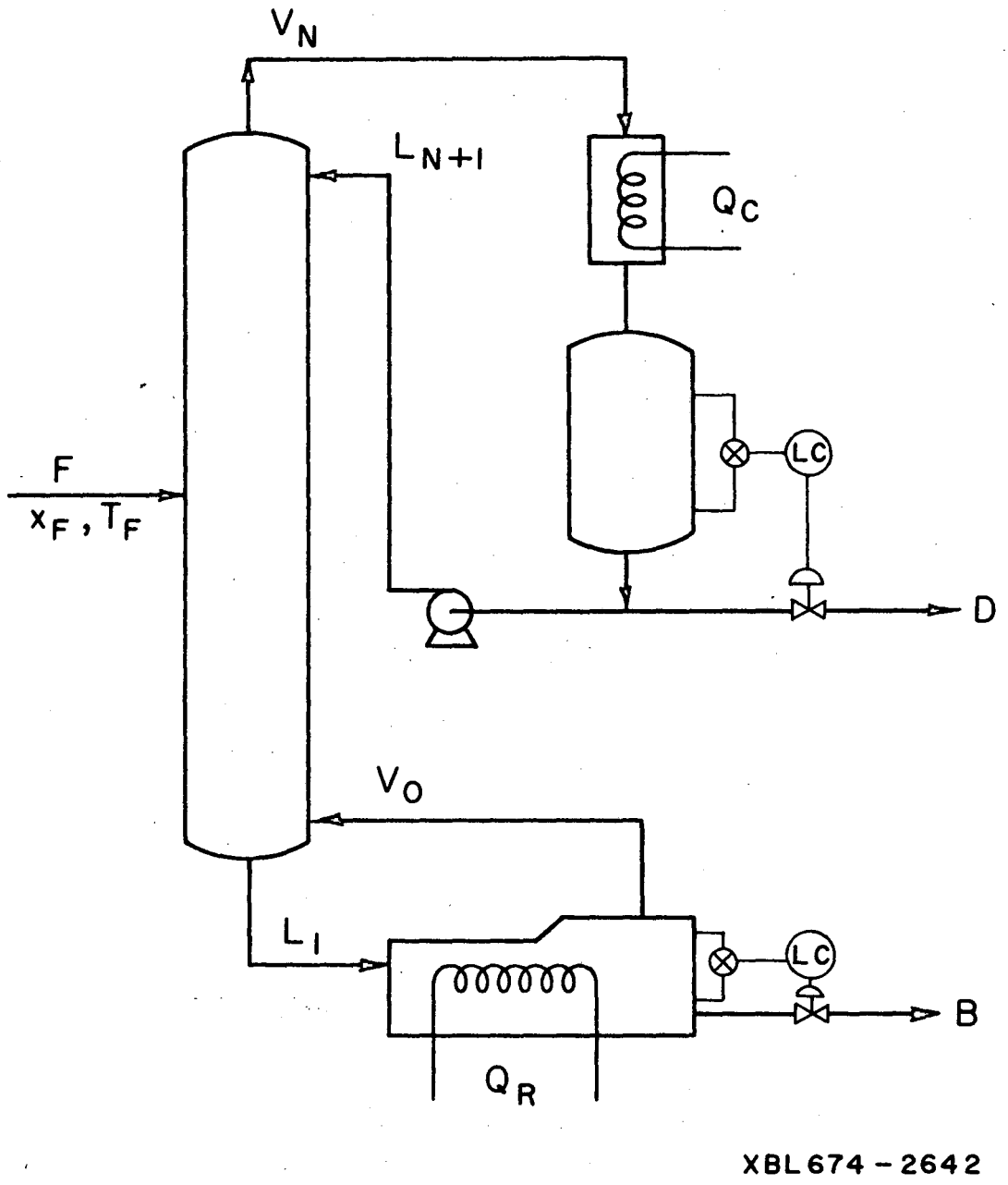

Fig. 4.2 Schematic diagram of the distillation column

liquid followed by a cooler that yields subcooled reflux and distillate. Both the condenser and the cooler are exposed to coolant that is at the same average temperature. Heat transfer to the condenser and cooler is governed by heat transfer coefficients that are calculated at steady state conditions, with the average coolant temperature, T_{CW}, determined by a specified average driving force. In modeling most industrial scale condensers there is no need for a cooler because they operate with negligible subcooling (unless there are inerts present or they have partially submerged tubes).[47]

This detailed model permits calculation of responses due to changes in nearly all common distillation input variables: feed flow rate, feed temperature, feed composition, reflux flow rate, reboiler steam temperature, and condenser coolant temperature. Many distillation models have used reboiler boilup rate as an input variable, but here the reboiler dynamics determine boilup rate as a function of steam temperature. Only a single, liquid phase feed stream is permitted, although it may be subcooled. Vapor or partially vaporized feeds are not allowed in the present form of the model. For the sake of simplicity, the average temperature of the condenser coolant, rather than its flow rate, is used as the input variable. The input variables that are classified as disturbances are feed flow rate, feed composition, and possibly feed temperature. The manipulated inputs are reflux flow rate, reboiler steam temperature and coolant temperature.

In conversion of the model to state space form the variables are reduced to dimensionless form and then linearized about steady state operating conditions. Although nondimensionalization is common practice, here it serves also to prevent elements corresponding to the variables

that undergo the greatest change in dimensional magnitude from overshadowing the other elements in the eigenvectors. In linearization parameters such as plate efficiencies, activity coefficients, heat transfer coefficients, and physical properties are held constant at their steady state values. The linearization is equivalent to the formation of a Taylor series expansion about the steady state with truncation after the first derivative terms.

When the three dimensionless, linearized differential equations for the i'th plate are written in terms of deviations in the state variables from steady state they have the form.

$$\frac{dh_i}{d\phi} = a_1 h_i + a_2 h_{i+1} + a_3 x_{i-1} + a_4 x_i + a_5 x_{i+1} + a_6 x_{i+2} + a_7 t_{i-1} + a_8 t_i + a_9 t_{i+1} \tag{3.1}$$

$$\frac{dx_i}{d\phi} = b_1 h_i + b_2 h_{i+1} + b_3 x_{i-1} + b_4 x_i + b_5 x_{i+1} + b_6 x_{i+2} + b_7 t_{i-1} + b_8 t_i + b_9 t_{i+1} \tag{3.2}$$

$$\frac{dt_i}{d\phi} = c_1 h_i + c_2 h_{i+1} + c_3 x_{i-1} + c_4 x_i + c_5 x_{i+1} + c_6 x_{i+2} + c_7 t_{i-1} + c_8 t_i + c_9 t_{i+1} \tag{3.3}$$

where the coefficients a_j, b_j, and c_j are, in general, different for each plate. These coefficients are complicated functions of physical parameters and steady state variables of the process as shown in Appendix B.1. The numbering of plates is from bottom to top and begins

with the reboiler as plate zero. For a ten-plate column there are 34 equations; three for each plate and two each for the reboiler and accumulator.

The state matrix $\underline{\underline{A}}$ for the entire distillation column is formed from the coefficients a_j, b_j, and c_j of the differential equations for all N plates, the reboiler and the accumulator. This matrix takes the form shown in Fig. 4.3. The state variables are arranged in the sequence; holdups, compositions, temperatures, with each group ordered from bottom to top of the column. The bands in the figure indicate the location of nonzero coefficients. Notice that the $\underline{\underline{A}}$ matrix may be partitioned into submatrices in which the coefficients form two, three, or four diagonals. The influence of each type of state variable on its own derivative is governed by the submatrices on the main diagonal, while interaction between the thermal, hydraulic and component accumulation processes is determined by the submatrices not on the main diagonal.

C. Simplified Models

Models 2,3, and 4 are considerably less detailed than Model 1. For each, all of the assumptions used for Model 1 are invoked along with additional restrictions.

In Model 2 the mass holdups throughout the column are treated as constant, but the formulation includes accumulation of heat and chemical species. This model seems reasonable if the change in mass held on a plate is usually small, so that the accumulation of enthalpy and components accounted for by this change in mass can be neglected. The assumption of constant mass requires that any liquid flow disturbances, which may arise from changes in input flows or enthalpies, be transmitted instantaneously down the column from the point of entry of the disturbance. Similarly, any vapor flow disturbances are transmitted instantaneously

$\underline{\underline{A}} =$

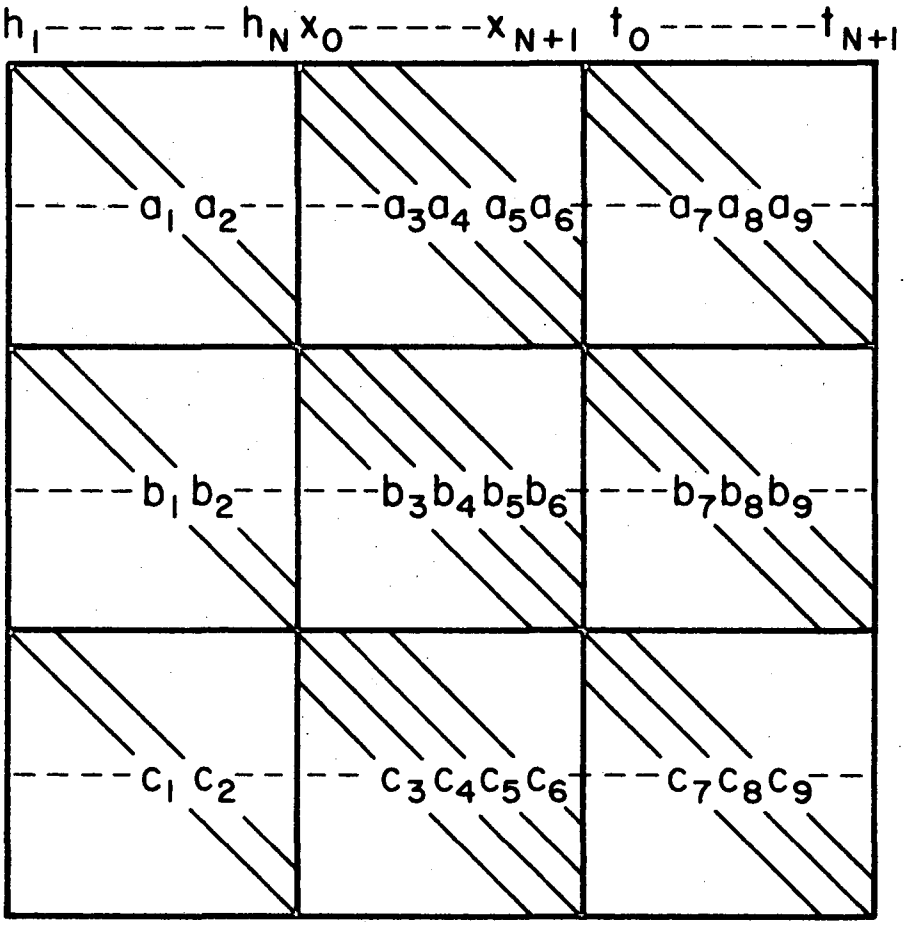

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Fig. 4.3 Form of the state space matrix for Model 1.

up the column. The version of Model 2 used by Huckaba, et al.[15,28,29] requires constant column pressure and has other restrictions on enthalpies. Nevertheless, these investigators observed reasonably good correspondence between predictions based on Model 2 and experimentally determined responses of compositions to changes in feed composition, feed flow rate, reflux flow rate, and reboiler heat duty. The experimental column had twelve bubble-cap plates and processed a binary mixture of methanol and tertiary butyl alcohol. Despite this success, there is nevertheless uncertainty regarding the applicability of Model 2 to columns other than the one used by Huckaba. Because of this uncertainty and because considerable effort would be required for the calculations, no further study was made of this model. The computational effort required for Model 2 would be nearly as great as that for Model 1 because the $\underline{\underline{B}}$ matrix must account for the instantaneous influence of some of the inputs at many plates in the column.

Models of type 3, which have been used widely, do not account for accumulation of enthalpy. However the effect of subcooled feed and reflux on flows at the feed plate and top plate may be included by special instantaneous enthalpy balances at those plates. Thus input variations in flow rate, composition, and temperature of the feed, reflux flow rate and reboiler steam temperature may be treated. Because, in Model 3, vapor flow rate does not influence holdup, vapor flow disturbances are transmitted instantaneously up the column. The derivation of a version of Model 3 very similar to that of Lamb, Pigford and Rippin[32] is given in Appendix B.2.

Model 3 has certain interesting properties that arise because the composition variables are partially decoupled from the holdup variables. This may be seen from the form of the state matrix shown in Fig. 4.4.

$\underline{\underline{A}} =$

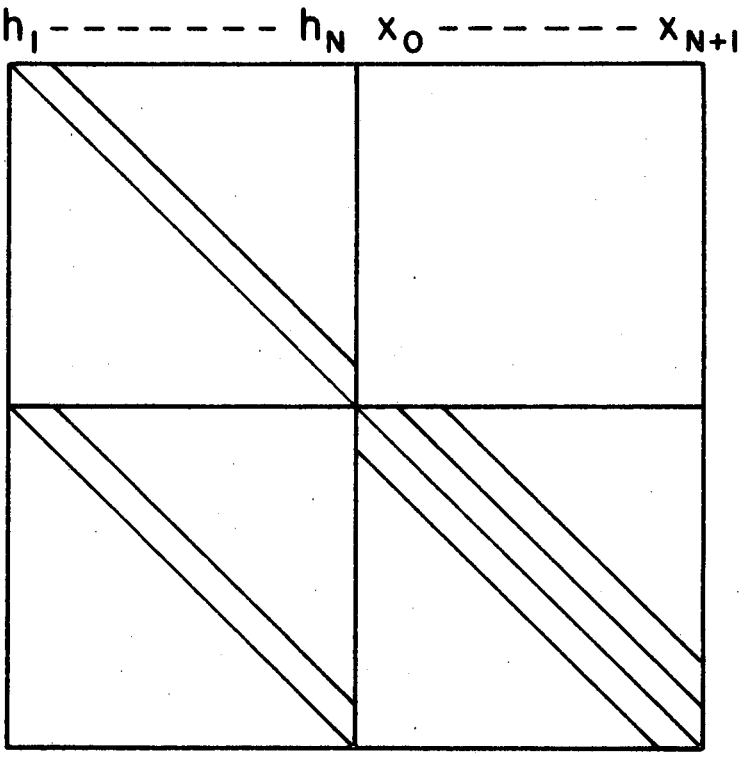

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Fig. 4.4 State space matrix for Model 3

Hydraulics influence the composition but compositions have no effect on mass holdups. Consequently the elements of the upper right submatrix are all zero. The eigenvalues of a state matrix such as this are all eigenvalues of either the upper left submatrix or the lower right submatrix. Thus the modes can be classified as either hydraulic or composition modes, as shown in Appendix A.3 and also demonstrated by Rosenbrock.[53] Until the calculations discussed in Chapter V are examined it is difficult to say whether the omission of the unsteady enthalpy balances seriously detracts from the utility of Model 3.

In Model 4, enthalpy and hydraulic effects are ignored, and there is an implicit assumption that component accumulation phenomena dominate the dynamics. If interactions with other phenomena are large this simple formulation cannot be used. The utility of Model 4 is also severely restricted because the only input variable is feed composition. However, its simple form makes this model worthy of study, and it is derived in Appendix B.3.

D. Data Requirements for Distillation Calculations

Prediction of distillation dynamics with a mathematical formulation such as Model 1 requires the selection of values for a large number of parameters. The basic data requirements may be subdivided into properties of the binary system being fractionated, parameters for the distillation column, and operating data that determine the steady state conditions. These are summarized in Table 4.2.

Values of parameters have been chosen to duplicate as closely as possible the behavior of the distillation column at the University of Delaware. Sources of data, the values used, and the specific form of the various correlations employed are given in Appendix D and Chapter V.

Table 4.2 Distillation data requirements

a. Properties of the binary system

1. Vapor-liquid equilibria for both components including pressure and temperature dependence.
2. Activity coefficient correlations
3. Enthalpy correlations for pure liquid and vapor; heat capacity correlations for pure liquids; heat of vaporization correlations
4. Density as a function of temperature for pure liquids
5. Vapor pressure correlations for both components
6. Molecular weight of both components

b. Basic distillation column parameters

1. Murphree efficiency correlation
2. Number of plates; feed plate (only a single feed allowed)
3. Correlations for hydraulics, vapor flow and effect of vapor rate on holdup
4. Reboiler and accumulator holdup
5. Plate area

c. Operating data (steady state)

1. Feed rate, enthalpy and concentration
2. Bottom product flow rate and reflux flow rate
3. Condenser pressure
4. Amount of reflux subcooling
5. Condenser temperature driving force
6. Reboiler temperature driving force

V. DISTILLATION COLUMN MODES AND RESPONSE: RESULTS AND INTERPRETATION

The results of the modal decomposition of a binary distillation column are examined in this chapter. Wherever possible the modes are analyzed in terms of their physical basis in order to establish a better understanding of distillation dynamics. Much of the interpretation of the nature of the modes is useful for the development of modal controllers.

A. Cases Studied

Modes have been calculated for a variety of combinations of steady state conditions and column models. The Model 1 simulation of typical operating conditions of the ten-plate column studied experimentally by Luyben, Verneuil, and Gerster[33] is taken as the basic case in this work. The generality of the findings and the influence of operating conditions, column design, and choice of model on the nature of the modes are studied by comparison with the modes that are obtained for other models and at other conditions.

The cases studied are listed in Table 5.1, and are identified by a code. For example, the code A-10-1 means steady state condition A (simulation of the experimental steady state), ten-plate column, and Model 1. The steady states B, C, D and E are variations of steady state A, as indicated in the table. These have been included to determine the influence of accumulator and reboiler holdups, reflux rate, and feed rate on the modes. Columns with five and three plates are studied to determine the effect of the number of plates on the dynamics. Models 3 and 4 have been included in order to evaluate their usefulness.

Table 5.1. Cases Calculated

Code	Steady State	Number of Plates	Model	Control
A-10-1	Experimental conditions	10	1	No control, Modal control, Pressure control, others
A-5-1	Experimental conditions	5	1	No control
A-3-1	Experimental conditions	3	1	No control
A-10-3	Experimental conditions	10	3	No control
A-10-4	Experimental conditions	10	4	No control
B-10-1	Small reboiler and accumulator holdups	10	1	No control
B-5-1	Small reboiler and accumulator holdups	10	1	No control
B-3-1	Small reboiler and accumulator holdups	10	1	No control
C-10-1	High reflux rate	10	1	No control
D-10-1	Small feed rate	10	1	No control
E-10-1	Small feed rate, small reflux rate	10	1	No control

Many other cases may be of interest but none are included here because only principal effects are sought.

The data required for the specification of a steady state are shown in Table 5.2, where case A-10 specifications are compared with the experimental conditions of Luyben, Verneuil, and Gerster.[33] Results of the steady state distillation calculations are given in Tables 5.3, 5.4, 5.5 and 5.6 for cases A-10, C-10, D-10, and E-10 respectively. The condenser heat load shown in these tables is appreciably larger than the reboiler heat load because the former includes the sensible heat that is required to subcool both the reflux and the distillate. No table has been included for case B-10 because it is identical to A-10 at steady state except for the reboiler and accumulator holdups, which are respectively 0.966 and 0.742 (dimensionless).

The McCabe-Thiele diagram for an experiment with Gerster's column,[33] given in Fig. 5.5, can be compared with the diagram for case A-10, given in Fig. 5.1. Discrepancies between the two figures are primarily due to differences in the vapor-liquid equilibrium data used, but, in addition, the seal pan, which serves as an inefficient plate (indicated in Fig. 5.5 by W), at the bottom of the experimental column was not simulated in this study. McCabe-Thiele diagrams for steady states C-10, D-10, and E-10 are presented in Figs. 5.2, 5.3, and 5.4. Tabulations and McCabe - Thiele diagrams for steady states A-5 and A-3, which are identical to A-10 except for number of plates, are given in Appendix E.

Examples of the state matrix $\underline{\underline{A}}$ and input matrix $\underline{\underline{B}}$ for cases A-10-1 and A-10-4 are presented in Appendix F, where, for A-10-1, $\underline{\underline{A}}$ is 34×34 and $\underline{\underline{B}}$ is 34×6. Matrices such as these were used for the calculation of modes.

Table 5.2. Data for Specification of the Steady State

	Steady State A-10	Luyben, Verneuil, Gerster[33] Run No. 7*
Number of Plates:	10	
Feed Plate:	Fifth from bottom	
Feed Rate:	0.0250 moles/sec	0.0248 moles/sec
Feed Temperature:	560°R	
Feed Composition:	$x_F = 0.5$	
Pressure at Condenser:	2.70 atm	
Bottom Product Flow Rate:	0.0100 moles/sec	0.0114 moles/sec
Reflux Flow Rate:	0.0160 moles/sec	0.0150 moles/sec
Subcooling of Reflux:	90°F	
Reboiler Holdup (includes holdup in reboiler piping):	67 gal (5.65 moles benzene)	
Accumulator Holdup (includes holdup in reflux piping):	67 gal (7.33 moles acetone)	
Temperature Driving Forces		
Reboiler:	$T_S - \bar{T}_0 = 60°F$	not known
Condenser:	$\bar{T}_{N+1} - T_{CW} = 10°F$	not known

* Only the conditions differing from those of steady state A-10 are entered.

Table 5.3. Steady State A-10

Plate No.	Temp., °R	Pressure, atm	Liquid Flow Rate, moles/sec	Liquid Composition, mole fraction	Murphree Efficiency	Dimensionless Holdup[4]
0	695.4	2.851	0.0100[2]	0.039	1.00	13.882
1	685.3	2.832	0.0511	0.123	0.83	0.965
2	674.5	2.814	0.0506	0.237	0.78	0.959
3	666.5	2.796	0.0506	0.357	0.74	0.950
4	661.7	2.779	0.0508	0.449	0.71	0.943
5	659.1	2.762	0.0510	0.508	0.71	0.937
6	657.4	2.750	0.0194	0.552	0.78	0.785
7	655.9	2.737	0.0195	0.603	0.78	0.781
8	654.5	2.725	0.0196	0.654	0.78	0.776
9	653.2	2.713	0.0197	0.704	0.78	0.772
10	652.1	2.702	0.0197	0.755	0.78	0.767
11	561.0[1]	2.700	0.0160[3]	0.807	1.00	$\frac{18.010}{40.527}$ = Total

Feed rate = 0.0250 moles/sec on Plate 5

Distillate flow rate = 0.0150 moles/sec

Condenser heat load = 701.7 Btu/sec

Reboiler heat load = 522.2 Btu/sec

Reflux ratio = 1.07

[1]Reflux temperature.

[2]Bottom product flow rate.

[3]Reflux flow rate.

[4]Holdup relative to residual holdup, H_W (H_W = 0.407 moles).

Table 5.4. Steady State C-10

Plate No.	Temp., °R	Pressure, atm	Liquid Flow Rate, moles/sec	Liquid Composition, mole fraction	Murphree Efficiency	Dimensionless Holdup[4]
0	704.1	3.543	0.0120[2]	0.082	1.00	13.882
1	690.4	3.449	0.1292	0.247	0.70	0.961
2	678.3	3.359	0.1289	0.387	0.70	0.922
3	670.2	3.271	0.1295	0.515	0.70	0.880
4	665.3	3.184	0.1301	0.605	0.70	0.840
5	662.4	3.098	0.1305	0.662	0.70	0.803
6	659.3	3.022	0.0984	0.730	0.70	0.616
7	656.8	2.946	0.0987	0.779	0.70	0.581
8	654.6	2.870	0.0988	0.816	0.70	0.547
9	652.6	2.793	0.0988	0.845	0.70	0.512
10	650.7	2.715	0.0988	0.867	0.70	0.476
11	560.1[1]	2.700	0.0800[3]	0.886	1.00	$\frac{18.010}{39.030}$ = Total

Feed rate = 0.0250 moles/sec on Plate 5

Distillate flow rate = 0.0130 moles/sec

Condenser heat load = 1610 Btu/sec

Reboiler heat load = 1475 Btu/sec

Reflux ratio = 6.15

[1] Reflux temperature

[2] Bottom product flow rate

[3] Reflux flow rate

[4] Holdup relative to residual holdup, H_W (H_W = 0.407 moles)

Table 5.5. Steady State D-10

Plate No.	Temp., °R	Pressure, atm	Liquid Flow Rate, moles/sec	Liquid Composition, mole fraction	Murphree Efficiency	Dimensionless Holdup[4]
0	694.4	2.786	0.00225[2]	0.0357	1.00	13.882
1	683.8	2.776	0.0255	0.124	0.86	0.953
2	671.8	2.766	0.0253	0.264	0.81	0.949
3	663.1	2.757	0.0255	0.419	0.77	0.943
4	658.2	2.748	0.0257	0.539	0.75	0.938
5	656.0	2.739	0.0258	0.616	0.74	0.934
6	653.9	2.731	0.0196	0.693	0.77	0.902
7	652.6	2.723	0.0197	0.752	0.77	0.899
8	651.7	2.716	0.0197	0.796	0.77	0.896
9	651.0	2.708	0.0198	0.830	0.77	0.894
10	650.5	2.701	0.0198	0.857	0.76	0.893
11	560.2[1]	2.700	0.0160[3]	0.880	1.00	$\frac{18.010}{41.093}$ = Total

Feed rate = 0.0050 moles/sec on Plate 5

Distillate flow rate = 0.00275 moles/sec

Condenser heat load = 326.7 Btu/sec Reflux ratio = 5.82

Reboiler heat load = 295.8 Btu/sec

[1]Reflux temperature

[2]Bottom product flow rate

[3]Reflux flow rate

[4]Holdup relative to residual holdup, H_W (H_W = 0.407 moles)

Table 5.6. Steady State E-10

Plate No.	Temp., °R	Pressure, atm	Liquid Flow Rate, moles/sec	Liquid Composition, mole fraction	Murphree Efficiency	Dimensionless Holdup[4]
0	682.4	2.756	0.00225[2]	0.104	1.00	13.882
1	671.1	2.749	0.00977	0.253	0.82	0.993
2	663.6	2.743	0.00979	0.380	0.79	0.992
3	659.7	2.737	0.00984	0.467	0.77	0.991
4	657.7	2.732	0.00987	0.518	0.76	0.990
5	657.0	2.726	0.00989	0.546	0.73	0.989
6	655.7	2.721	0.00358	0.584	0.87	0.960
7	654.5	2.715	0.00359	0.632	0.86	0.959
8	653.5	2.710	0.00360	0.680	0.86	0.958
9	652.5	2.705	0.00362	0.727	0.86	0.958
10	651.6	2.700	0.00363	0.774	0.85	0.957
11	560.8[1]	2.700	0.00294[3]	0.824	1.00	$\frac{18.010}{41.639}$ = Total

Feed rate = 0.0050 moles/sec on Plate 5

Distillate flow rate = 0.00275 moles/sec

Condenser heat load = 128.6 Btu/sec

Reboiler heat load = 96.53 Btu/sec

Reflux ratio = 1.07

[1] Reflux temperature

[2] Bottom product flow rate

[3] Reflux flow rate

[4] Holdup relative to residual holdup, H_W (H_W = 0.407 moles)

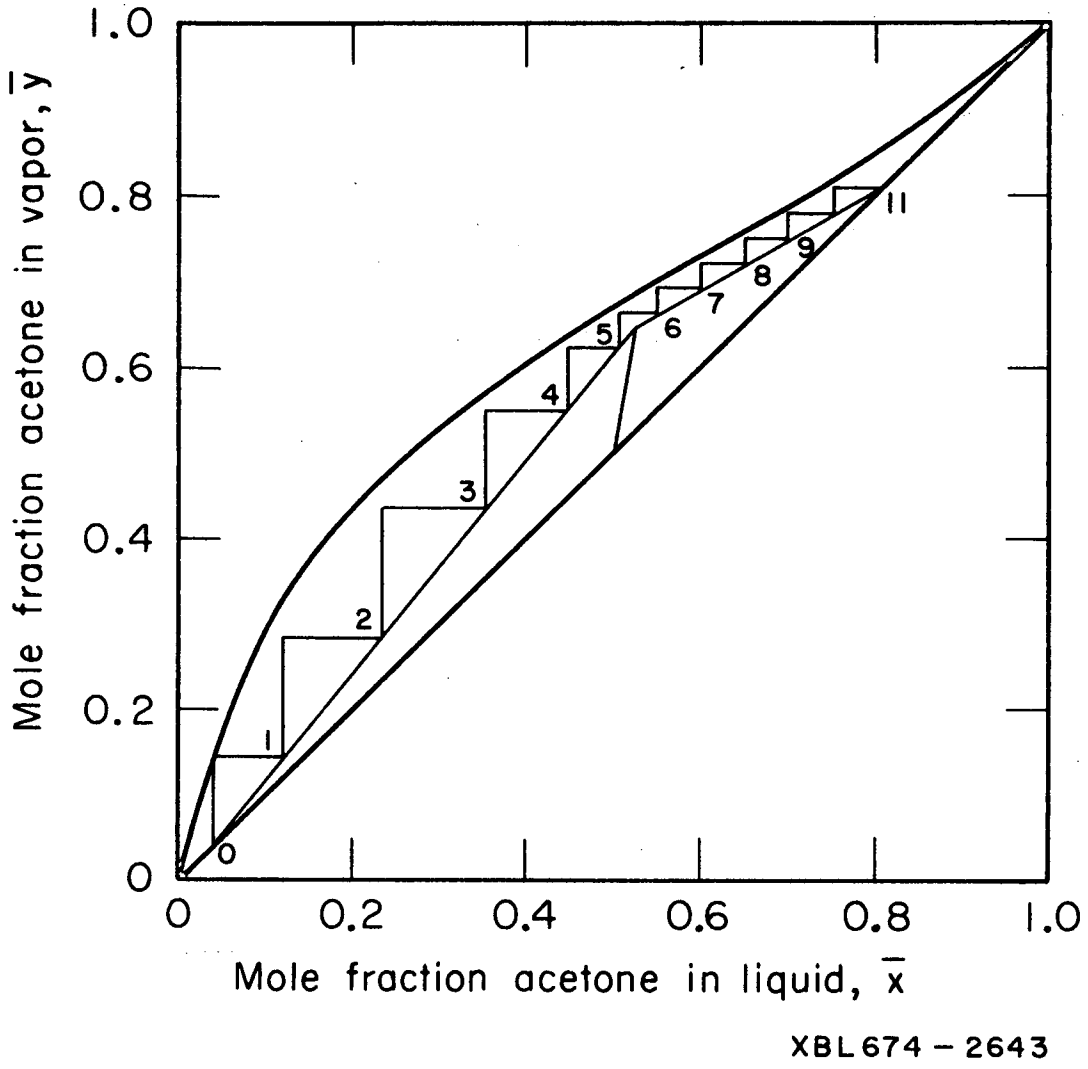

Fig. 5.1. McCabe-Thiele diagram for Case A-10.

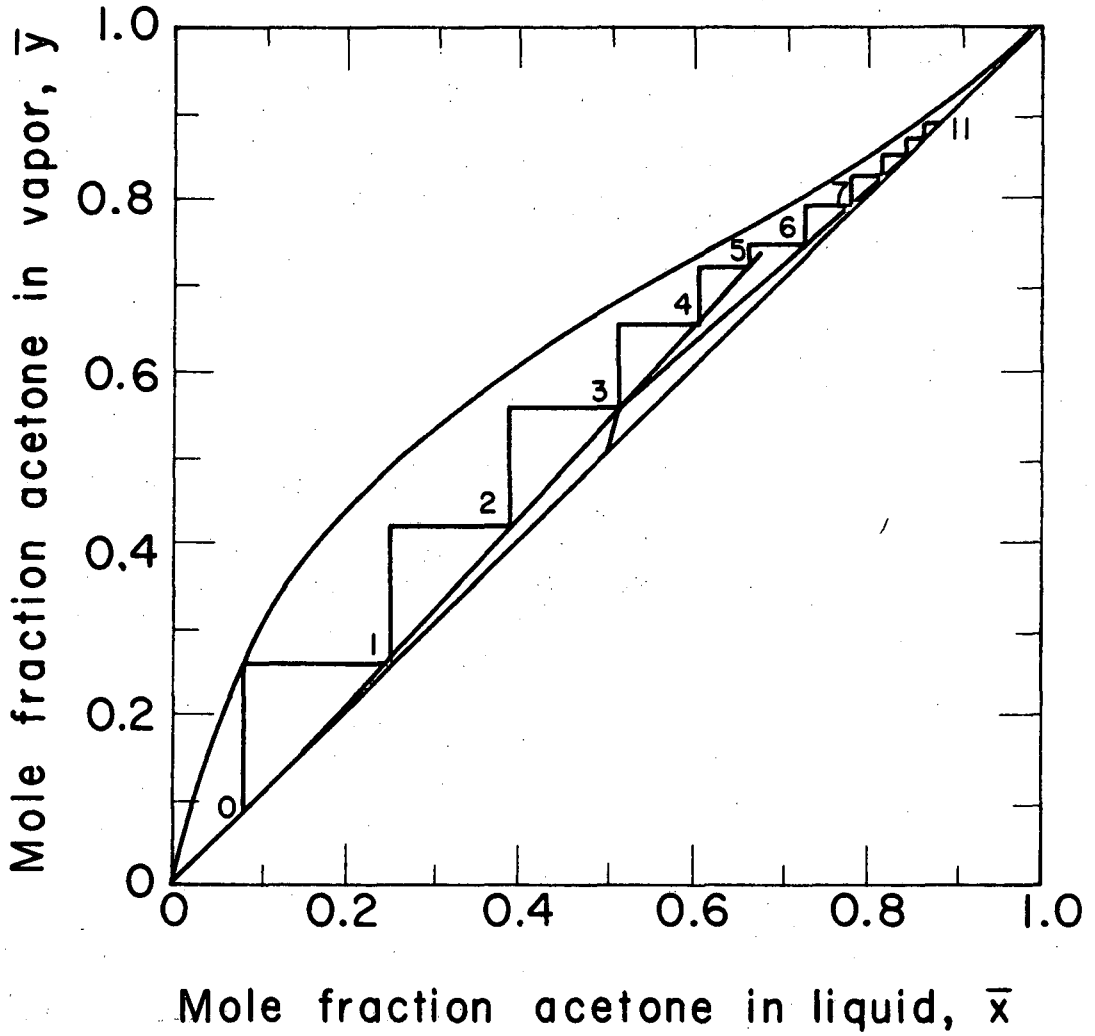

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Fig. 5.2 McCabe-Thiele diagram for Case C-10.

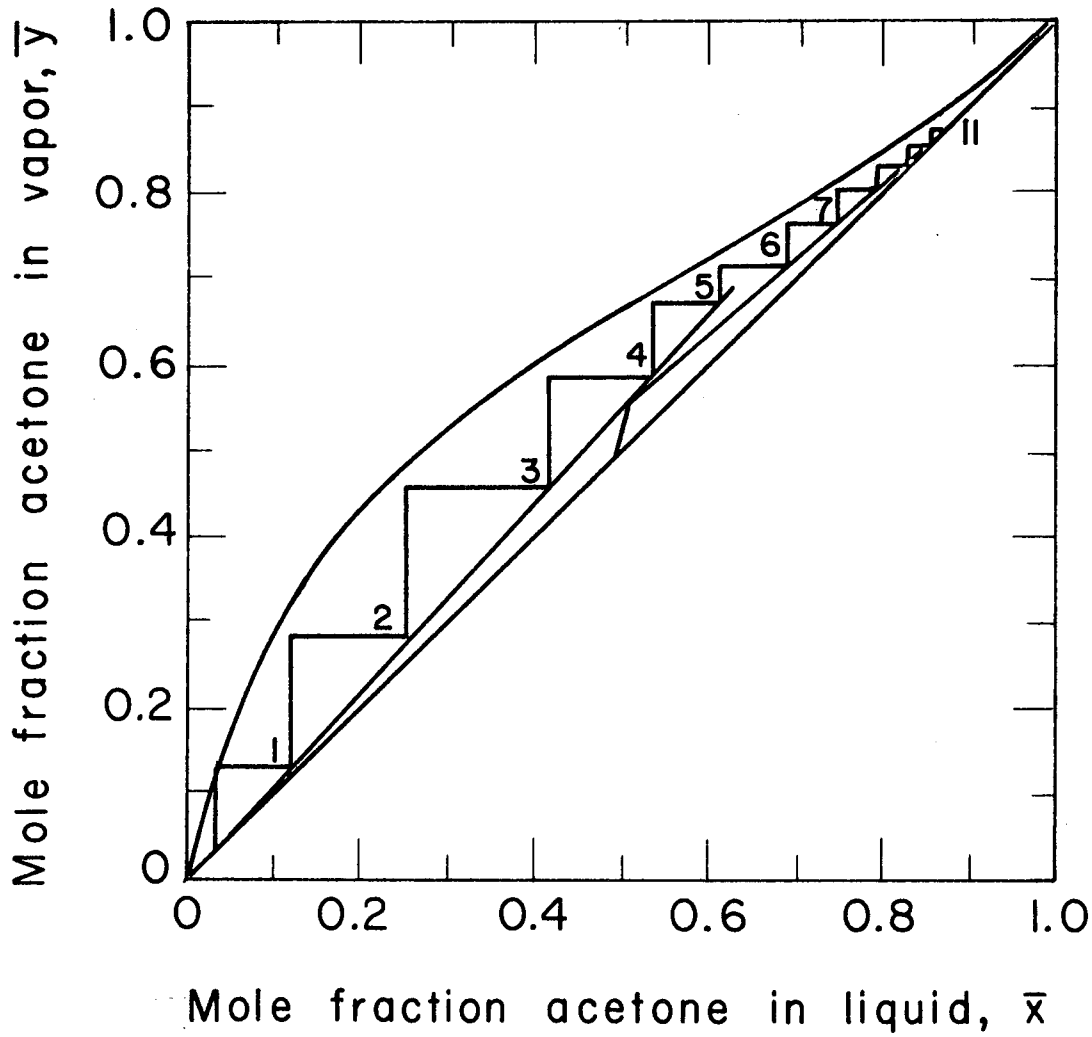

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Fig. 5.3 McCabe-Thiele diagram for Case D-10.

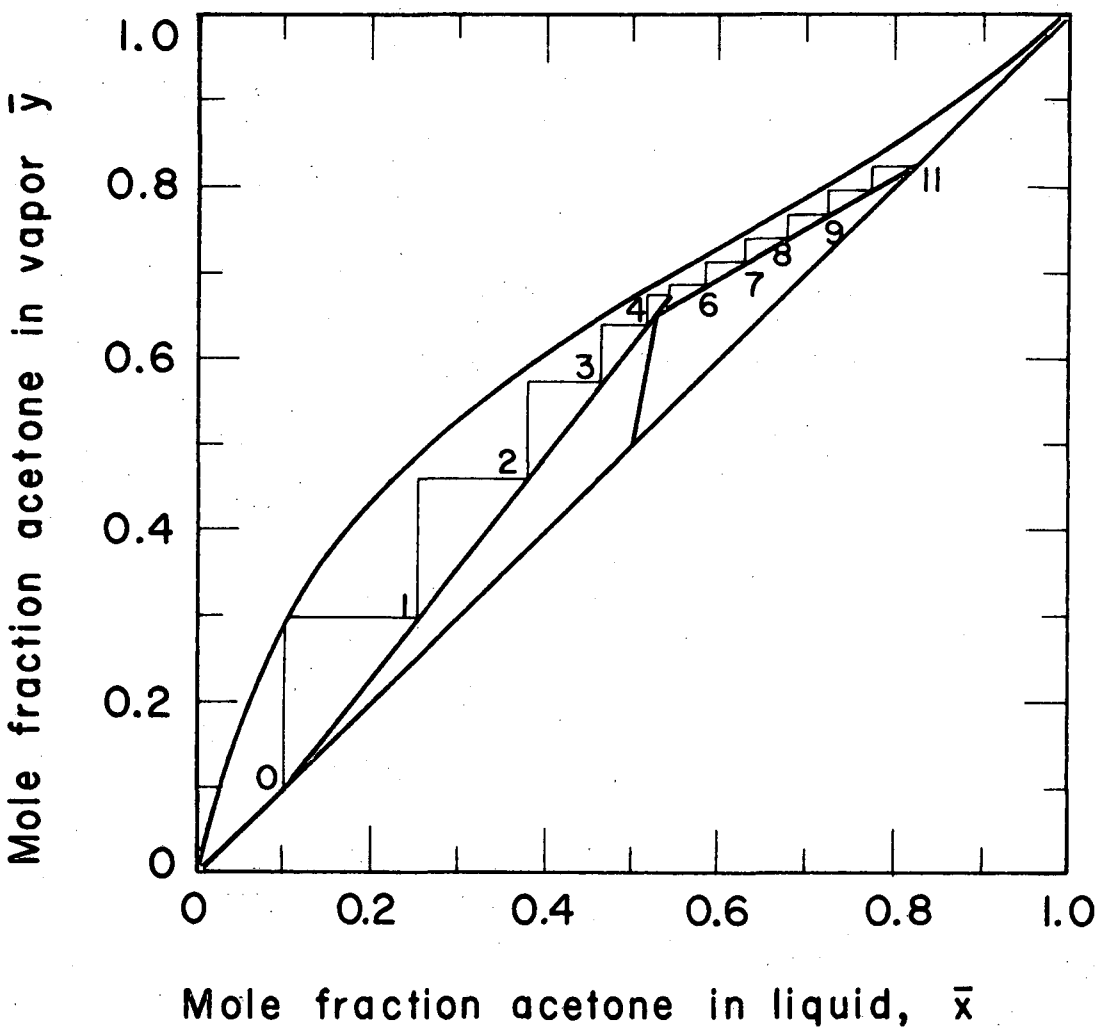

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Fig. 5.4 McCabe-Thiele diagram for Case E-10.

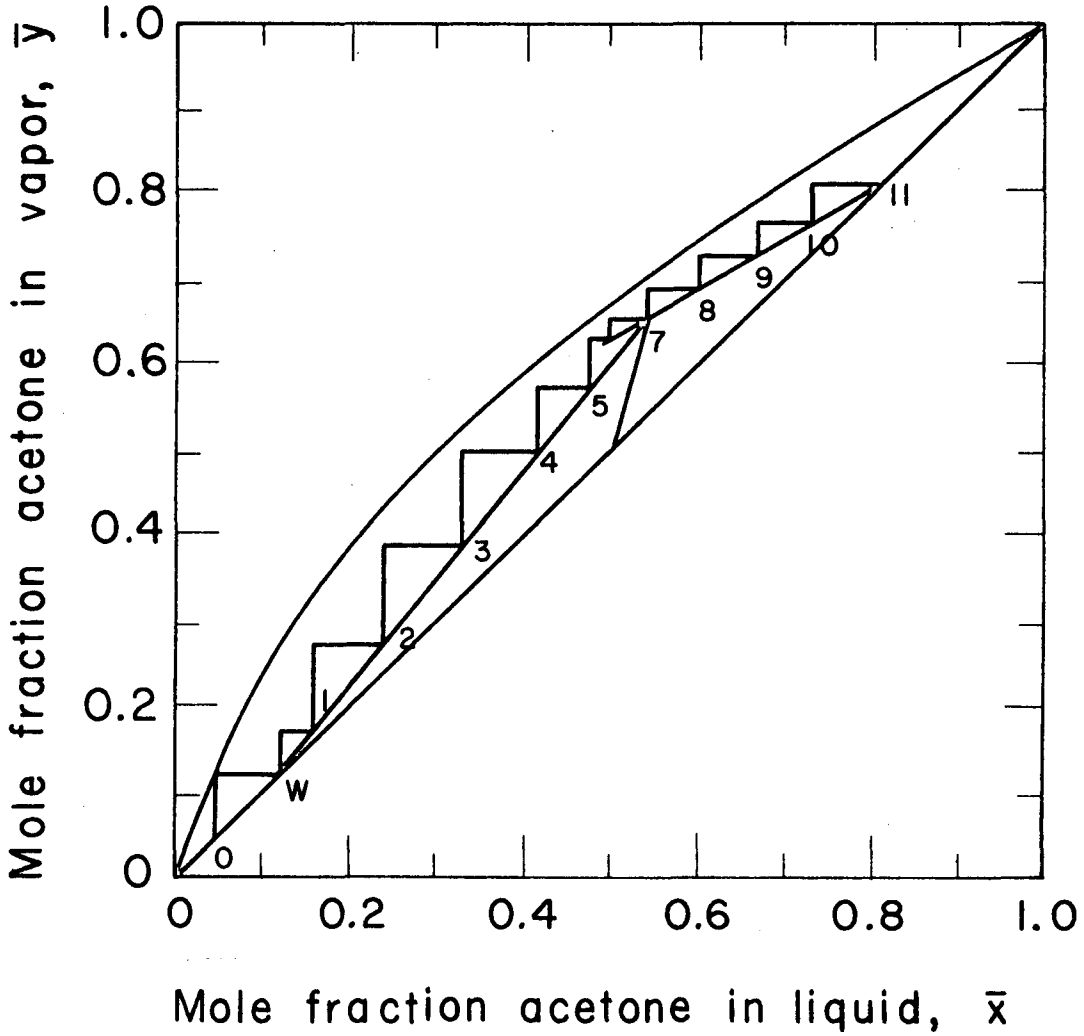

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Fig. 5.5 McCabe-Thiele diagram for the distillation column of Luyben, Verneuil, and Gerster,[33] Run No. 7.

Each of the input variables shown in Table 5.7 was changed stepwise from its initial steady state to generate a response of the state vector that was calculated by summing the contributions of the modes. All of these inputs were not used for Models 3 and 4; Model 3 does not include coolant temperature, and Model 4 has only feed composition as an input. The magnitudes of the step changes were chosen arbitrarily to be approximately one percent changes based on values at steady state A. But, for case B calculations, the step change in reflux rate was approximately one percent of the case B reflux rate. It should be noted that a one percent change in the absolute value of the steam temperature or coolant temperature corresponds to much more than a one percent change in driving force. However, the magnitudes chosen here are not particularly important because the models are linear.

B. Modes for Case A-10-1

This section is restricted to an analysis of the modes for the basic case, A-10-1. The eigenvalues and the corresponding time constants (derived from the matrix $\underline{\underline{A}}$ shown in Appendix F) for all 34 modes are listed in Table 5.8. In Appendix F, additional significant figures for the eigenvalues, and the eigenvectors (right and left) of the six slowest modes are presented. The eigenvalues are given in order of increasing modulus, and, therefore, the largest time constant appears first. The thirteen slowest of the 34-dimensional modes (right eigenvectors) are represented in Fig. 5.6 by bar graphs in which the length of each bar is proportional to the magnitude of the corresponding eigenvector element. Absolute magnitudes are not indicated because eigenvectors may always be scaled by an arbitrary constant. The

Table 5.7. Magnitude of Step Inputs

	Dimensional	Dimensionless
Feed rate:	0.000250 moles/sec	0.00940
Feed temperature:	5.58°R	0.154
Feed composition:	0.005 mole fraction	0.005
Reflux rate:	0.000160 moles/sec	0.010
Steam temperature:	7.30°R	0.0202
Coolant temperature:	5.61°R	0.0155

Table 5.8. Eigenvalues and Time Constants
Case A-10-1 (no control)

Mode	Eigenvalue (dimensionless), λ	Time Constant (min), τ*
1	-0.0453	9.37
2	-0.108	3.94
3	-0.130	3.26
4	-0.477	0.889
5	-0.782	0.542
6	-1.06	0.400
7	-2.11	0.201
8	-3.96 + 1.04i	0.107
9	-3.96 - 1.04i	0.107
10	-4.92 + 2.05i	0.0862
11	-4.92 - 2.05i	0.0862
12	-6.99 + 3.92i	0.0607
13	-6.99 - 3.92i	0.0607
14	-8.70	0.0487
15	-8.93 + 1.14i	0.0475
16	-8.93 - 1.14i	0.0475
17	-9.65 + 4.29i	0.0440
18	-9.65 - 4.29i	0.0440
19	-12.1 + 3.20i	0.0351
20	-12.1 - 3.20i	0.0351
21	-12.2	0.0347
22	-13.4 + 0.948i	0.0316
23	-13.4 - 0.948i	0.0316
24	-17.2	0.0246
25	-70.3	0.00603
26	-457	0.000928
27	-1,170	0.000361
28	-2,210	0.000192
29	-3,350	0.000127
30	-4,630	0.0000916
31	-5,920	0.0000716
32	-6,950	0.0000610
33	-9,000	0.0000471
34	-11,000	0.0000384**

* $\tau = -0.424/\lambda'$.

** 2.30 milliseconds.

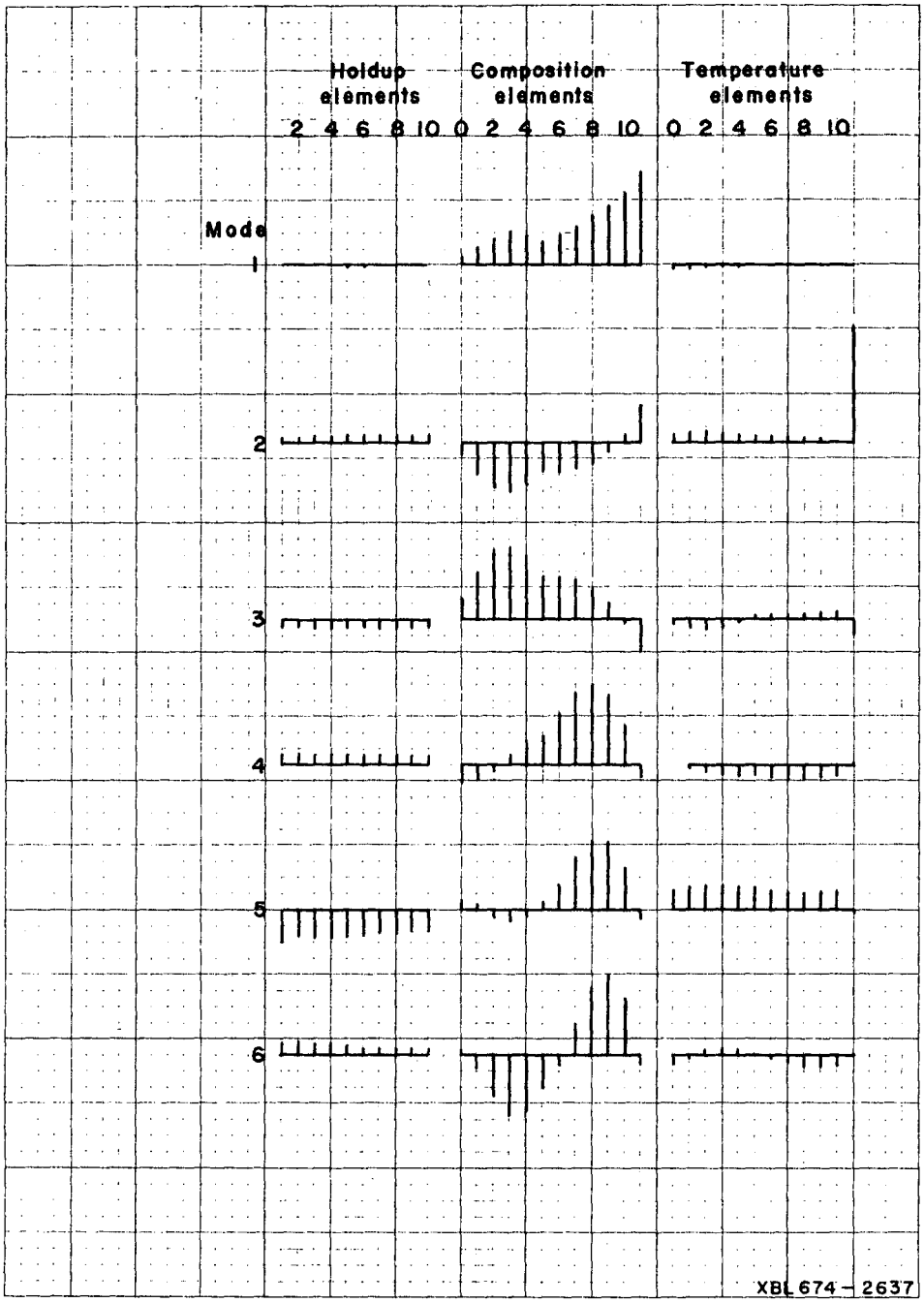


Fig. 5.6 Modes for Case A-10-1, no control.

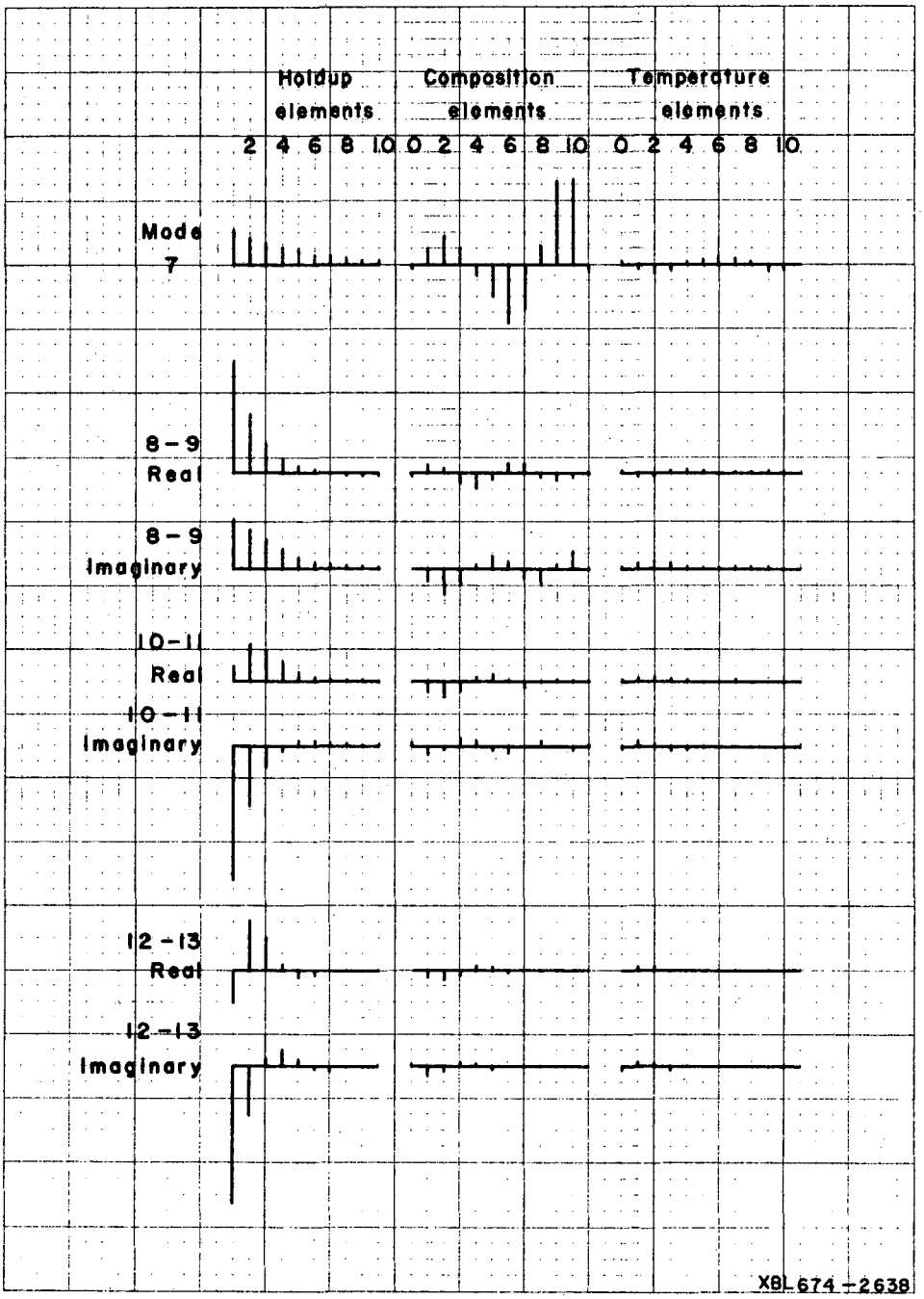


Fig. 5.6 Modes for Case A-10-1, no control.

elements of the eigenvectors correspond to state variables and are arranged in the sequence: holdups (plate 1 through plate 10), compositions (reboiler through accumulator), and temperatures (reboiler through accumulator). Plate numbers are indicated at the top of the figure.

The time constant of a mode determines whether that mode can potentially be important in determining the process dynamics. However, a mode with a relatively large time constant is actually important only if it is activated appreciably by some or all of the possible inputs. The activations of the first seven modes that are caused by step changes in each of the six inputs are given in Table 5.9. These are the activations determined by Eq. (2.9) or (A.1.8), and as such are relative weights that apply for the specific input having the dimensionless magnitudes shown. The activations shown for a particular input cannot be compared directly with the corresponding activations for other inputs, that is, comparisons can be made only vertically in this table. Since the activation of the first mode is nearly as large or larger than the activation of any other of the slow modes for every input, it is concluded that the slowest mode is indeed the most important one.

As shown in Fig. 5.6, the dominant mode, which has a time constant of 9.37 minutes, affects only composition variables appreciably. All plates, including reboiler and accumulator, are influenced, and all compositions are driven in the same direction. This indicates that the dominant dynamic effect concerns the accumulation and transfer of chemical species throughout the column. It is of interest that, even though the condenser and reboiler are primary contributors to the total

Table 5.9. Activation of Modes by Step Inputs

Case A-10-1 (No Control)

Mode	Input Variable and Magnitude of Step					
	f = 0.00940	t_F = 0.0154	x_F = 0.0050	ℓ_{11} = 0.0100	t_s = 0.0202	Δt_{cw} = 0.0155
1	0.01121	-0.006378	0.01354	0.01463	-0.07668	0.1110
2	0.002273	-0.0005056	0.001860	0.001955	-0.009786	0.03361
3	0.01389	-0.008469	0.01388	0.01578	-0.1320	0.1478
4	0.001528	-0.002295	0.004806	0.002436	-0.009314	0.01458
5	0.001978	0.005687	-0.000027	-0.002866	0.08836	-0.002690
6	-0.004232	-0.003768	-0.002365	0.0004504	-0.05680	-0.03072
7	0.001430	0.001974	-0.001065	0.001900	0.01322	0.04567

holdup, and hence to the dominant time constant, the influence of the first mode is nevertheless distributed rather uniformly throughout the column.

The second mode, which has a time constant of 3.94 minutes, is 2.4 times faster than the slowest and is much less strongly activated. It is interesting, however, because the accumulator temperature component is very large, as may be seen in Fig. 5.6, and because no other mode has any similarity to this one. To verify that mode 2 is associated with the accumulator, a time constant τ_A of 3.94 minutes may be calculated as accumulator holdup divided by throughput rate (reflux plus distillate rate). This is the same as the time constant for the second mode and suggests that the accumulator responds as a nearly decoupled, well-stirred tank. The nearly independent response can be predicted intuitively because the accumulator has only one-way liquid flow whereas all the plates and the reboiler generate both vapor and liquid streams. Vapor streams provide alternate channels for rapid transmission of disturbances, but upsets entering the accumulator can only be transmitted to the liquid effluent.

It seems somewhat surprising that there is a mode (the second) with a large accumulater temperature component, while there are no modes that are dominated by temperature components corresponding to plates. The reason for this is related to the mechanisms for accumulation of enthalpy. On the plates, and in the reboiler, most of the heat absorbed is used to generate vapor, and only a fraction serves to raise the fluid temperature. In fact, most of the temperature changes observed on the plates probably are induced by pressure changes.

However, in the accumulator all of the heat absorbed is used to raise the fluid temperature, and therefore enthalpy changes have a much more pronounced effect on accumulator temperature than on plate temperatures.

The third mode, with a time constant of 3.26 minutes, is not exclusively related to the reboiler, even though the reboiler has a large holdup only slightly less than the accumulator holdup. The reboiler is not decoupled from the rest of the column because it behaves very much as a plate. The physical basis for mode 3 is not entirely evident, although it can be considered as a composition mode much like mode 1 because its holdup and temperature elements are small compared to the composition elements. In fact, modes 1 and 3 appear to be closely related because the activations for both are of the same magnitude and sign for every input, as can be seen in Table 5.9. This suggests that it is not possible to identify every mode with a specific phenomenon or group of phenomena in the column.

Modes that have time constants smaller than those of the third or fourth mode are not of great importance when control is considered but nevertheless have very interesting characteristics. For instance, the faster the response of a mode, the more frequently its composition elements change sign between the bottom and top of the column. At mode 6 there is a cyclic trend in the composition components that might be considered as the first harmonic of a standing wave of composition. Lamb, Pigford, and Rippin[32] mention the propagation and "reflection" of disturbances in a distillation column that could result in standing waves analogous to those generated in distributed processes that have reflections at one or both ends. The possibility of composition harmonics has been suggested by Rosenbrock in the discussion following

reference 1. Only composition, and possibly temperature, standing waves can be expected; flow distrubances are absorbed in the product streams through the action of the level controllers at both ends of the column. It may be reasonable to call mode 4 the fundamental mode for composition standing waves, and then modes 6, 7, and 8 (imaginary part) may be considered as the first, second, and third harmonics. Each of these four modes has a time constant that is approximately a factor of two smaller than its predecessor; they are 0.889, 0.400, 0.201, and 0.107 minutes respectively. Interactions between hydraulic and composition phenomena in these modes prevent a clear-cut sequence of composition harmonics from appearing.

One or more of the intermediate modes should have a time constant near to the characteristic time for change of inventory on a single plate, which is approximately 0.13 minutes in the stripping section and 0.27 minutes in the rectifying section. These numbers bracket the time constant for mode 7, which is the fastest of the 13 modes shown that is dominated by compositions. It should be noted that between modes 1 and 7, the faster the mode, the less significant are the composition components corresponding to the reboiler and accumulator. The large holdups seem to contribute only to the slowest modes.

Modes 8 through 23 all have relatively insignificant composition components; rather they are dominated by holdup components. Therefore they are referred to as flow modes or hydraulic modes, and all have a character similar to the ones shown (modes 8-13) in Fig. 5.6. The time constants for the flow modes lie in the range 0.107 to 0.0316 minutes, which is 12 to 87 percent of the typical time for change of inventory for a plate. However a typical decay time for hydraulic effects on a

single plate is based on a liquid holdup less than the total plate holdup, because the hydraulics are governed by the height of liquid above the weir.

Fourteen of the hydraulic modes occur as complex conjugate pairs. The appearance of complex modes is evidence that interactions between hydraulic effects and thermal or component accumulation phenomena are significant. However, complex modes must not be considered a necessary result of interactions; conceivably many kinds of interaction do not produce them. On the other hand, when the phenomena are completely decoupled the modes must all be real. The simplest example of this is given by Model 4, which generates a tridiagonal state matrix. It can be proven mathematically that all of the eigenvalues of such a tridiagonal matrix are real.[34] For Model 3 the hydraulic modes are decoupled because the coefficients in the state matrix that link the holdup equations to composition (and temperature) variables are all zero. Further discussion of hydraulic modes is deferred to a later section.

The successive time constants of the next few modes after the last hydraulic mode (mode 23) decrease in magnitude very sharply. Modes 24 and 25 have some significant composition and temperature components, while modes 26 through 34 have only holdup and temperature elements, or temperature elements alone, that are important. The range of time constants for modes 26 through 34 is 55.7 milliseconds to 2.30 milliseconds. The physical basis for the slower of these modes is not entirely clear. They must be associated with hydraulic and thermal phenomena. The fastest modes are almost certainly associated with the transmission of pressure disturbances up the column. To achieve an

increase in pressure on a plate, liquid is heated by condensation of part of the vapor stream. At short times, before the composition changes appreciably, the pressure and temperature on the plate must change simultaneously. A time constant for this mechanism at one plate is on the order of 6 milliseconds, which is the order of magnitude of the time constant for the fastest mode (2.30 milliseconds).

Additional information about the distillation column modes is available from the eigenvalue sensitivities. Sensitivities of 14 eigenvalues to changes in 19 parameters or groups of parameters, calculated by Eq. (2.18), are listed in Table 5.10, where the entries give the ratio of the relative change in the eigenvalue to that in the parameter. The previous identification of the physical basis for some of the modes is substantiated by the sensitivities to steady state values of liquid holdups. The accumulator holdup affects only the first two modes significantly. For the second mode the sensitivity is -1.07, which means that a one percent increase in accumulator holdup causes a one percent decrease in the eigenvalue (increase in time constant). The reboiler holdup influences modes 3, 4, and 5 predominantly and has almost no effect on mode 1 or 2. The sum of the sensitivities to steady state holdups on plates one through ten is largest for modes 6, 7, 8, and 9, and significant for many other modes, but it is reasonable that many modes are influenced by plate holdups.

The dominant modes are strongly affected by vapor-liquid equilibria parameters, but the large influence occurs partly because these parameters appear in the exponents of the equilibrium correlations. Except for plate area, A_T, the rest of the parameters listed have relatively little effect on any of the eigenvalues. Plate area is important for the intermediate (hydraulic) modes.

Table 5.10. Eigenvalue Sensitivities to Values of Parameters

Case A-10-1 (No Control)

Mode	Vapor-Liquid Equilibria				Activity Coefficients A_{12} and A_{21}	Hydraulics α	Vapor Flow β	Overhead Vapor Flow β_N	Heat of Vaporization		Heat Capacity	
	a_1	a_2	b_1	b_2					a_{VH}	b_{VH}	a_{CP}	b_{CP}
1	3.76	-0.70	-4.21	1.08	0.07	0.00	0.00	0.00	-0.01	0.01	0.00	0.00
2	0.86	0.59	-0.77	-0.68	-0.04	0.01	0.00	0.00	0.03	-0.01	0.00	0.00
3	0.85	-3.14	-5.25	3.26	0.31	-0.02	0.02	0.00	-0.21	0.04	-0.09	-0.08
4	-7.31	-4.06	7.93	4.68	0.35	0.00	0.00	0.00	-0.02	-0.02	0.02	0.01
5	-1.53	-1.01	1.58	1.10	0.07	-0.08	0.00	0.00	0.18	-0.09	0.16	0.15
6	-3.00	-2.94	2.32	3.32	0.12	0.00	0.00	0.00	-0.05	-0.04	0.05	0.05
7	0.18	-4.12	-1.37	5.04	0.16	-0.06	0.00	0.00	-0.07	-0.01	-0.04	-0.04
8-9 real	1.78	-4.09	-2.72	5.13	0.09	-0.03	0.00	0.00	0.06	-0.03	-0.22	-0.21
8-9 imag.	6.66	1.99	-6.63	-1.93	-0.05	-0.48	0.00	0.00	0.17	0.04	-0.08	0.08
10-11 real	-4.69	0.48	4.73	-0.92	0.10	-0.95	0.01	0.00	-0.14	0.03	0.32	0.31
10-11 imag.	0.15	-0.74	-0.52	0.97	0.04	0.17	-0.01	0.00	0.03	0.01	0.09	0.09
12-13 real	0.00	-0.16	0.03	0.18	0.01	-0.92	0.01	0.00	0.02	0.00	-0.04	-0.04
12-13 imag.	-0.98	1.19	1.13	-1.53	0.04	0.17	0.01	0.00	-0.03	0.02	0.17	0.16
14	1.27	2.84	-0.85	-3.47	-0.10	-1.70	0.00	0.00	0.02	0.01	0.07	0.07

Table 5.10 (Continued)

Mode	Density Correlation		Vapor Flow	Steady State Holdups			Plate Area
	a_{RHO}	b_{RHO}	K	$\bar{h}_{11}$	$\bar{h}_0$	$\bar{h}_1-\bar{h}_{10}$	A_T
1	0.00	0.00	0.00	-0.80	-0.03	-0.16	0.00
2	-0.02	0.01	-0.02	-1.07	0.04	0.04	0.01
3	0.08	-0.03	0.08	-0.04	-0.47	-0.55	-0.01
4	-0.02	0.01	-0.01	-0.03	-0.40	-0.55	0.00
5	-0.09	0.04	-0.08	-0.01	-0.43	-0.40	-0.08
6	0.01	-0.01	0.01	-0.01	-0.22	-0.77	0.01
7	-0.05	0.02	-0.05	-0.01	-0.06	-0.82	-0.06
8-9 real	-0.10	0.04	-0.09	0.00	-0.11	-0.77	-0.02
8-9 imag.	-0.12	0.05	-0.10	0.00	-0.04	0.62	-0.48
10-11 real	0.10	-0.04	0.09	0.00	0.12	-0.23	-0.96
10-11 imag.	-0.04	0.02	-0.02	0.00	0.02	-0.17	0.17
12-13 real	0.00	0.00	0.00	-0.00	0.01	-0.05	-0.93
12-13 imag.	0.03	-0.01	0.03	0.00	0.06	0.10	-0.18
14	0.03	-0.01	0.02	0.00	0.12	0.58	-1.71

C. Calculated and Experimental Transient Response

Transient response of the state variables calculated with Model 1 can be used to evaluate the accuracy of the model through comparisons with experimental response data. In this work responses to step changes of inputs are calculated by summation of the contributions of the modes according to Eqs. (2.14) and (A.1.9), even though the usual and more direct procedure for finding transient response is by integration of the original differential equations. The use of the modes in the response calculation provides a check on the entire computational procedure. Distillation response to a step input can be determined alternately by the evaluation of the initial and final steady states. The difference between the state vectors at these two steady states is used as an initial condition, and the column can be treated as an autonomous system that decays to its (final) steady state. This procedure is built into the computer programs as an option but has not been used here.

While the response of the entire state vector (holdups, compositions, and temperatures) has been calculated for step changes at time zero of all six of the inputs for Model 1, only the composition responses are considered here. They are presented in Figs. 5.7 - 5.12. The initial steady state is case A-10, which was described in the first section of this chapter, and the magnitudes of the step changes are given in Table 5.7. The ordinates are labeled "change in state variable", but in every case this can be interpreted as "change in composition." The responses are mole fraction changes from initial steady state and are identified by x_0 through x_{11} for reboiler through accumulator compositions, but

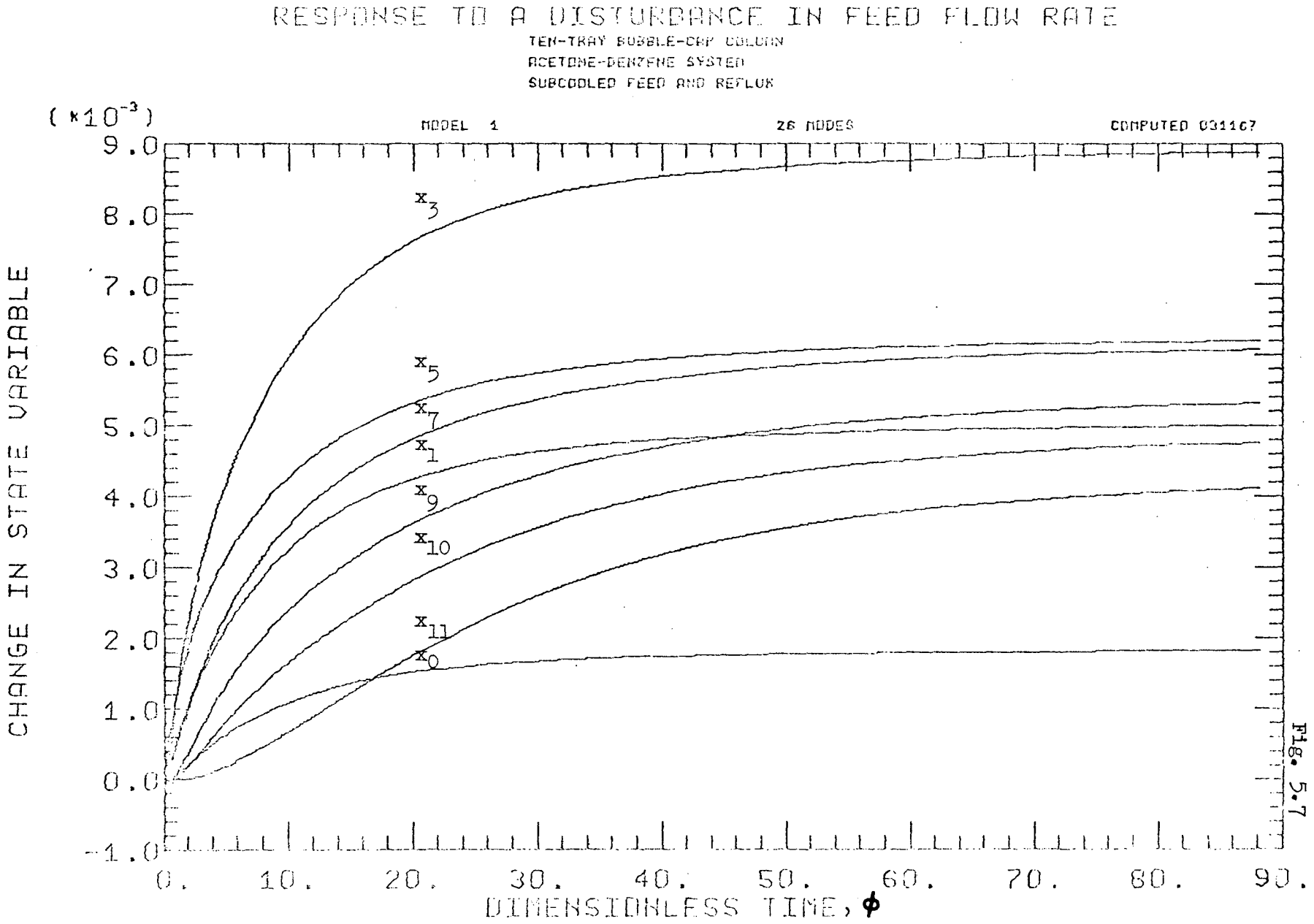

RESPONSE TO A DISTURBANCE IN FEED FLOW RATE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 1
26 NODES
COMPUTED 031167
(x10^-3)
CHANGE IN STATE VARIABLE
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
x3
x5
x7
x1
x9
x10
x11
x0
0.
10.
20.
30.
40.
50.
60.
70.
80.
90.
DIMENSIONLESS TIME, φ

Fig. 5.7

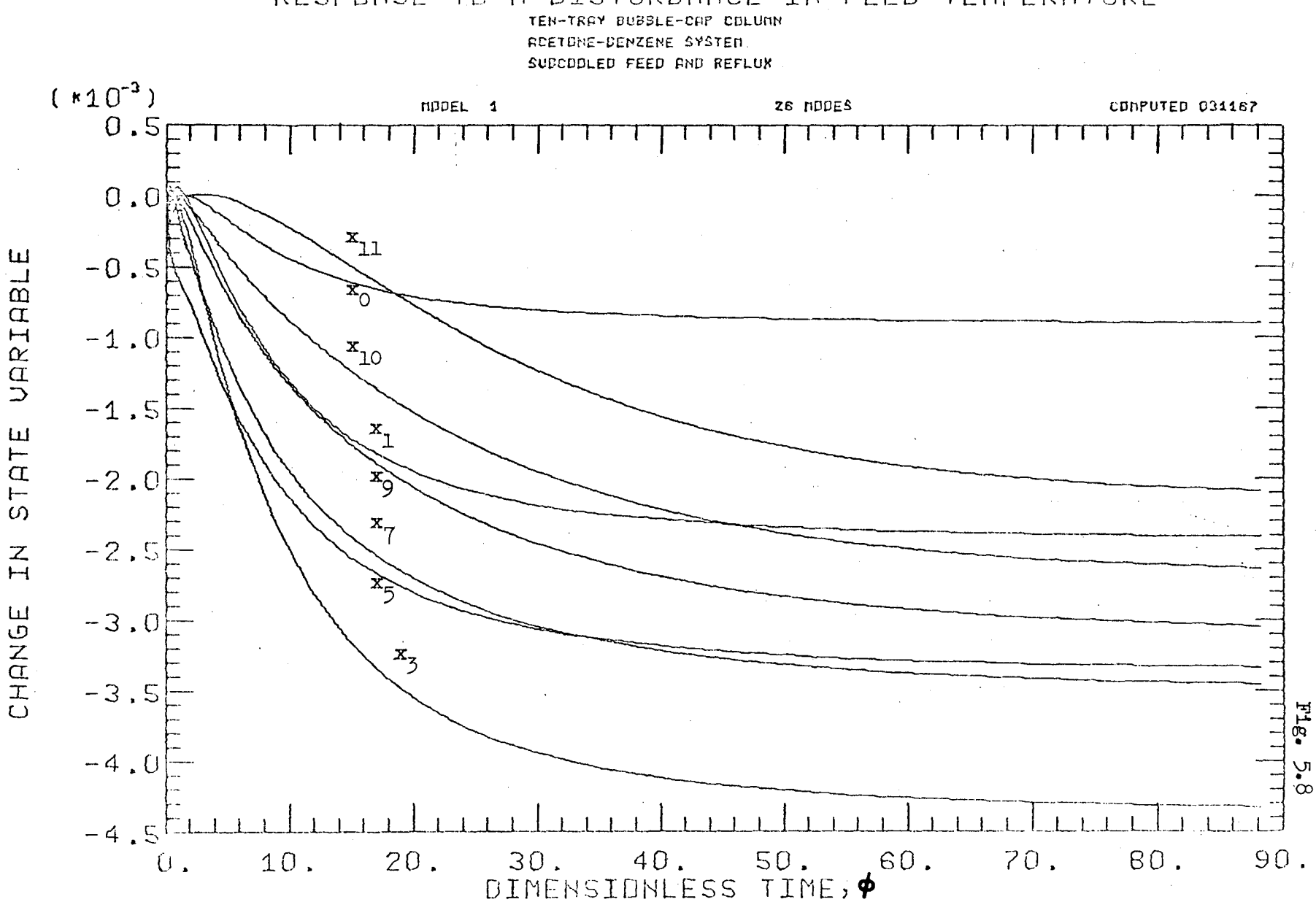

RESPONSE TO A DISTURBANCE IN FEED TEMPERATURE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 1
26 NODES
COMPUTED 031167
(×10⁻³)
CHANGE IN STATE VARIABLE
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
-4.0
-4.5
x11
x0
x10
x1
x9
x7
x5
x3
0.
10.
20.
30.
40.
50.
60.
70.
80.
90.
DIMENSIONLESS TIME, φ

Fig. 5.8

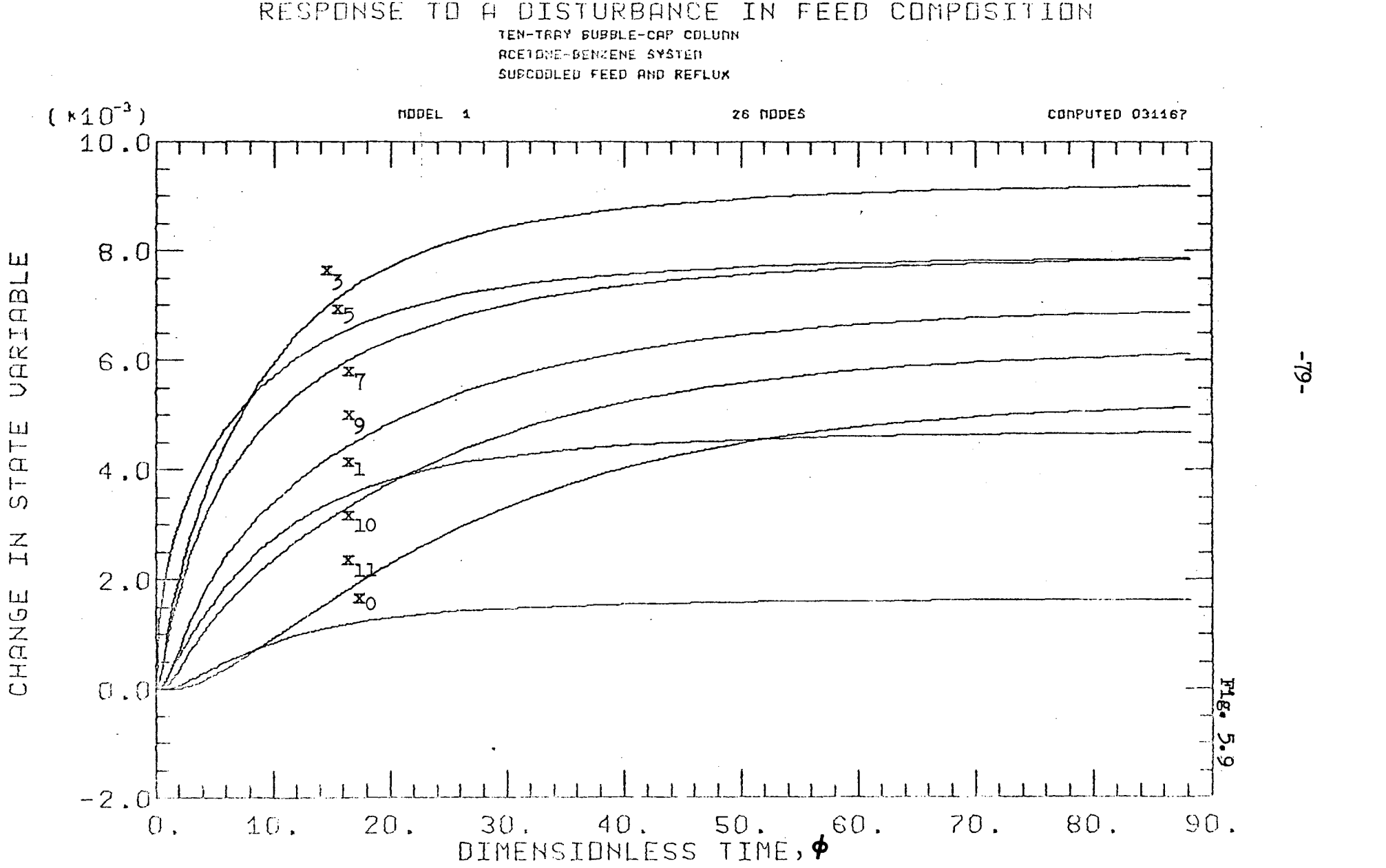

RESPONSE TO A DISTURBANCE IN FEED COMPOSITION
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 1
26 NODES
COMPUTED 031167
(x10^-3)
CHANGE IN STATE VARIABLE
10.0
8.0
6.0
4.0
2.0
0.0
-2.0
x3
x5
x7
x9
x1
x10
x11
x0
0.
10.
20.
30.
40.
50.
60.
70.
80.
90.
DIMENSIONLESS TIME, φ

Fig. 5.9

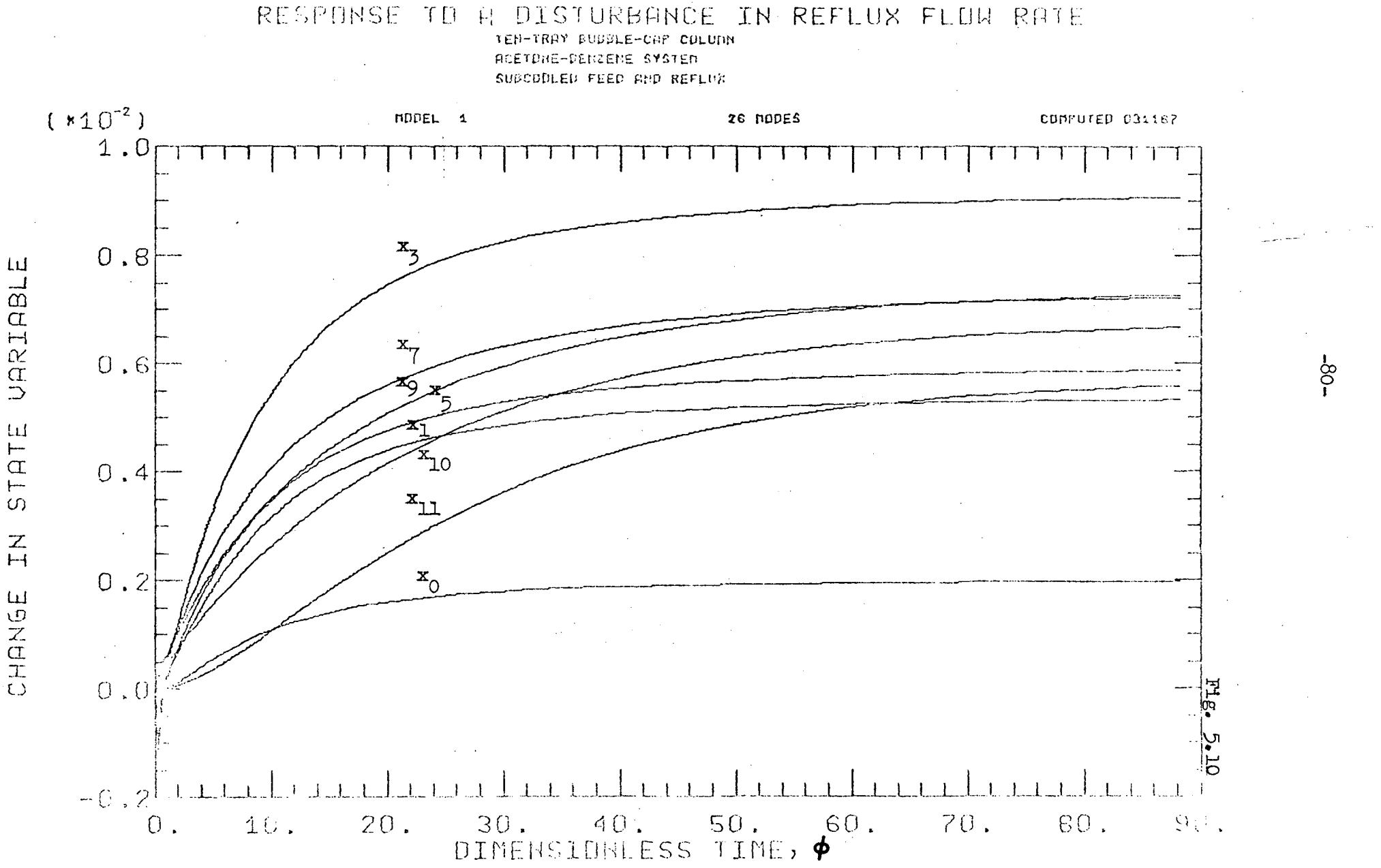

RESPONSE TO A DISTURBANCE IN REFLUX FLOW RATE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
(*10^-2)
MODEL 1
26 NODES
COMPUTED 031187
CHANGE IN STATE VARIABLE
1.0
0.8
0.6
0.4
0.2
0.0
-0.2
x3
x7
x9
x5
x1
x10
x11
x0
0.
10.
20.
30.
40.
50.
60.
70.
80.
DIMENSIONLESS TIME, φ

Fig. 5.10

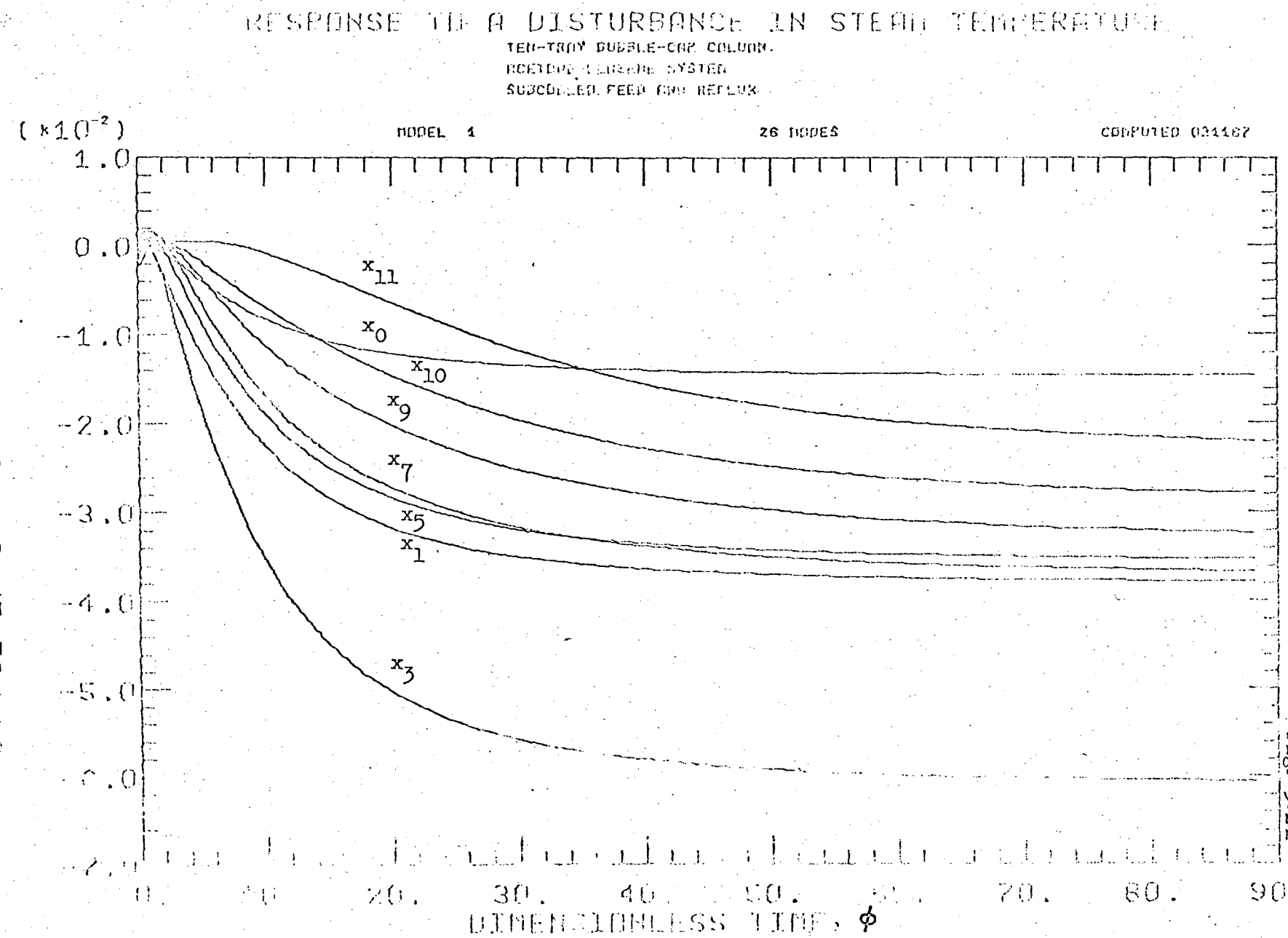

RESPONSE TO A DISTURBANCE IN STEAM TEMPERATURE
TEN-TRAY BUBBLE-CAP COLUMN
SUBCOOLED FEED AND REFLUX
(x10⁻²)
MODEL 1
26 MODES
COMPUTED 031187
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
x11
x0
x10
x9
x7
x5
x1
x3
0.
10.
20.
30.
40.
50.
70.
80.
90.
DIMENSIONLESS TIME, φ

Fig. 5.11

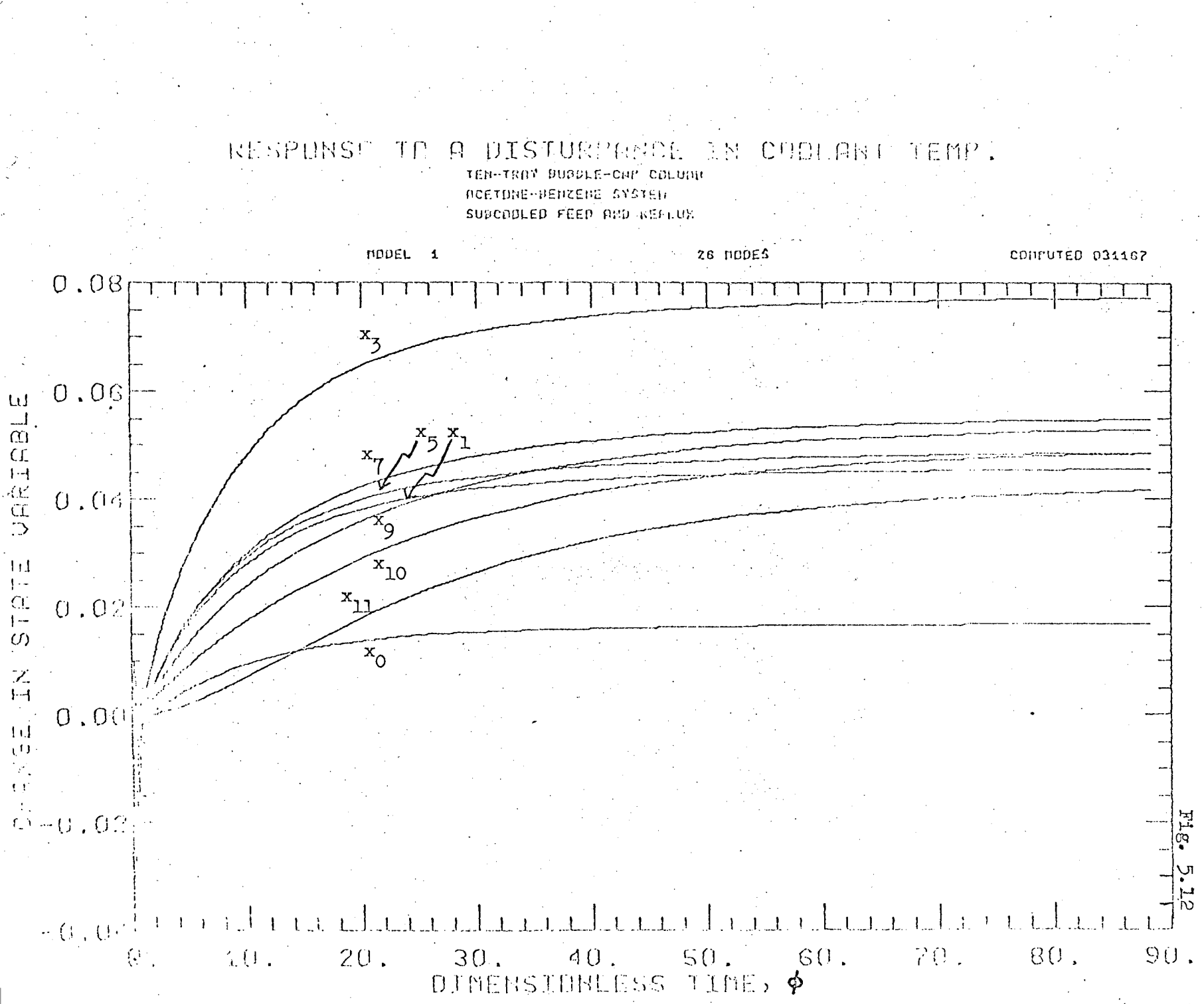

RESPONSE TO A DISTURBANCE IN COOLANT TEMP.
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 1
26 MODES
COMPUTED 031167
0.08
0.06
0.04
0.02
0.00
-0.02
-0.0
DEVIATION IN STATE VARIABLE
x_3
x_5
x_1
x_7
x_9
x_{10}
x_{11}
x_0
0.
10.
20.
30.
40.
50.
60.
70.
80.
90.
DIMENSIONLESS TIME, ϕ

Fig. 5.12

not every plate is included. The heading "26 modes" indicates that the contributions of 26 modes were included in the calculation of the response, and therefore only the eight shortest-lived modes were ignored. In all cases the activations of the modes neglected were small enough to justify this. The dimensionless time used for the abscissa can be converted to time in minutes through multiplication by 0.424. At very small times some of the response graphs indicate erratic behavior. This results from slight errors in a few of the intermediate modes that are highly activated and is a symptom of the problem of nearly identical modes that is discussed in Appendix A.2. Fortunately these modes die away very quickly and do not influence the long time response.

Luyben, Verneuil and Gerster[33] present experimental composition responses to step disturbances in feed flow rate, feed composition, reflux flow rate and vapor boilup rate. These data may be compared with Figs. 5.7, 5.9, 5.10, and 5.11 respectively. For the purposes of this work an exact quantitative comparison is not needed. In fact close agreement cannot be expected because pressure in the experimental column was held constant during transients by the introduction of nitrogen to the accumulator, while no attempt was made to restrict pressure changes artificially in Model 1. Responses have been calculated for Model 1 with a simulated pressure controller that receives a measurement of condenser pressure and manipulates coolant temperature proportionally. However, such a controller does not satisfactorily simulate the nitrogen injection, even though it eliminates approximately ninety percent of the uncontrolled pressure variation.

The calculated responses of the uncontrolled column agree semi-quantitatively with the experimental responses. For instance, in all cases the experimental column has nearly reached its new steady state

after 20 minutes (47 on the dimensionless scale used here), and the simulated column behaves likewise. After a step change in the feed composition (Fig. 5.9), the initial slope of the feed plate response is the steepest, and the accumulator and reboiler responses are the least steep, while the slopes of the other initial responses lie in between. The farther a plate is from the feed plate, the more its response is delayed.

Responses to steps in feed flow rate and reflux flow rate also show agreement in all principal trends, but response to a step in steam temperature (Fig. 5.11) cannot easily be compared with the experimental response to a step change in boilup rate. Figure 8 of Luyben, Verneuil, and Gerster[33] shows increasing compositions following what is claimed to be an increase in boilup rate, but the change must actually have been a step decrease. Also, it seems that a true step change in boilup rate was not even approximated in the experiment because after twenty minutes the compositions still rise at a nearly constant and appreciable rate. The most interesting behavior of the calculated response for this case is the very slight rise in the accumulator composition followed by a very gradual fall after about three minutes. The experimental reflux composition seems to follow the same course.

The directions in which compositions move after process upsets depend primarily on the relative magnitudes of changes in liquid and vapor flows (changes in reflux ratio). The calculated compositions follow expected trends. The changes in temperatures and holdups are not shown, but they also seem reasonable. There are no experimental data with which temperature or holdup responses may be compared.

It may be concluded that Model 1 predicts composition responses that compare favorably with available experimental responses. It also predicts other response behavior that is not confirmed experimentally but is in agreement with intuitive expectations.

D. Modes of Simplified Models

The modes of Models 3 and 4 are examined in order to evaluate the usefulness of these models, and also to uncover fundamental effects that are obscured in the more detailed model.

Model 4, which predicts only the behavior of compositions on each plate, has dominant modes as shown in Fig. 5.13 and eigenvalues as listed in Table 5.11 for the conditions of case A-10. The time constant of the slowest mode is quite close to the first time constant for case A-10-1. This mode resembles the composition portion of the first mode of Model 1, although the former has only small components for the bottom half of the column. It may be that the major difference between modes 1 of Model 4 and of Model 1 arises from the constant pressure condition of the former case. When pressure control is applied vapor flow below the feed plate becomes much less sensitive to disturbances, and the first mode of case A-10-1 resembles the first mode of A-10-4 quite closely.

The second mode of Model 4 has a time constant only half as large as the second mode of Model 1 and is not closely related to the accumulator. This is not surprising because the discussion in a previous section showed the second mode of Model 1 to be primarily a temperature mode. The subsequent time constants span the range of the modes referred to as hydraulic modes in Model 1. However, in Model 4 there

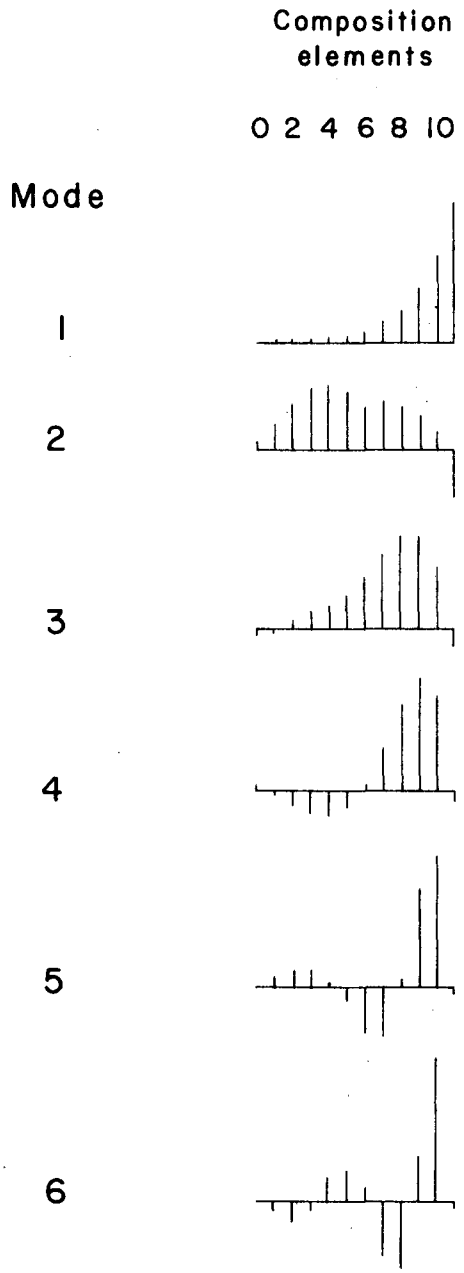


Fig. 5.13 Modes for case A-10-4, no control.

Table 5.11. Eigenvalues and Time Constants

Case A-10-4, No Control

Mode	Eigenvalue (dimensionless), λ	Time Constant (min), τ^*
1	-0.0485	8.75
2	-0.206	2.06
3	-0.650	0.652
4	-1.33	0.319
5	-3.02	0.141
6	-4.87	0.0871
7	-7.09	0.0598
8	-9.52	0.0446
9	-11.6	0.0366
10	-13.1	0.0324
11	-17.2	0.0247
12	-21.8	0.0195

* $\tau = -0.424/\lambda'$

Table 5.12. Activation of Modes by Step Change in Feed Composition

Case A-10-4, No Control

$x_F = 0.0050$

Mode	Activation
1	0.01311
2	0.007261
3	0.006218
4	-0.002873
5	-0.001586
6	0.001635
7	-0.0003325
8	-0.0005367
9	-0.0006587

can only be composition modes, and therefore many or all of the Model 1 modes in this range arise from interactions between hydraulic effects and component accumulation effects. The very fast modes do not appear in Model 4 at all.

The components of the first mode of Model 4 all have the same sign, while successive modes have components that alternate in sign between the reboiler and the accumulator. Each mode has one more alternation of sign than the preceding one, a trend that was noted, but with less regularity, for Model 1.

The only possible input, feed composition, activates mainly the dominant mode with each successively faster mode activated somewhat less than the preceding one (see Table 5.12).

The response curves are shown in Fig. 5.14 and are very similar to the composition responses for Model 1 except for the final steady state that is approached.

Model 3 incorporates a description of column hydraulics, but, as shown in Appendix A.3, the composition modes and the flow modes are completely decoupled. The composition modes are the same as the modes of Model 4, while all ten hydraulic modes are identical because of the form of the state matrix. They have a time constant of 0.0459 minutes, as shown in Table 5.13.

The degenerate situation caused by the identical flow modes was discussed in Chapter II and is demonstrated in Appendix A.2. For Model 1 the flow modes are distinct because of interactions with thermal and composition effects. However, these modes have closely spaced time constants, and the associated condition numbers are large. Furthermore, they have a tendency to resemble the identical hydraulic modes of

Fig. 5.14

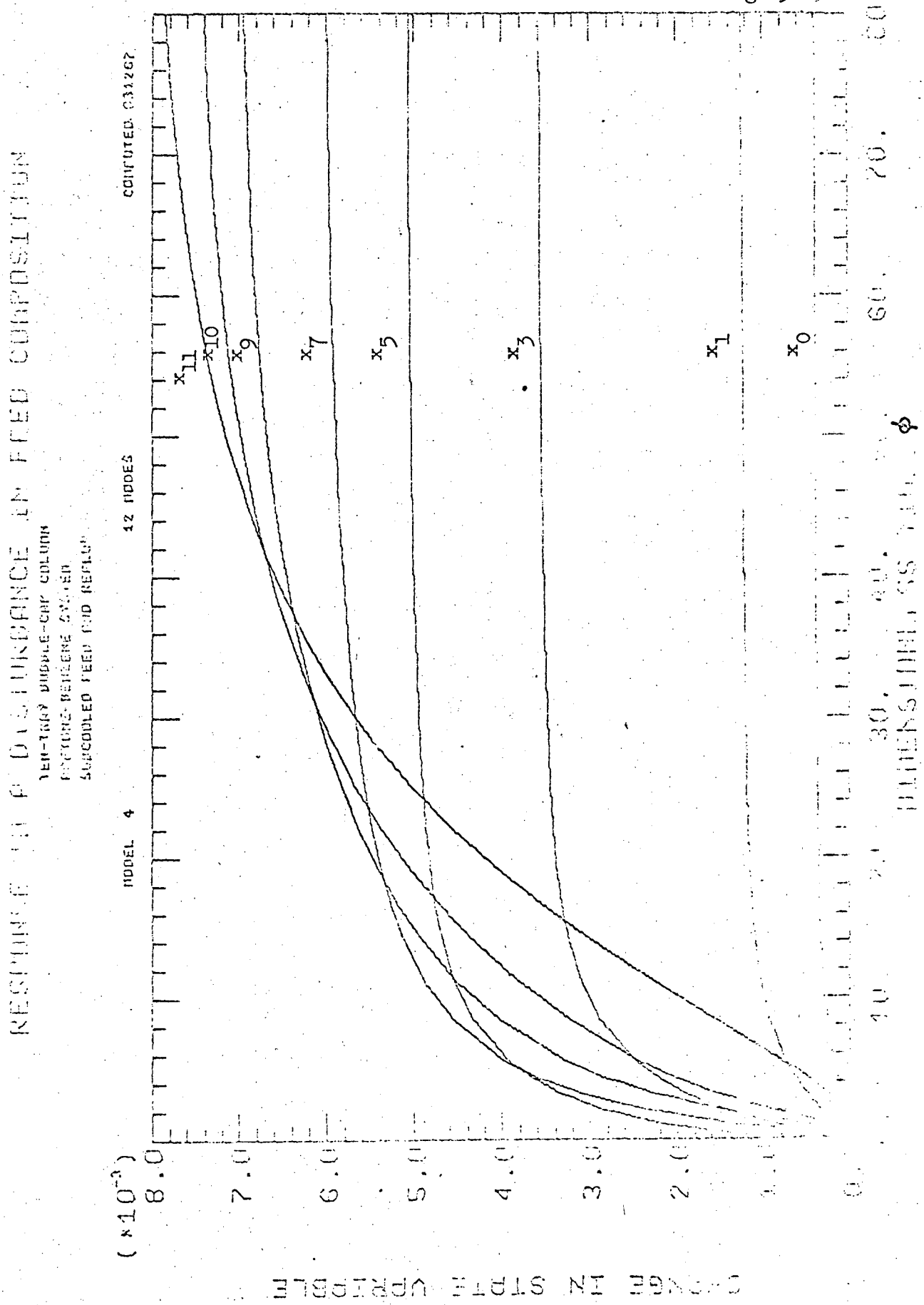

RESPONSE OF THE DISTILLATE TO FEED COMPOSITION
TEN-TRAY BUBBLE-CAP COLUMN
BENZENE-TOLUENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 4
12 NODES
COMPUTED RESPONSE
x_{11}
x_{10}
x_9
x_7
x_5
x_3
x_1
x_0
$(\times 10^{-3})$
8.0
7.0
6.0
5.0
4.0
3.0
2.0
0.
30.
60.
90.
120.
150.
180.
ϕ
CHANGE IN STATE VARIABLE

Table 5.13. Eigenvalues and Time Constants
Case A-10-3, No Control

Mode	Dimensionless Eigenvalue, λ	Time Constant, Minutes, τ^*
1	-0.0485	8.75
2	-0.206	2.06
3	-0.650	0.652
4	-1.33	0.319
5	-3.02	0.141
6	-4.87	0.0871
7	-7.09	0.0598
8-17	-9.25	0.0459
18	-9.52	0.0446
19	-11.6	0.0366
20	-13.1	0.0324
21	-17.2	0.0247
22	-21.8	0.0195

* $\tau = -0.424\ \lambda'$.

All significant eigenvector elements for vectors 1-7 are like those of Case A-10-4 eigenvectors.

Table 5.14. Activation of Modes for Step Input
Case A-10-3, No Control

Mode	Input Variable and Magnitude of Step				
	f = 0.00940	t_f = 0.0154	x_F = 0.0050	ℓ_{11} = 0.0100	t_s = 0.0202
1	0.04215	-0.05953	0.01311	0.01662	-0.02785
2	0.03164	-0.04469	0.007261	0.01370	-0.02723
3	0.01215	-0.01716	0.006218	0.001782	-0.001907
4	-0.01781	0.02516	-0.002873	-0.006917	0.01676
5	0.05751	-0.08122	-0.001586	0.02934	-0.07208

Model 3; the only large holdup components are those corresponding to plates near the bottom of the column.

State variable responses for Model 3 are not presented because only the first seven modes can be treated by methods developed here, and these are identical to modes of Model 4. However Model 3 does incorporate five inputs, and therefore the activations of the dominant modes by step changes are of interest and are shown in Table 5.14. Modes other than the slowest are activated significantly in every case, but the first mode is always important. The relatively large activation of the fifth mode contrasts with the activations found for modes of Model 1 that have time constants of similar magnitude. This discrepancy and its possible consequences has not been investigated.

Although Models 3 and 4 demonstrate the basis for the prevailing effects for most of the modes of Model 1, they do not resolve the question of which formulation is most appropriate for describing distillation dynamics. It is possible that Model 1 contains more detail than is necessary; perhaps some of the enthalpy balances and secondary relationships could be omitted. However, Model 1 avoids the inconsistencies presented by simpler models, and all inputs are easily treated.

E. Effect of Reboiler and Accumulator Holdup

There are many examples of dynamic studies of distillation columns in which the holdups of the reboiler and accumulator used in the model were either negligible or equal to the holdup on a single plate.[8,13,46] This is not ordinary practice with industrial columns, and the recurring use of this simplification in simulation suggests that the significance of liquid holdup in determining the major dynamic effects has not been fully appreciated.

The effect of small accumulator and reboiler holdups is investigated by examination of the modes of case B-10-1, which is identical to A-10-1 except that the reboiler and accumulator holdups are approximately equal to plate holdups at steady state. The eigenvalues and time constants of the dominant modes for case B-10-1 are listed in Table 5.15. The first time constant is 3.12 minutes compared to 9.37 minutes for case A-10-1. In Fig. 5.15, which shows the six slowest modes, the dominant mode can be seen to remain a composition mode much like case A-10-1.

Of the six slowest modes, only mode 6 bears any resemblance to the mode that is associated with the accumulator in case A-10-1. The time constant for mode 6 is 0.169 minutes, while the change-of-inventory time, τ_A, for the accumulator is 0.162 minutes. It appears that this mode is associated to a large degree with the accumulator, which probably behaves as a nearly decoupled tank again. However some composition effects are combined in mode 6.

A few eigenvalue sensitivities are given in Table 5.16 to further substantiate the nature of the modes, and it can be seen that only mode 6 is very sensitive to changes in accumulator holdup. Reboiler holdup has little effect on any mode, but the cumulative effect of changes in all ten plate holdups is significant, especially for the first three modes. The coefficient in the plate hydraulics correlation and the plate area are important in the third or fourth modes, as well as some faster modes, whereas for case A-10-1 the slowest mode influenced is the eighth.

To complete the picture, activations of the dominant modes by step changes of inputs are listed in Table 5.17. The activation of the first mode is significant for all six inputs and therefore it governs the response at long times. The response to a step change in feed composition

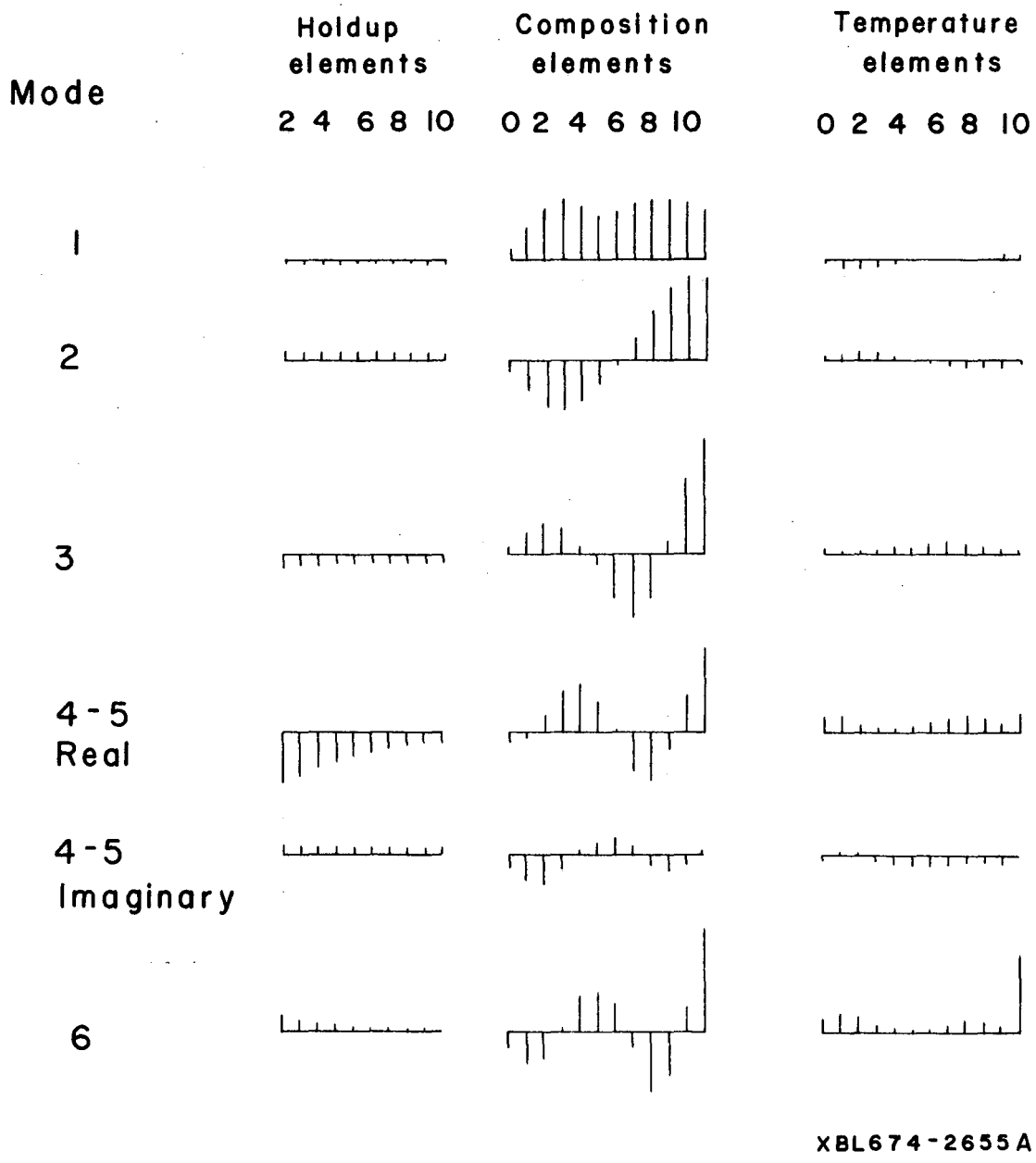


Fig. 5.15 Modes for case B-10-1.

Table 5.15. Eigenvalues and Time Constants
Case B-10-1 (No Control)

Mode	Eigenvalue (dimensionless), λ	Time Constant (min), τ^*
1	-0.136	3.12
2	-0.509	0.833
3	-1.43	0.296
4	-1.96 + 0.347i	0.216
5	-1.96 - 0.347i	0.216
6	-2.51	0.169
7	-3.36	0.126
8	-4.15 + 3.36i	0.102
9	-4.15 - 3.36i	0.102
10	-4.21	0.101

* $\tau = -0.424/\lambda'$.

Table 5.16. Eigenvalue Sensitivities to Values of Parameters
Case B-10-1 (No Control)

	Steady State Holdups			Hydraulics	Plate Area
Mode	$\bar{h}_{11}$	$\bar{h}_0$	$\bar{h}_1-\bar{h}_{10}$	α	A_T
1	-0.03	-0.02	-0.97	0.00	0.01
2	-0.12	-0.02	-0.96	0.03	0.03
3	-0.28	0.03	-0.98	0.32	0.32
4-5 real	0.02	-0.15	-0.28	-0.67	-0.67
4-5 imag.	-0.08	0.05	0.01	0.10	0.10
6	-1.08	0.01	0.09	0.13	0.13
7	-0.05	-0.04	-0.75	-0.15	-0.15
8-9 real	-0.01	-0.08	-0.02	-0.89	-0.89
8-9 imag.	0.00	0.02	0.26	-0.34	-0.34
10	-0.30	0.02	-0.60	-0.04	-0.04

Table 5.17. Activation of Modes by Step Inputs
Case B-10-1 (No Control)

Mode	Input Variable and Magnitude of Step					
	f = 0.00940	t_F = 0.0154	x_F = 0.0050	ℓ_{11} = 0.0100	t_s = 0.0202	t_{CW} = 0.0155
1	0.02219	-0.01339	0.02596	0.02703	-0.1742	0.2253
2	-0.005558	0.003953	-0.003515	-0.006151	0.08407	-0.07528
3	-0.001127	-0.006683	-0.001856	0.008585	-0.1333	0.08696
4-5 real	-0.0008109	0.004008	0.001831	-0.01149	0.1053	-0.1699
4-5 imag.	0.01235	0.02682	-0.003505	-0.01266	0.3485	-0.01988
6	0.0006127	0.0006752	-0.0004018	0.001758	0.001683	0.05749
7	0.005070	0.006845	0.0009998	0.002045	0.08745	0.08423

is chosen as representative of responses predicted by case B-10-1 and is shown in Fig. 5.16.

In summary, the small reboiler and accumulator holdups cause the column response to be considerably more rapid than the response of the conventional column. Furthermore, the parameters associated with the plates are much more important in determining the response characteristics.

It would be unwise to use the results of models that treat reboiler and accumulator holdups as small for the prediction of the dynamic behavior of real columns in which these holdups are usually large, because the influence of holdup is very significant. However, it may be advantageous to change column design to reduce the amount of reboiler and accumulator holdup. If the large reboiler and accumulator are used merely for the purpose of averaging disturbances in the product streams, this should be accomplished instead by mixing tanks external to the distillation system.

F. Effect of Number of Plates

In this section the effect of the number of plates on the character of the modes, and especially on the magnitude of the dominant mode time constant is investigated. For this purpose modal decomposition is carried out with cases A-5-1 and A-3-1, which are identical to A-10-1, except that five plates and three plates, respectively, are used. The eigenvalues and time constants are given in Tables 5.18 and 5.19, and the modes for case A-3-1 are shown in Fig. 5.17; those for case A-5-1 are not shown because they are not significantly different. The modes of the small columns are very similar to the modes of the ten-plate column and therefore need not be examined in detail. In every case

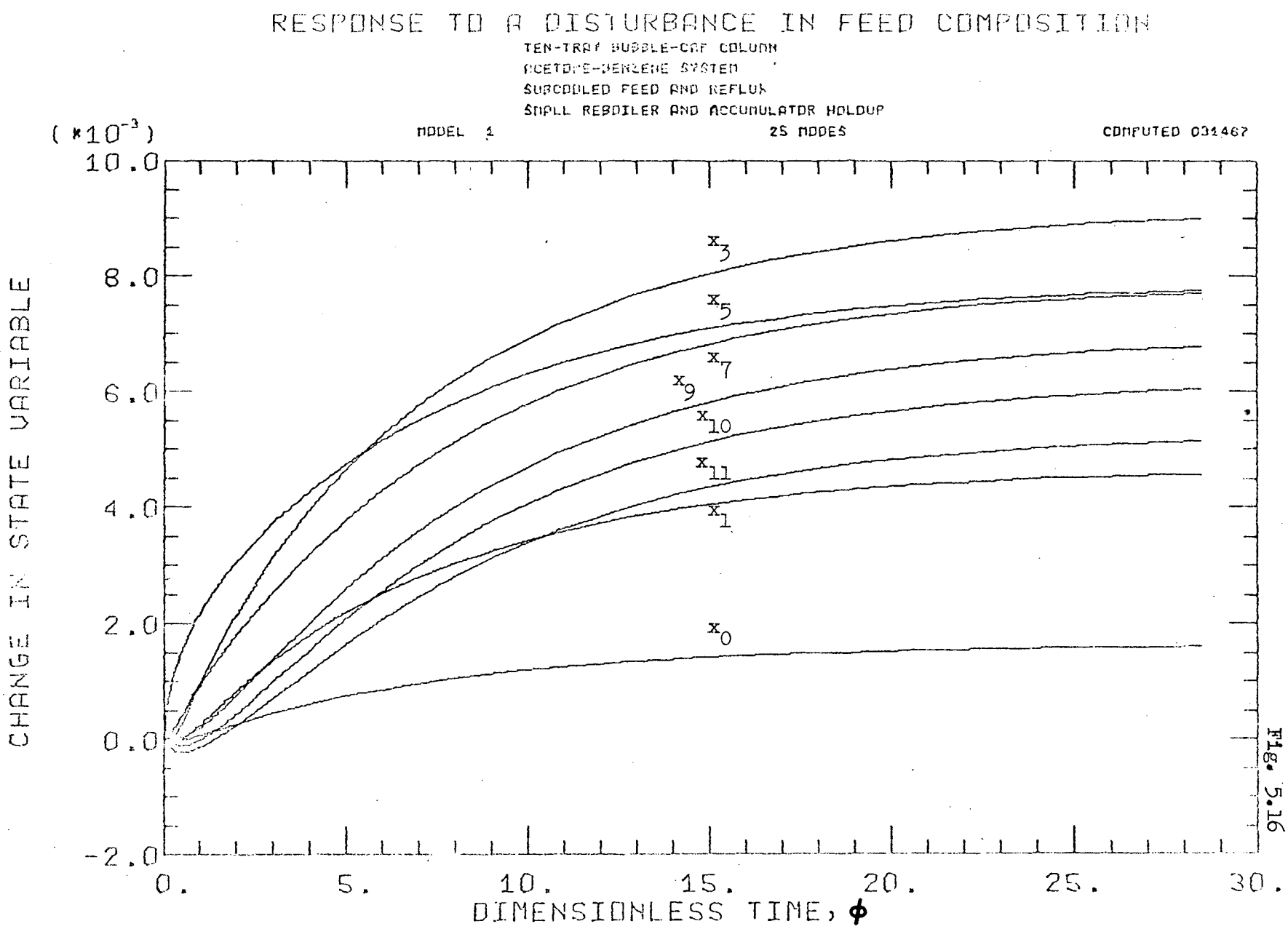

RESPONSE TO A DISTURBANCE IN FEED COMPOSITION
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
SMALL REBOILER AND ACCUMULATOR HOLDUP
MODEL 1
25 MODES
COMPUTED 031467
(*10^-3)
CHANGE IN STATE VARIABLE
10.0
8.0
6.0
4.0
2.0
0.0
-2.0
0.
5.
10.
15.
20.
25.
30.
DIMENSIONLESS TIME, φ
x3
x5
x7
x9
x10
x11
x1
x0

Fig. 5.16

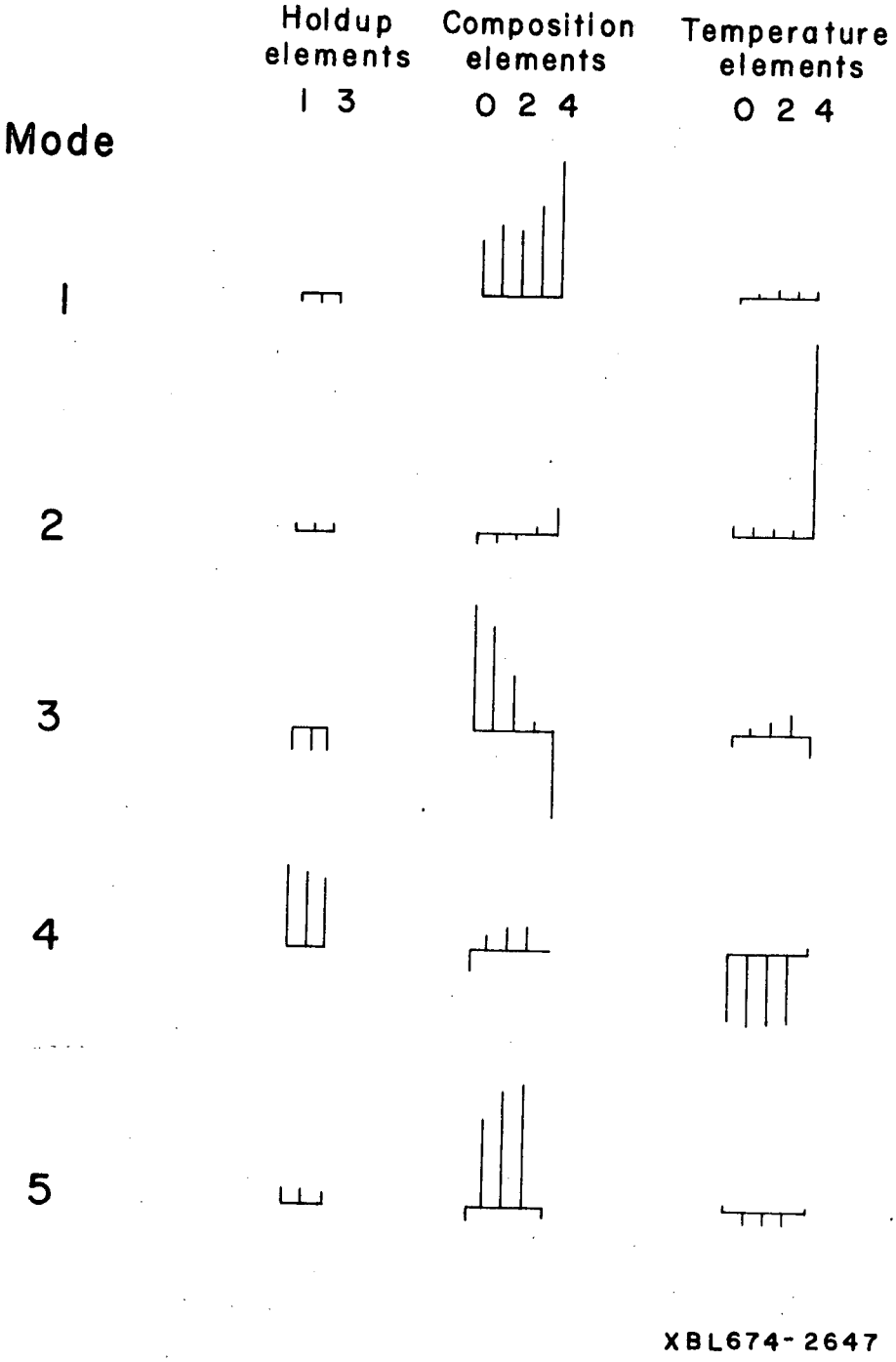


Fig. 5.17 Modes for case A-3-1.

Table 5.18. Eigenvalues and Time Constants
Case A-5-1, No Control

Mode	Dimensionless Eigenvalue, λ	Time Constant, minutes, τ^*
1	-0.0518	8.18
2	-0.107	3.96
3	-0.141	3.01
4	-1.03	0.412
5	-1.13	0.375
6	-3.10	0.137
7	-5.68	0.0746
8	-7.53 + 2.10i	0.0563
9	-7.53 - 2.10i	0.0563
10	-8.84	0.0480
11	-10.3 + 2.25i	0.0411
12	-10.3 - 2.25i	0.0411
13	-11.7	0.0362
14	-14.0	0.0302
15	-218	0.00194
16	-1540	0.000275
17	-3650	0.000116
18	-5940	0.0000714
19	-8880	0.0000477

* $\tau = -0.424/\lambda'$.

Table 5.19. Eigenvalues and Time Constants
Case A-3-1, No Control

Mode	Dimensionless Eigenvalue, λ	Time Constant, minutes, τ^*
1	-0.0530	8.00
2	-0.106	4.00
3	-0.151	2.81
4	-1.26	0.337
5	-2.00	0.212
6	-6.18	0.0686
7	-8.58 + 0.708i	0.0494
8	-8.58 - 0.708i	0.0494
9	-10.7	0.0396
10	-11.8	0.0359
11	-483	0.000878
12	-3410	0.000124
13	-6900	0.0000615

*$\tau = -0.424/\lambda'$.

mode 2 has a large accumulator temperature element and almost exactly the same time constant.

According to the discussion in previous sections, the largest time constant is determined to a great extent by the total liquid holdup, and consequently the columns with fewer plates would be expected to have only slightly smaller dominant time constants. The values are 8.00, 8.18, and 9.37 minutes for the three, five, and ten plate columns respectively, and the corresponding total holdups are 34.5, 36.3, and 40.5 moles at steady state. The ratios of the time constants are nearly the same as the ratios of the holdups, and on this basis the dominant time constant seems to increase linearly with the number of plates.

The linear dependence of the dominant time constant on number of plates is not consistent with the results of Pigford[46] and Lamb, Pigford and Rippin,[32] who concluded that the dominant time constant should increase approximately with the square of the number of plates. However this conclusion is based on columns with no holdup in the condenser-accumulator and either zero holdup in the reboiler, or holdup equal to that on a plate. The calculations of the authors cited above were performed with models somewhat like Model 4. In this work, similar calculations were made, but the results are inconclusive. With Model 1 it appears that the dominant mode time constant may depend on the square of the number of plates for large columns (20 plates or more) when reboiler and accumulator holdups are small. However, with fewer plates the dependence is nearly linear. If the dominant time constant ever does depend on the square of the number of plates, this must occur when the total liquid holdup on the plates is large compared to the combined accumulator and reboiler holdups; a condition that is probably seldom met in practice.

G. Effect of Operating Conditions

In this section the effects of reflux flow rate, feed flow rate (column throughput), and the purity of the products on the nature of the distillation column modes and their time constants are examined. These effects are considered in order to determine whether conclusions about the modes that were based on case A-10-1 need to be modified when operating conditions are changed.

When the reflux rate is increased by a factor of five compared to case A-10-1, the modes are as shown in Fig. 5.18, with time constants as given in Table 5.20. The large reflux rate results in high internal circulation rate so that composition disturbances are transmitted through the column more rapidly than for case A-10-1. The dominant time constant is only 5.14 minutes, compared to 9.37 minutes for case A-10-1. Dominant time constants for all of the cases studied are summarized in Table 5.21. The modes for this high reflux rate case (C-10-1) are not greatly different from those of A-10-1 except that they have shorter time constants and more significant holdup elements.

Much slower responses result for case D-10-1, which has a steady state feed flow rate one-fifth as large as that for A-10-1 but an undiminished reflux rate. The eigenvalues and time constants are given in Table 5.22, and the modes in Fig. 5.19 where it can be seen that again the modes are similar in nature to those of case A-10-1. The dominant time constant is 37.2 minutes, larger than that of A-10-1 by a factor of four. The second mode (real part), which is associated with the accumulator, has a time constant of only 6.90 minutes, less than twice as large as the second time constant of A-10-1. However, the change-of-inventory time for the accumulator is 6.48 minutes, and

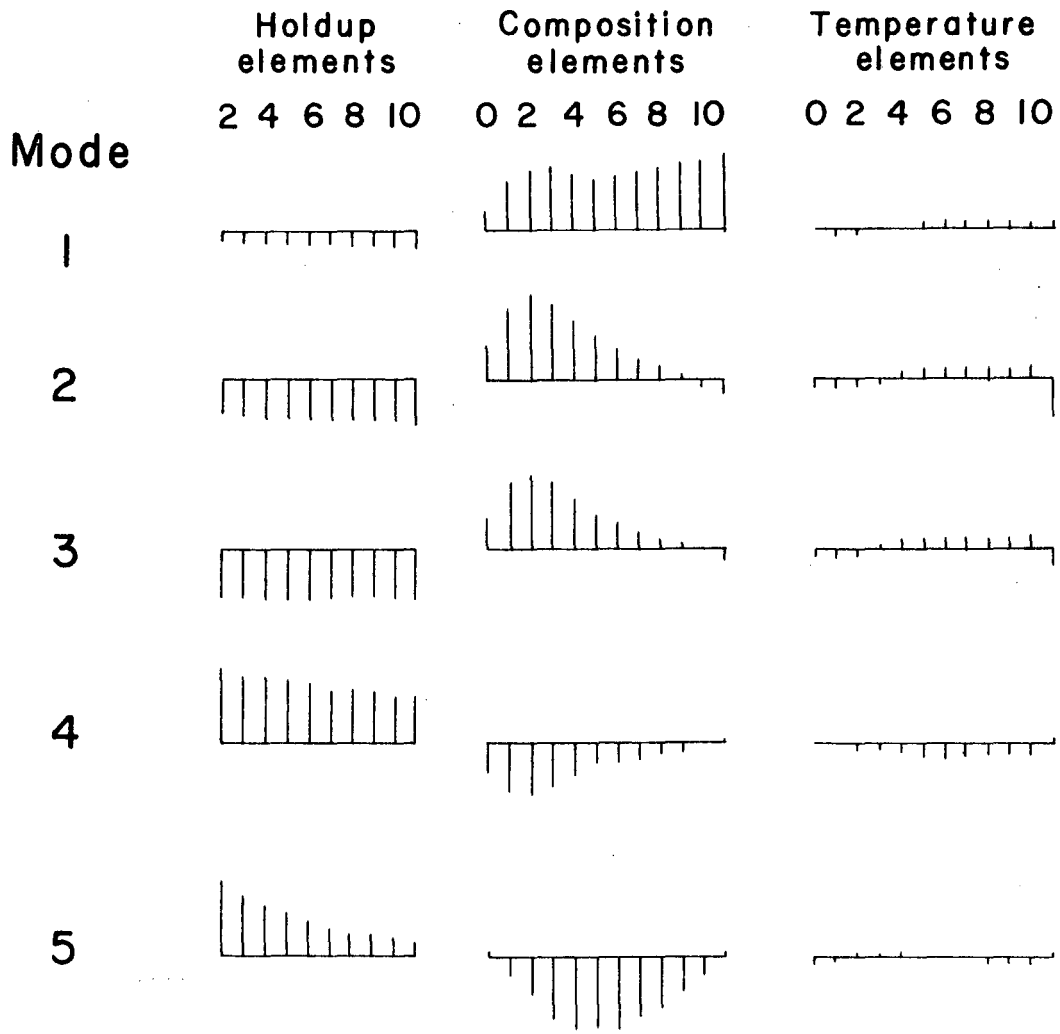


Fig. 5.18. Modes for Case C-10-1.

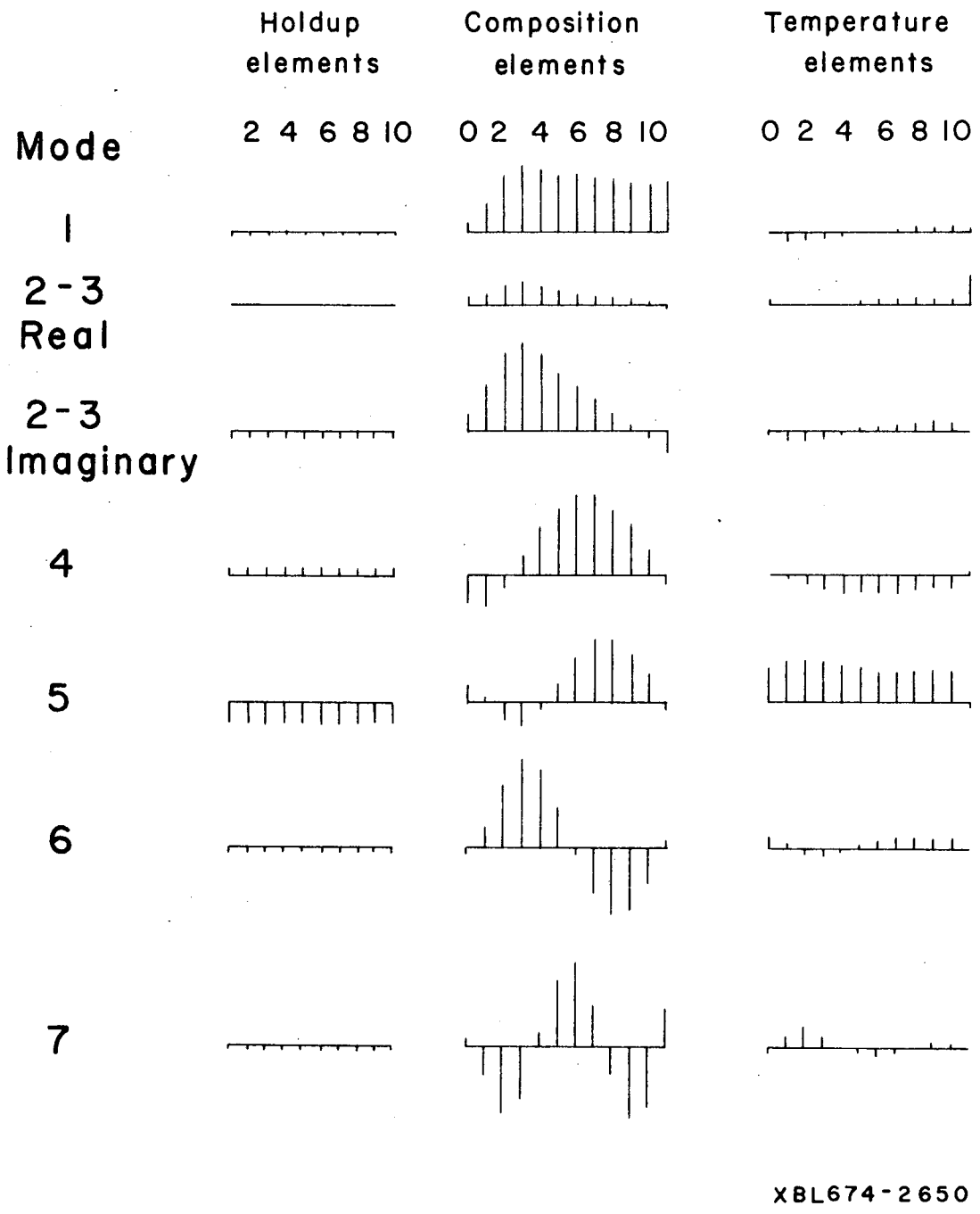


Fig. 5.19 Modes for Case D-10-1.

Table 5.20. Eigenvalues and Time Constants
Case C-10-1, No Control

Mode	Dimensionless Eigenvalue*, λ	Time Constant, minutes, τ**
1	-0.0165	5.14
2	-0.0717	1.18
3	-0.0898	0.944
4	-0.156	0.543
5	-0.331	0.256
6	-0.701 + 0.703i	0.121
7	-0.701 - 0.703i	0.121
8	-0.822	0.103
9	-1.35 + 1.08i	0.0627
10	-1.35 - 1.08i	0.0627
11	-1.81	0.0468

**$\tau = -0.848/\lambda'$.

* The dimensionless eigenvalues cannot be compared with other cases because they are non-dimensionalized with the high reflux rate (0.0800 moles/sec).

Table 5.21. Comparison of Time Constants

Mode	A-10-1 No Control	A-5-1 No Control	A-3-1 No Control	A-10-3 or A-10-4 No Control	A-10-1 Pressure Control	(Small Holdups) B-10-1 No Control	B-5-1 No Control
1	9.37	8.18	8.00	8.75	8.04	3.12	1.42
2	3.94	3.96	4.00	2.06	3.94	0.833	0.329
3	3.26	3.01	2.81	0.652	1.11	0.296	0.170
4	0.889	0.412	0.337	0.319	1.11	0.216	
5	0.542	0.375	0.212	0.141	0.582	0.216	
6	0.400	0.137	0.0686	0.0871	0.348	0.169	
7	0.201	0.0746	0.0494	0.0598	0.189	0.126	
8	0.107	0.0563			0.128	0.102	

Mode	B-3-1 No Control	(Large Reflux Rate) C-10-1 No Control	(Small Feed Rate) D-10-1 No Control	(Small Feed Rate and Reflux Rate) E-10-1 No Control
1	0.987	5.14	37.2	48.1
2	0.201	1.18	6.90	21.6
3	0.168	0.944	6.90	21.6
4		0.543	1.71	5.96
5		0.256	0.922	2.77
6		0.121	0.709	2.44
7		0.121	0.334	1.34
8		0.103	0.190	0.783

Table 5.22. Eigenvalues and Time Constants
Case D-10-1, No Control

Mode	Dimensionless Eigenvalue, λ	Time Constant, minutes, τ^*
1	-0.0114	37.2
2	-0.0615 + 0.00620i	6.90
3	-0.0615 - 0.00620i	6.90
4	-0.248	1.71
5	-0.460	0.922
6	-0.598	0.709
7	-1.27	0.334
8	-2.23	0.190
9	-3.08	0.138
10	-4.58 + 0.695i	0.0926
11	-4.58 - 0.695i	0.0926
12	-5.63 + 1.49i	0.0754
13	-5.63 - 1.49i	0.0754

$^*\tau = -0.424/\lambda'$

Table 5.23. Eigenvalues and Time Constants
Case E-10-1, No Control

Mode	Dimensionless Eigenvalue, λ	Time Constant, minutes, τ^*
1	-0.0480	48.1
2	-0.107 + 0.00669i	21.6
3	-0.107 - 0.00669i	21.6
4	-0.387	5.96
5	-0.833	2.77
6	-0.945	2.44
7	-1.72	1.34
8	-2.95	0.783
9	-4.09	0.564
10	-5.43	0.425

$^*\tau = -2.31/\lambda'$

therefore provides a good estimate of the second time constant.

The sensitivities of case D-10-1 eigenvalues to changes in selected parameters, shown in Table 5.24, also confirm that these modes are much like those of case A-10-1 (for which sensitivities are given in Table 5.10). However, in this case with low feed rate and high reflux ratio, the steady state plate holdups have a considerably greater effect on the first two eigenvalues, while the accumulator holdup has a correspondingly decreased influence.

When both the feed and reflux rate are reduced to one-fifth the values used for A-10-1, the time constants for the modes are approximately five times greater, as shown in Table 5.23. In nearly every respect, these modes (case E-10-1) are merely slower versions of the A-10-1 modes.

To determine the effect of a pinched region, the steady state product flow rates of case D-10-1 are changed slightly so that a very pure bottom product is produced. For such a case, the time constants associated with every mode but the first are close to those for D-10-1, but slightly smaller. However, the dominant time constant is 87.8 minutes, 2.36 times larger than that for D-10-1. The problem of a pinch caused by the requirement for a pure product was mentioned in Chapter IV, where the concern was for the nonlinearities introduced by such a pinch.[38] Although these nonlinear effects make response calculations for this pure product case invalid, it is still interesting to see the strong effect of the pinched region on the dominant time constant. The pinch results in a slower response because the compositions in the pinched region are relatively insensitive to disturbances. Consequently a long time is required to transmit a composition disturbance

Table 5.24 Eigenvalue Sensitivities to Values of Parameters
Case D-10-1, No Control

	Vapor-Liquid Equilibria				Activity Coefficients	Hydraulics	Vapor Flow	Heat of Vaporization	Heat Capacity
Mode	a_1	a_2	b_1	b_2	A_{12} and A_{21}	α	β	a_{VH}	a_{CP}
1	12.55	6.78	-9.60	-7.15	-0.05	0.00	0.01	-0.11	-0.07
2-3 real	3.51	-1.52	-7.01	1.52	0.15	0.00	0.00	-0.11	-0.05
2-3 imag	-3.72	-0.06	5.35	0.12	-0.02	-0.01	0.00	0.06	0.01
4	-8.67	-1.87	10.68	2.09	0.38	0.00	0.00	-0.06	0.00
5	-0.89	-0.60	1.07	0.64	0.07	-0.03	0.00	0.30	0.14
6	-1.96	-2.82	1.22	3.21	0.14	0.00	0.00	-0.07	0.02
7	-1.44	-3.89	0.42	4.59	0.17	0.00	0.00	-0.12	-0.01
8	-3.91	-3.89	3.11	4.39	0.15	0.06	0.00	-0.17	0.00
9	0.83	-3.59	-1.84	4.46	0.17	-0.11	0.00	-0.04	-0.03

Table 5.24 (Continued)

Mode	Density Correlation a_{RHO}	Vapor Flow κ	Steady State Holdups $\bar{h}_{11}$	$\bar{h}_0$	$\bar{h}_1 - \bar{h}_{10}$	Plate Area A_T
1	0.01	0.01	-0.64	-0.05	-0.29	0.01
2-3 real	0.02	0.02	-0.62	-0.14	-0.23	0.00
2-3 imag	0.01	0.01	-0.10	0.02	0.07	-0.01
4	-0.01	0.00	-0.04	-0.50	-0.46	0.00
5	-0.07	-0.05	-0.01	-0.49	-0.44	-0.03
6	0.01	0.01	-0.02	-0.23	-0.76	0.00
7	-0.01	-0.01	-0.01	-0.04	-0.93	0.00
8	0.03	0.02	0.00	-0.01	-1.05	0.06
9	-0.08	-0.06	0.00	-0.01	-0.80	-0.11

through a pinched region to the product stream. The disturbance tends to be held in the mid-region of the column where there is appreciable composition change on each plate.

The preceding sections have shown that the dominant mode time constant depends on column holdup, feed rate, reflux rate, number of plates, and the degree of separation attained, but in this work no attempt has been made to predict this time constant from information concerning the steady state. However, there have been some predictions for the effect of factors such as holdup, internal circulation rate, number of plates, and the nature of the equilibrium relationship on column time constants.[20a,36,38,46] Moczek, Otto, and Williams[38] use the concept of change of inventory, which successfully predicts the effect of pinched regions on the major time constant. Perhaps some of these results could be extended and used to estimate the dominant time constants calculated here. More fundamental methods for making such estimates are needed.

VI. DISTILLATION COLUMN CONTROL BASED ON MODAL INFORMATION

The modal control procedure described in Chapter II has been applied to the simulated distillation column. Since the object here was to obtain preliminary information about the usefulness and limitations of the method, the modal controllers were designed by rather crude short-cut methods that do not provide solutions to all of the problems considered in Chapter II. All of the control calculations are applied to the basic case, A-10-1.

A. Implications of Modal Decomposition

Much of the information about the modes that was discussed in Chapter V is relevant to the control of the distillation column. The first mode was found to be highly activated by all inputs and nearly 2.5 times slower than the second. Thus a modal controller applied only to mode 1 could improve the time required for the column to recover from disturbances by a factor of 2.5. If modal controllers could be applied to the first three modes, the improvement in recovery time would be more than a factor of ten.

The first mode is a composition mode, which means that it is impossible to detect its activation unless at least one composition is measured. This is unfortunate because it is usually difficult to measure compositions rapidly, although the compositions of the two-component mixtures used here can be determined uniquely by pressure and temperature measurements (see Appendix B.1). In general composition measurements are considered undesirable, and no more than two are used by the controllers developed here.

In the previous chapter, the slowest mode was observed to retain the same character over a wide range of operating conditions. As a consequence, a modal controller designed for this mode should be effective in most situations.

B. Design of Modal Controllers

As discussed in Chapter II, it is impossible to determine the activation of any single mode or to drive the state vector in any direction in state space when both the number of measurements and the number of manipulated inputs are less than the number of state variables. The previous discussion showed how these restrictions affect the choice of measured and manipulated variables in the design of modal controllers, but the methods used here have not incorporated all of the recommended procedures. In the following, the development of modal controllers is described with no justification for the methods other than the effectiveness of their results.

For this study the composition and temperature state variables were assumed to be measurable; fortunately there was no need to measure holdups. The manipulated inputs available were taken to be reflux flow rate ℓ_{N+1}, reboiler steam temperature t_s, and condenser coolant temperature t_{cw}. The modal controllers were designed for one mode at a time, with the slowest taken first. As an aid to this discussion, the six slowest modes of case A-10-1 are reproduced in Fig. 6.1.

The controller for the slowest mode was designed to use three measurements that were combined in proportion to the three largest elements of the first left eigenvector, which is shown in Table 6.1. These elements are x_{11}, x_0, and t_{11} with relative magnitudes 1.409, 0.669, and -0.202 respectively. Thus,

Table 6.1 Left Eigenvectors for Case A-10-1
No Control

		Mode 1	Mode 2	Mode 3
holdup elements	1	0.00487	0.00309	0.0257
	2	0.0127	0.00723	0.0619
	3	0.0214	0.0115	0.0999
	4	0.0285	0.0147	0.129
	5	0.0333	0.0167	0.147
	6	0.0372	0.0181	0.161
	7	0.0419	0.0193	0.173
	8	0.0468	0.0202	0.183
	9	0.0518	0.0207	0.190
	10	0.0567	0.0211	0.195
composition elements	0	0.669	0.464	3.529
	1	0.0582	0.0322	0.263
	2	0.0631	0.0314	0.265
	3	0.0667	0.0300	0.258
	4	0.0701	0.0276	0.243
	5	0.0736	0.0240	0.217
	6	0.0659	0.0147	0.140
	7	0.0682	0.00954	0.0968
	8	0.0687	0.00523	0.0598
	9	0.0680	0.00173	0.0287
	10	0.0663	-0.00103	0.00331
	11	1.409	-0.0954	-0.751
temperature elements	0	-0.169	-0.0512	-0.835
	1	-0.0119	-0.00351	-0.0577
	2	-0.0119	-0.00338	-0.0564
	3	-0.0119	-0.00317	-0.0544
	4	-0.0121	-0.00284	-0.0516
	5	-0.0125	-0.00234	-0.0475
	6	-0.0109	-0.00129	-0.0343
	7	-0.0110	-0.000740	-0.0294
	8	-0.0109	-0.000368	-0.0259
	9	-0.0107	-0.000122	-0.0233
	10	-0.0105	0.000034	-0.0216
	11	-0.202	1.534	1.160

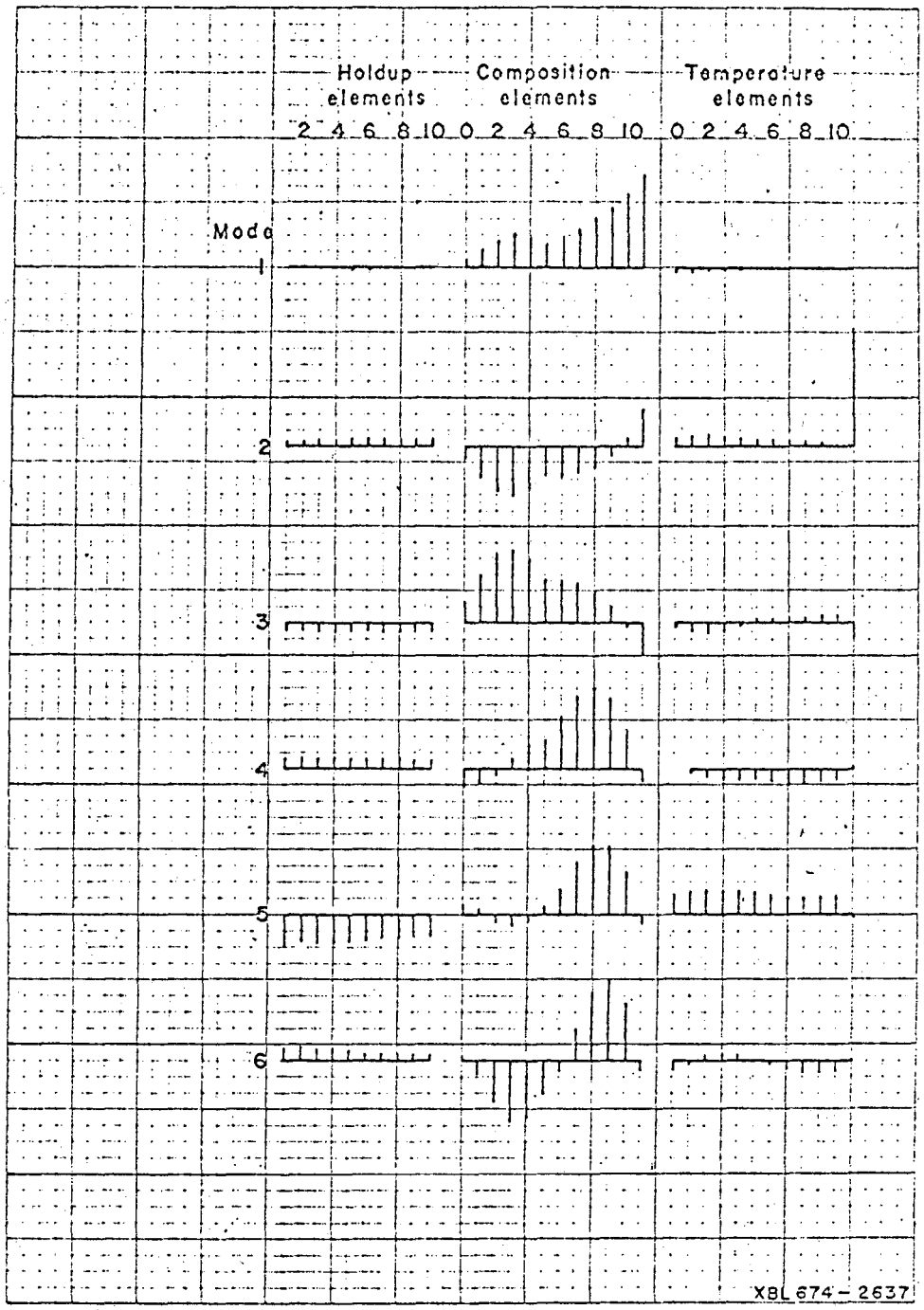


Fig. 6.1 Modes for Case A-10-1, no control.

$$\underline{e}^{(1)^T} = [0.669, \quad 1.409, \quad -0.202] \tag{6.1}$$

A suitable combination of the manipulated variables was sought by examination of the influence of each, individually, in the state space. In Chapter II the p vectors $\underline{\underline{C}}\,\underline{g}$ in n-space that result from the p inputs were considered, but here the final values of the state vectors $\underline{z}\,(\infty)$ that result from a step change in each input were used instead. These two sets of vectors are quite similar because

$$\underline{z}\,(\infty) = \sum_{i=1}^{n} - \frac{1}{\lambda_i} \left(\underline{v}^{(i)^T}\,\underline{\underline{C}}\,\underline{g}\right) \underline{u}^{(i)} \tag{6.2}$$

Whenever $\underline{\underline{C}}\,\underline{g}$ is coincident with $\underline{u}^{(i)}$ then, because $\underline{u}^{(i)}$ is orthogonal to all left eigenvectors but $\underline{v}^{(i)}$, $\underline{z}\,(\infty)$ takes the direction of $\underline{u}^{(i)}$. The final steady state vectors generated by a step change in each of the inputs (including disturbances) are shown in Fig. 6.2.

The problem was then to find a linear combination of the manipulable inputs that gave a vector $\underline{z}(\infty)$ coincident or nearly coincident with the direction of the first mode ($\underline{u}^{(1)}$). This problem does not seem particularly difficult because all of the $\underline{z}(\infty)$ vectors in Fig. 6.2 are surprisingly similar to mode 1. All have large composition elements, but relatively small holdup and temperature elements. Some combinations of ℓ_{11}, t_s, and t_{cw} were chosen by inspection, and $\underline{z}(\infty)$ vectors were generated, which are shown in Fig. 6.3. Combination (g) is very much like $\underline{u}^{(1)}$ except for composition elements at the top few plates, and therefore this combination was used as vector $\underline{f}^{(1)}$ in the controller. The elements, in the sequence ℓ_{11}, t_s, t_{cw}, are 0.010, 0.00101, -0.00078. Thus the linkages for the modal controller can be expressed as

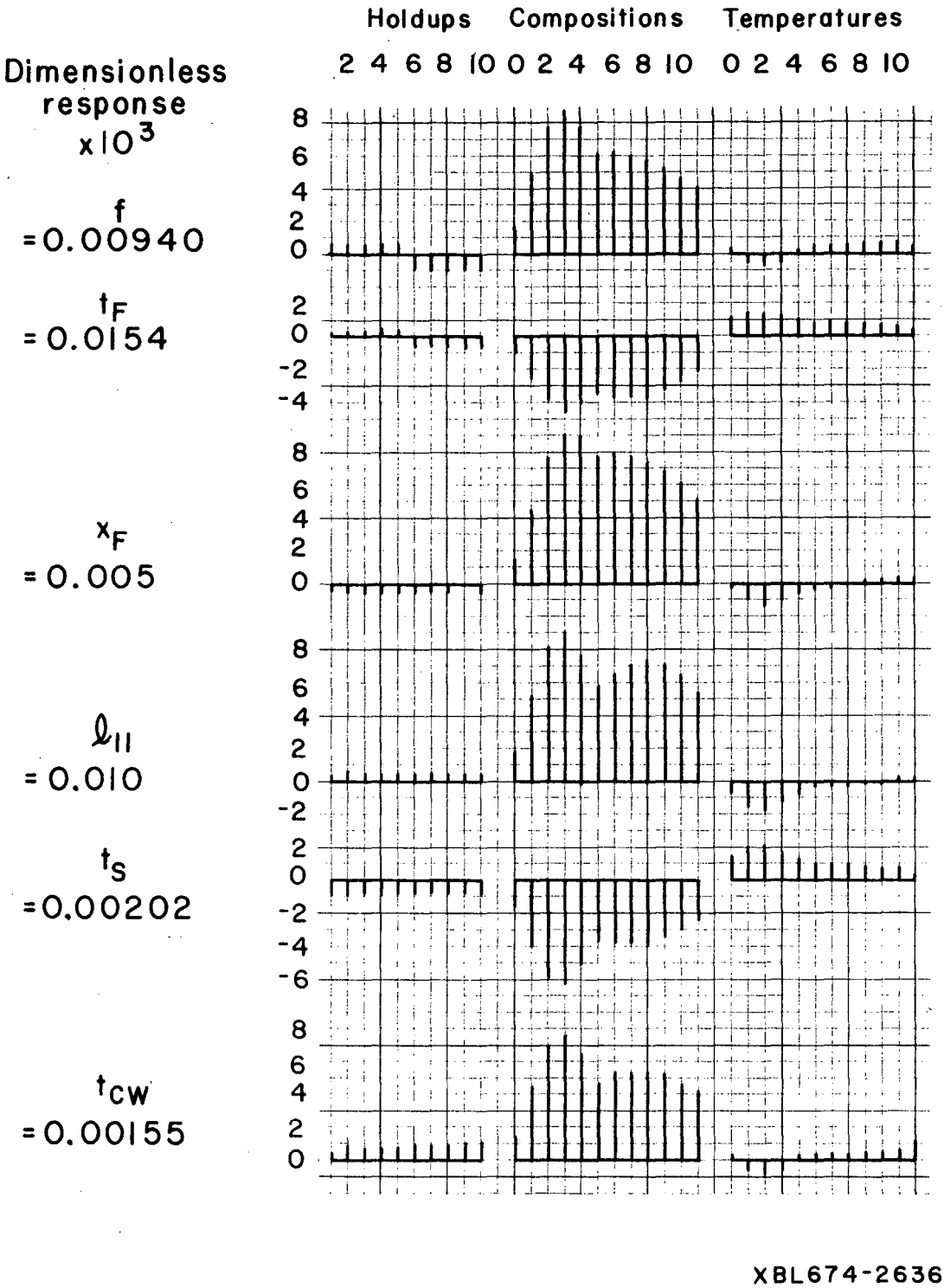


Fig. 6.2 Final steady state, $\underline{z}(\infty)$, for case A-10-1 following step changes of single inputs.

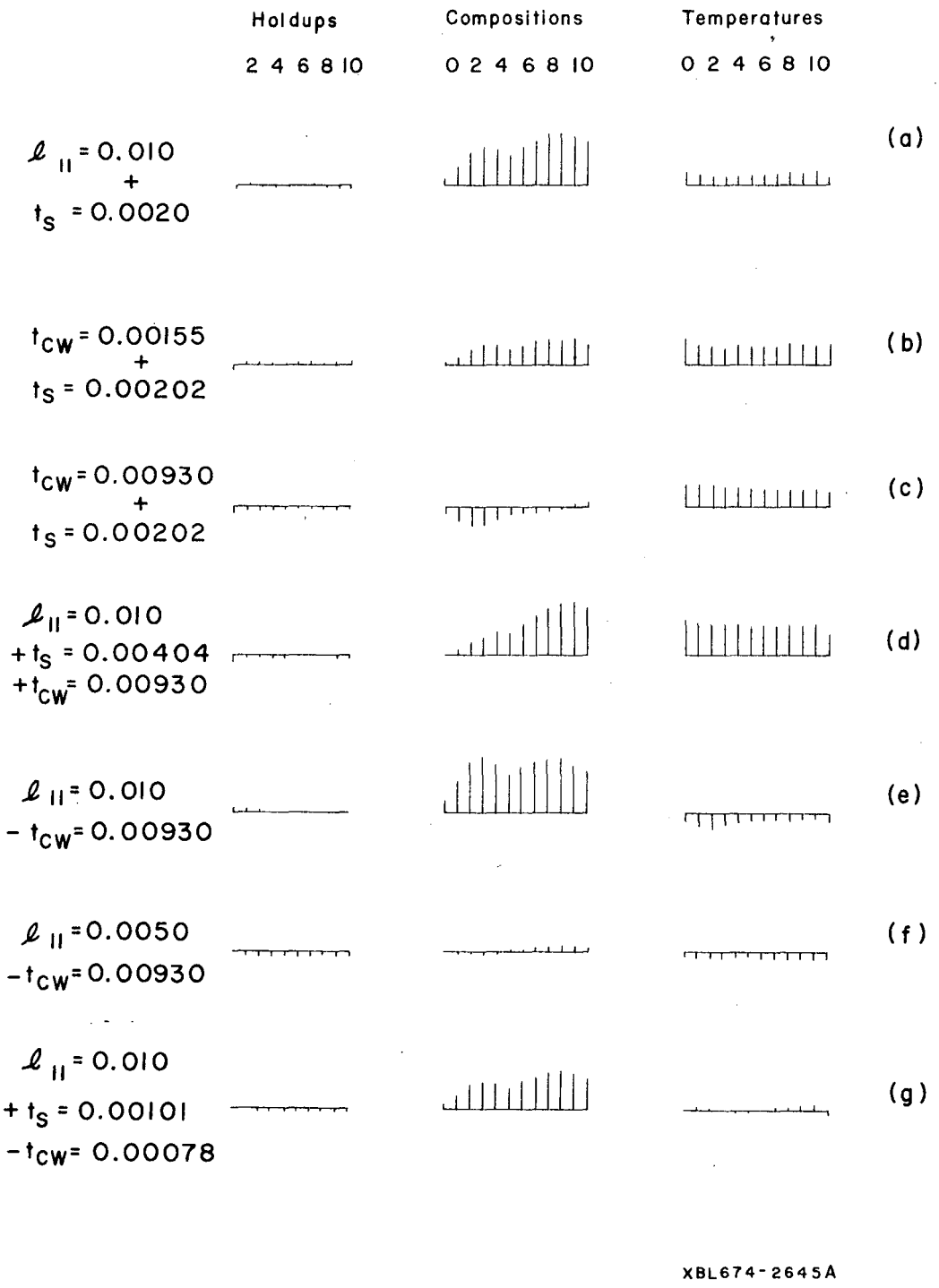


Fig. 6.3 Final steady state, $\underline{z}(\infty)$, for case A-10-1 following combinations of step inputs.

$$\ell_{11} = 0.010 \quad (0.669x_0 + 1.409\ x_{11} - 0.202\ t_{11})(-k_1)$$

$$t_s = 0.00101\ (0.669x_0 + 1.409\ x_{11} - 0.202\ t_{11})(-k_1) \qquad (6.3)$$

$$t_{cw} = -0.00078\ (0.669x_0 + 1.409\ x_{11} - 0.202\ t_{11})(-k_1)$$

In Chapter II it was shown that an ideal modal controller with gain $-k_i$ resulted in a controlled process having for mode i an eigenvalue equal to $(\lambda_i - k_i)$. However the values of k_1 used here cannot be expected to have this significance, because the control and measurement vectors ($\underline{f}^{(1)}$ and $\underline{e}^{(1)^T}$) have not been normalized. Even if these vectors were normalized, this approximate controller probably would not change the eigenvalue to $(\lambda_1 - k_1)$ because the control vector is not aligned exactly with mode 1. The constant k_1 must be considered as a proportionality factor or gain whose value is chosen arbitrarily to give a desired reduction in time constant. Various values of k_1 are used in the numerical studies of the controller performance to be presented in the next section.

Because the $\underline{z}(\infty)$ vector corresponding to a step change in reflux rate resembles the first mode so closely, it was also of interest to consider a simpler controller for the first mode. This controller was based on one manipulable input, ℓ_{11}, and one measurement, x_{11}. Therefore its linkage is given by

$$\ell_{11} = 0.010\ (1.409x_{11})(-k_1') \qquad (6.4)$$

where the numerical coefficients were chosen arbitrarily to make values for k_1' somewhat comparable to values used for k_1. The performance of this simple controller is also examined in the next section.

If it is assumed that the time constant of the slowest mode can be reduced at least to the magnitude of the second mode time constant, consideration should be given to the design of a modal controller for the second mode. However, if the $\underline{z}(\infty)$ vectors (Fig. 6.2) are compared with the second mode (Fig. 6.1) it can be seen that no combination of the $\underline{z}(\infty)$ can approximate the large accumulator temperature element of the mode.

Possibly an approximate controller for mode 1 could alter the higher modes (as a result of interactions) in such a way that the state vector could be driven in the direction of the slowest of these altered modes. However, it will be shown that the second mode retained approximately the same direction in variable space when the controller was applied to mode 1. Therefore, a modal controller for mode 2 cannot be built through use of the methods attempted here.

C. Results of Modal Control

The performance of these modal controllers was evaluated by response calculations for case A-10-1. The controller that uses three measurements and three manipulated variables (hereafter referred to as the 3×3 controller) is discussed first. The time constants for the five slowest modes of the controlled process for several values of the feedback proportionality factor k_1 are given in Table 6.2. The modal controller reduced the dominant time constant by 33 percent when k_1 was 100 and by 56 percent when k_1 was 200, but higher values gave very little additional improvement. The effect of the controller on the modes can be seen by examination of Fig. 6.4, which includes modes of the controlled and the uncontrolled process for comparison. At k_1 = 100 the second and third modes (and all

Table 6.2 Dominant Time Constants of the Controlled Process
Case A-10-1, Control of First Mode

Mode	No Control	3 Measured Variables and 3 Manipulated Inputs					1 Measured Variable and 1 Manipulated Input	
		k_1=100	k_1=200	k_1=250	k_1=300	k_1=400	k_1' = 100	k_1' = 200
1	9.37 min.	6.26	4.15	3.93	3.90	3.90	4.52	4.61
2	3.94	3.96	4.15	3.93	3.76	3.44	4.52	4.61
3	3.26	3.40	3.77	3.89	3.76	3.44	4.05	4.06
4	0.888	0.910	0.935	0.947	0.961	1.00	0.934	0.912
5	0.542	0.545	0.546	0.548	0.549	0.550	0.521	0.531

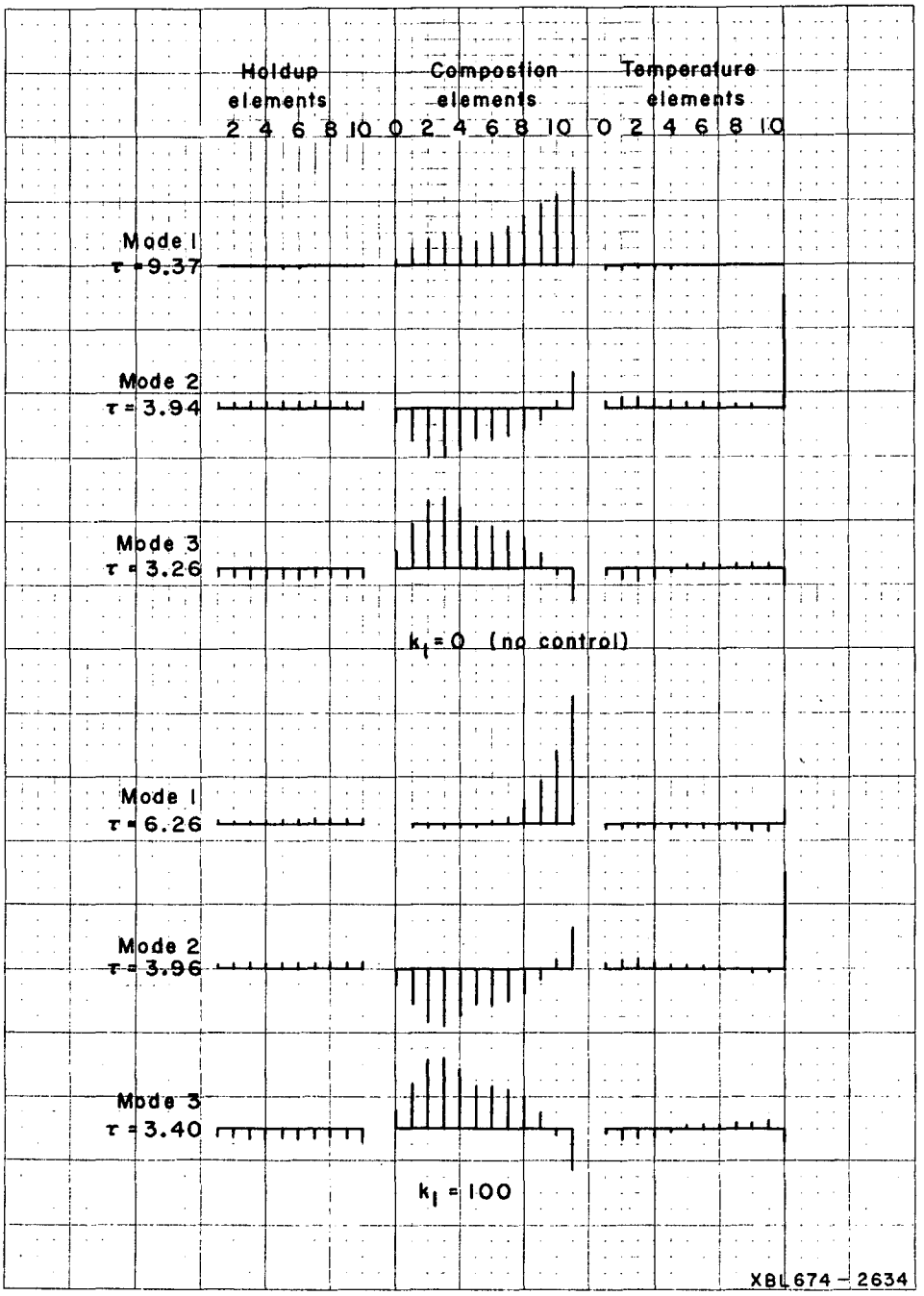


Fig. 6.4 Modes for case A-10-1 with the 3×3 modal controller.

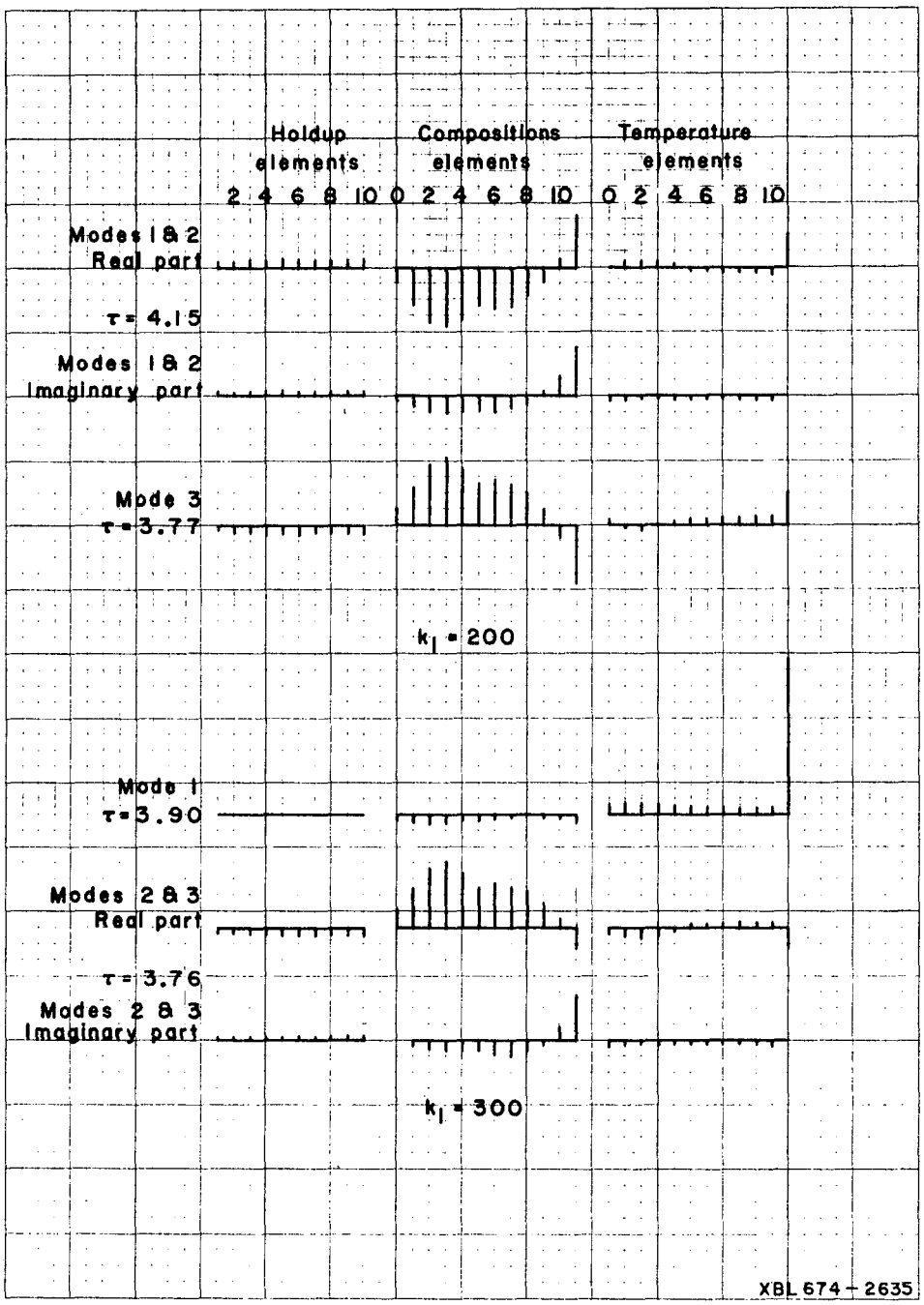


Fig. 6.4 Modes for case A-10-1 with the 3×3 modal controller.

higher modes) were essentially unchanged from the uncontrolled process. However, the first mode appeared much like the difference between the first mode of the uncontrolled process and the $\underline{z}(\infty)$ vector generated by the controller. The most significant elements of the controlled mode were those corresponding to the components that were most poorly matched. The term "controlled mode" refers to the modified mode that results when a modal controller is applied to a specific mode of the uncontrolled process. If the controller is sufficiently effective it is possible to distinguish the controlled mode from the uncontrolled modes even when the time constant of the former has been reduced appreciably.

As k_1 was increased above 100 the modes were not quite so clearly related to those of the uncontrolled process. At $k_1 = 200$ modes 1 and 2 became a complex conjugate pair, where the original mode 2 was the real part and the controlled mode the imaginary part. However, there was some mixing or "interaction" among the first three modes. When k_1 was 300 and larger, the controlled mode had a time constant faster than the former mode 2 (associated with the accumulator), and the latter again became a nearly pure, decoupled mode with a large accumulator temperature element. Also at $k_1 = 300$ or 400 the mode that was third for the uncontrolled process became the real part of a complex conjugate pair and the controlled mode the imaginary part. Thus, increasing k_1 did continue to decrease the time constant of the controlled mode, but when it reached the vicinity of modes 2 and 3 (of the uncontrolled process) there was strong interaction that would not have occurred if the controller were ideal. The result of this interaction was to reduce the effectiveness of increased controller gain, but was not very important, because at $k_1 = 300$ the accumulator mode was already dominant.

The modal controller that measured one variable and manipulated one input (hereafter referred to as the 1×1 controller) was slightly less effective than the 3×3 controller, as shown by the time constants in Table 6.2 and the modes in Figure 6.5. When k_1' was 100 the dominant time constant was reduced 52 percent, but at $k_1' = 200$ it had actually increased slightly. The controlled mode joined as the real part of a complex pair with former mode 3 as the imaginary part. However, there was considerable interaction among the three modes, and the controlled mode showed evidence of poorer matching by the 1×1 controller than was achieved with the 3×3 controller. Although the 1×1 controller could not achieve unlimited reduction of the controlled mode time constant, it was successful in gaining significant improvement.

The fourth and faster modes have not been included in the previous discussion, because the modal controllers had very little influence on any of them. The effect on the time constants of modes 4 and 5 can be seen in Table 6.2. The 3×3 controller with $k_1 = 200$ changed the sixth time constant by 0.7 percent and the subsequent ones by 0.5 percent or less. Even the 1×1 controller at $k_1' = 100$ changed the sixth and higher time constants by 1.5 percent or less.

The most conclusive evidence for the success of the modal controller was given by the process response, which was calculated using the 3×3 controller with $k_1 = 200$. This controller improved the process recovery from disturbances nearly as much as is possible with control of only one mode. The activation of the first five modes by step changes in the six possible inputs is given in Table 6.3, where manipulated inputs as well as disturbance inputs are included, because it is possible to have disturbances superimposed on the controlled changes of ℓ_{11}, t_s, and t_{cw}.

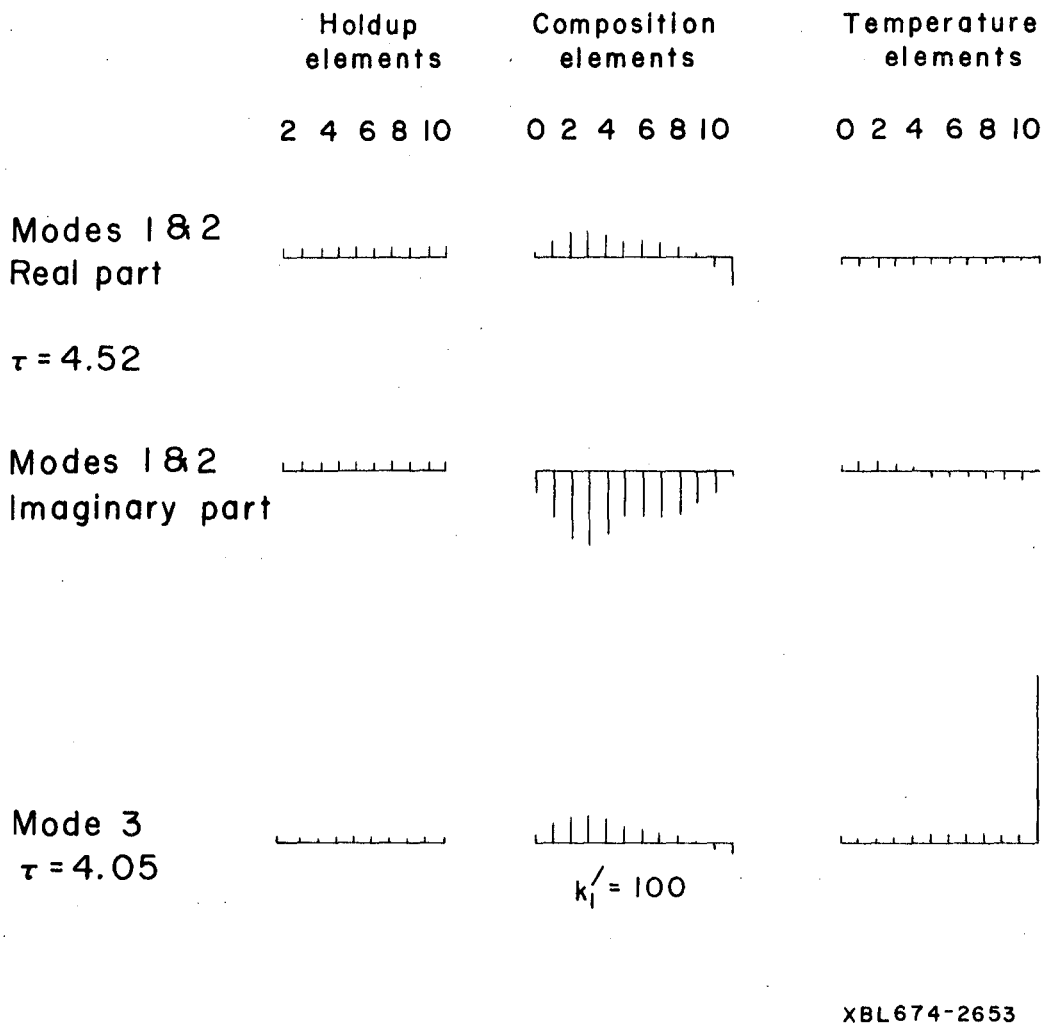


Fig. 6.5 Modes for case A-10-1 with the 1x1 modal controller

Table 6.3 Activation of Modes by Step Changes of Inputs
Case A-10-1 with Control of Mode 1 (3×3) k_1 = 200

	Input Variable and Magnitude of Step					
Mode	f =0.00940	t_F =0.0154	x_F =0.0050	ℓ_{11} =0.0100	t_S =0.0202	t_{cw} =0.0155
1-2 real	-0.0124	0.00968	-0.0141	-0.0160	0.140	-0.110
1-2 imag.	-0.0362	0.0221	-0.0414	-0.0448	0.297	-0.371
3	0.0131	-0.00689	0.0134	0.0146	-0.102	0.148
4	0.00169	-0.00242	0.00525	0.00273	-0.00887	0.0162
5	0.00169	0.00569	-0.000536	-0.00293	0.0861	-0.00432

The controlled mode (the imaginary part of the complex pair) was the most strongly activated of the first five modes. It is interesting that the activations of the real part of mode 1 had magnitudes like those for mode 3, but the signs were opposite in every case. The responses of compositions for the six step inputs are shown in Figures 6.6 through 6.11, and may be compared with the uncontrolled responses in Figures 5.7 through 5.12. These comparisons show that this response time was reduced by more than a factor of two, but that the final steady states were nearly as far from the initial steady states as they were with no control. If the final steady state is viewed as the desired state for the process, then the modal controller drove it there in less than half the time required without control. The magnitude of the controller proportionality factor k_1, is such that the manipulated inputs are moved no more than one percent of their steady state values when the measured variables undergo a five percent change from steady state.

It has been shown that the approximate modal controlled reduced the response time of the column, but did not appreciably diminish the magnitudes of the responses to step inputs. In Chapter II it was demonstrated that a factor $(\frac{1}{\lambda-k})$ appears in the activation of every controlled mode when a step input is applied. Consequently the use of a large controller gain should make the contribution of the controlled mode small. Apparently the gain used here was not sufficiently large to decrease the activation greatly. Furthermore, some of the higher modes contributed significantly to the response magnitude even though they have relatively small time constants.

Further improvement might be achieved by modal control if the mode associated with the accumulator could be either controlled or made

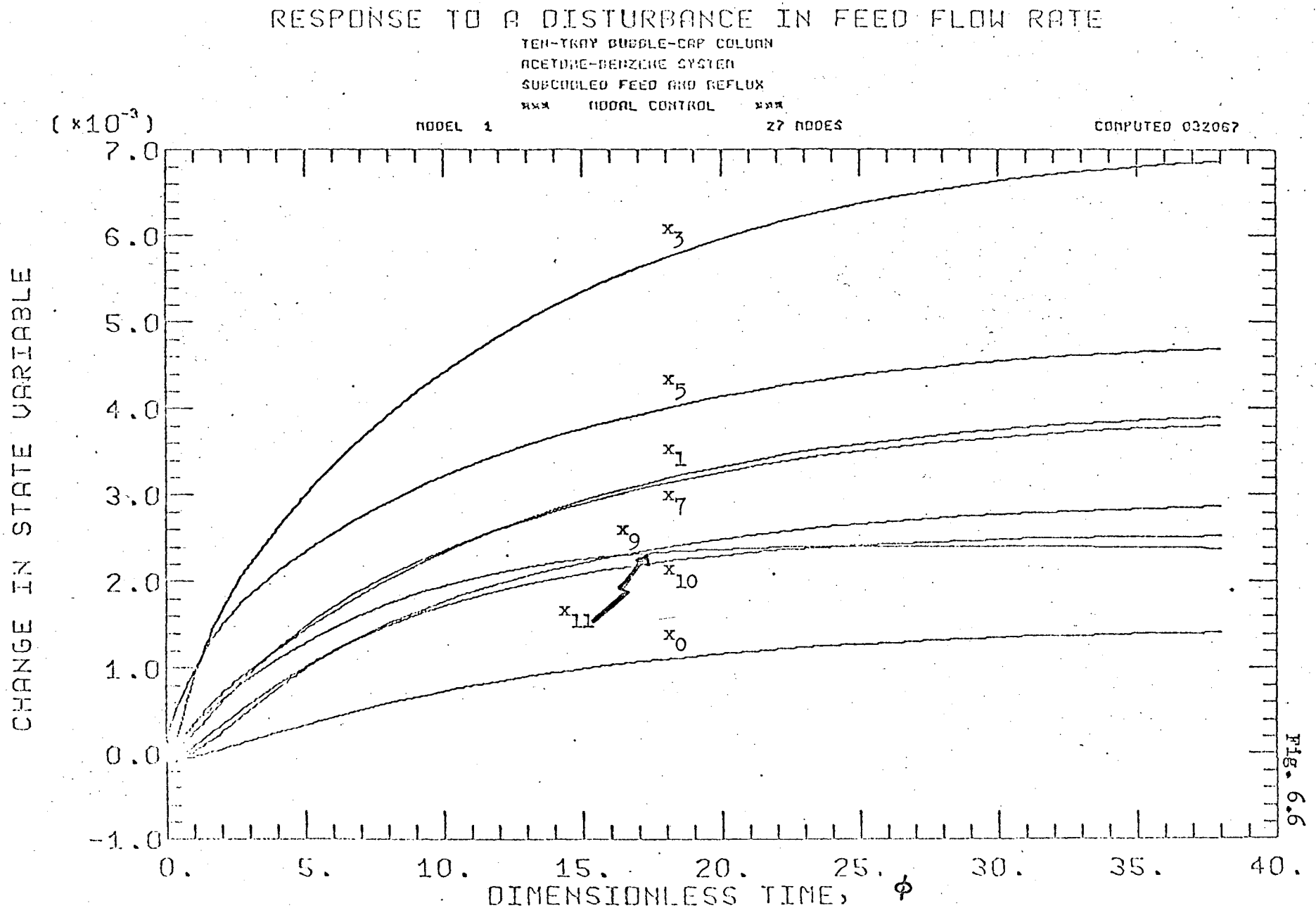

RESPONSE TO A DISTURBANCE IN FEED FLOW RATE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 MODES
COMPUTED 032067
(x10^-3)
CHANGE IN STATE VARIABLE
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, φ
x3
x5
x1
x7
x9
x10
x11
x0

Fig. 6.6

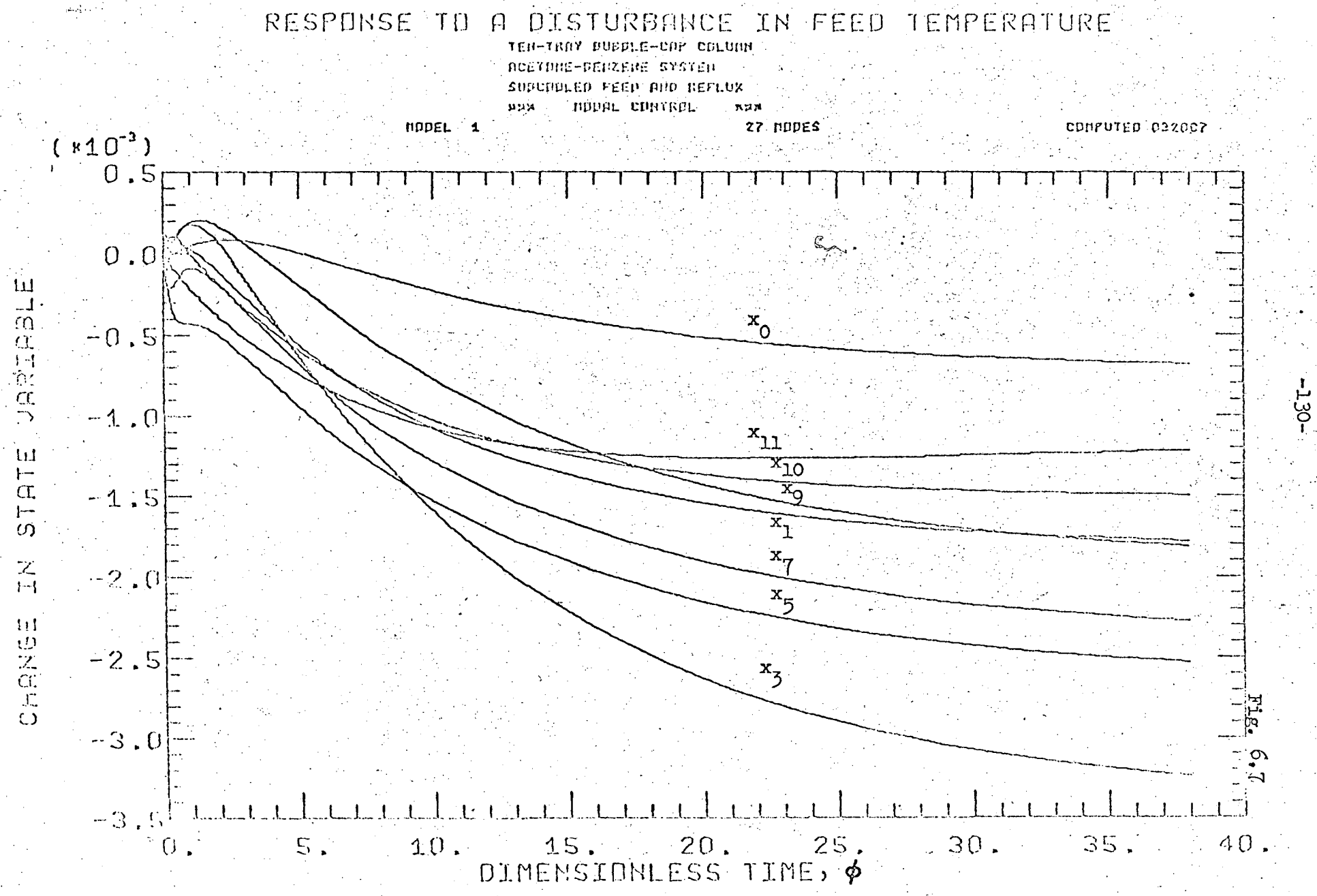
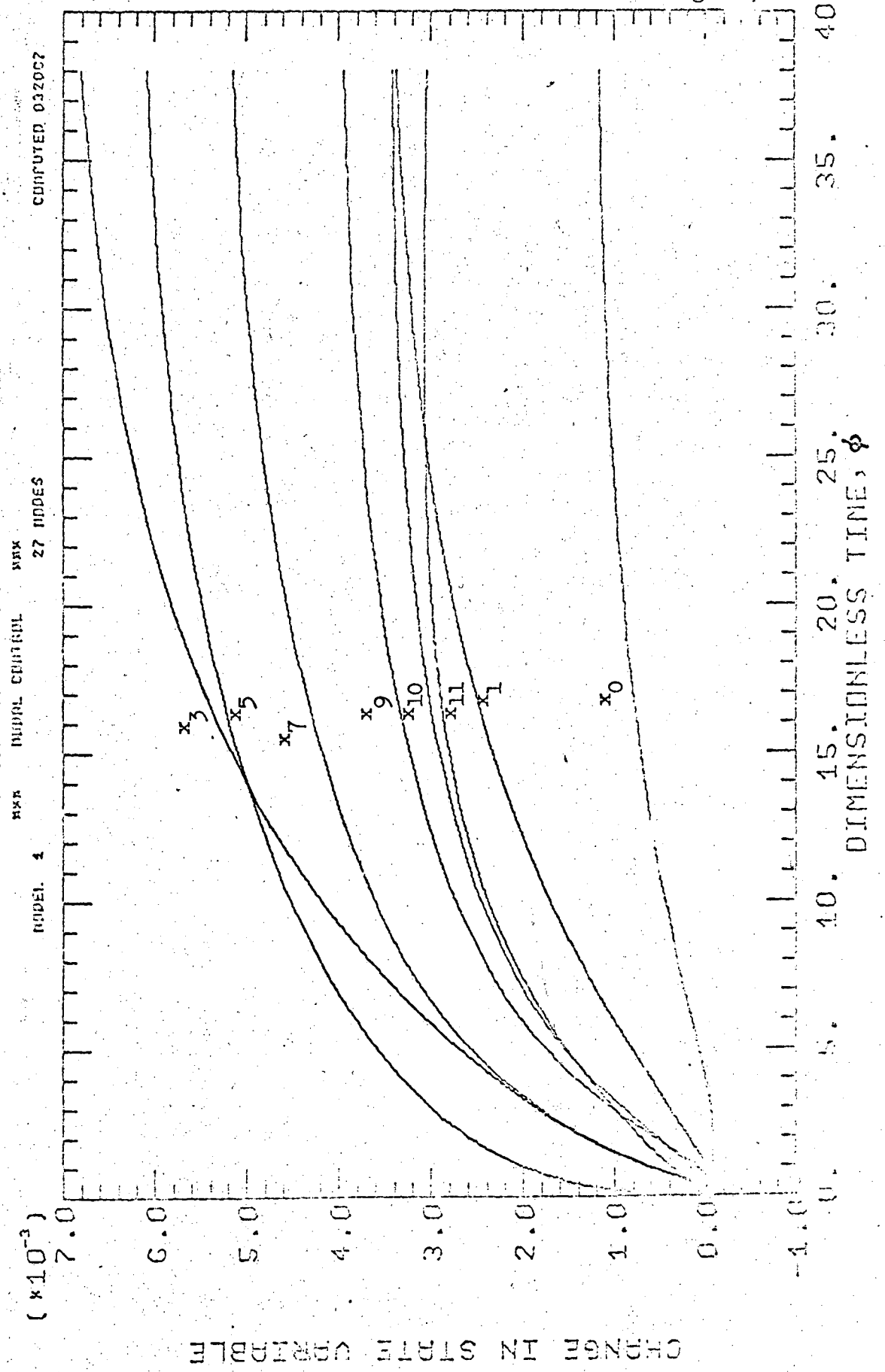

RESPONSE TO A DISTURBANCE IN FEED TEMPERATURE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 MODES
COMPUTED 032007
(×10⁻³)
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
CHANGE IN STATE VARIABLE
x0
x11
x10
x9
x1
x7
x5
x3
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, ϕ

Fig. 6.7

Fig. 6.8


RESPONSE TO A DISTURBANCE IN FEED COMPOSITION
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
MODEL 4 MODAL CONTROL 27 MODES
COMPUTED 03ZOC7
x_3
x_5
x_7
x_9
x_{10}
x_{11}
x_1
x_0
CHANGE IN STATE VARIABLE
($\times 10^{-3}$)
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, ϕ

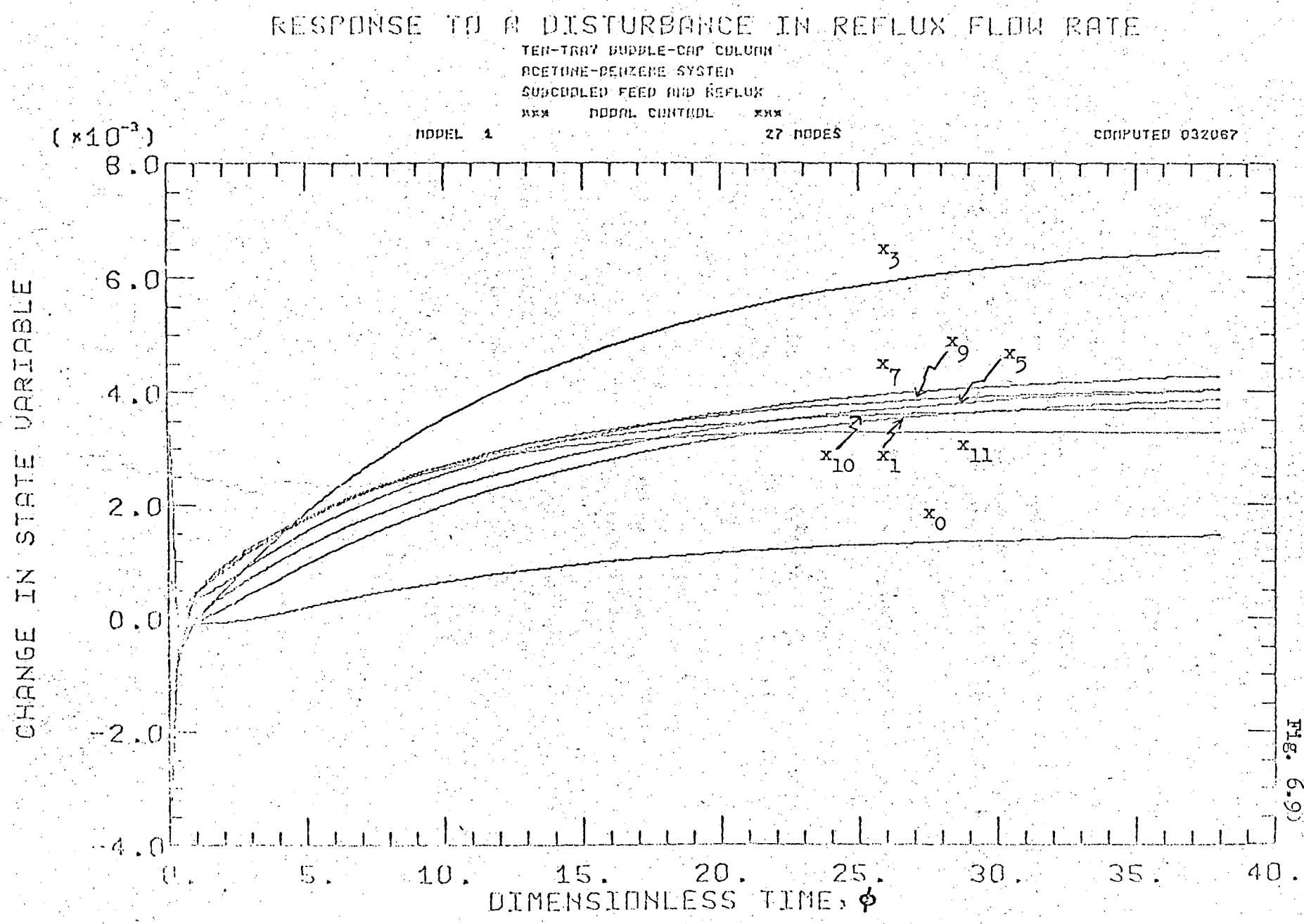

RESPONSE TO A DISTURBANCE IN REFLUX FLOW RATE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** NORMAL CONTROL ***
MODEL 1
27 NODES
COMPUTED 032067
(×10⁻³)
8.0
6.0
4.0
2.0
0.0
-2.0
-4.0
0.
5.
10.
15.
20.
25.
30.
35.
40.
CHANGE IN STATE VARIABLE
DIMENSIONLESS TIME, φ
x3
x7
x9
x5
x10
x1
x11
x0

Fig. 6.9

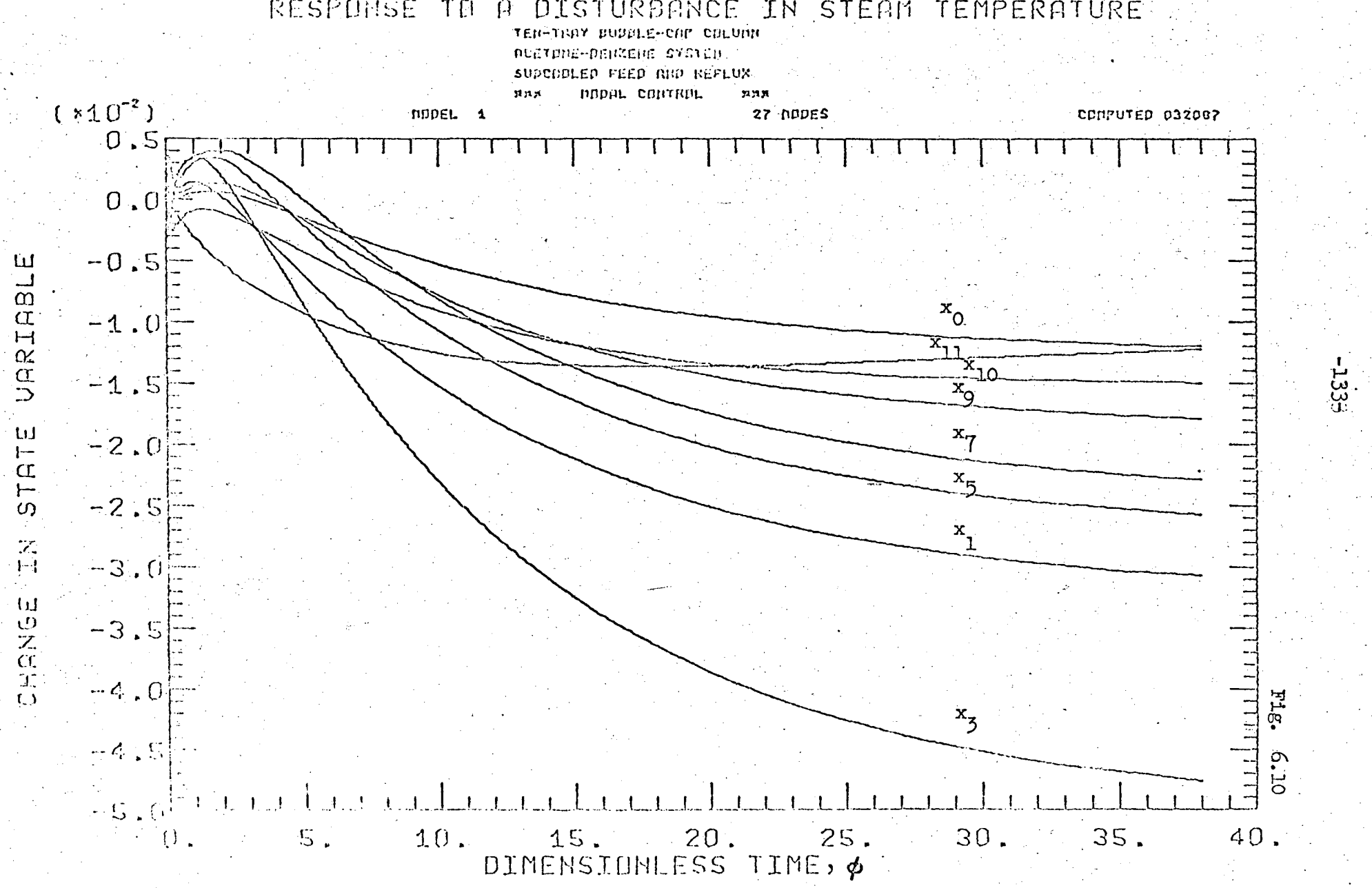

RESPONSE TO A DISTURBANCE IN STEAM TEMPERATURE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 MODES
COMPUTED 032087
(×10⁻²)
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
-3.0
-3.5
-4.0
-4.5
-5.0
CHANGE IN STATE VARIABLE
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, φ
x_0
x_{11}
x_{10}
x_9
x_7
x_5
x_1
x_3

Fig. 6.10

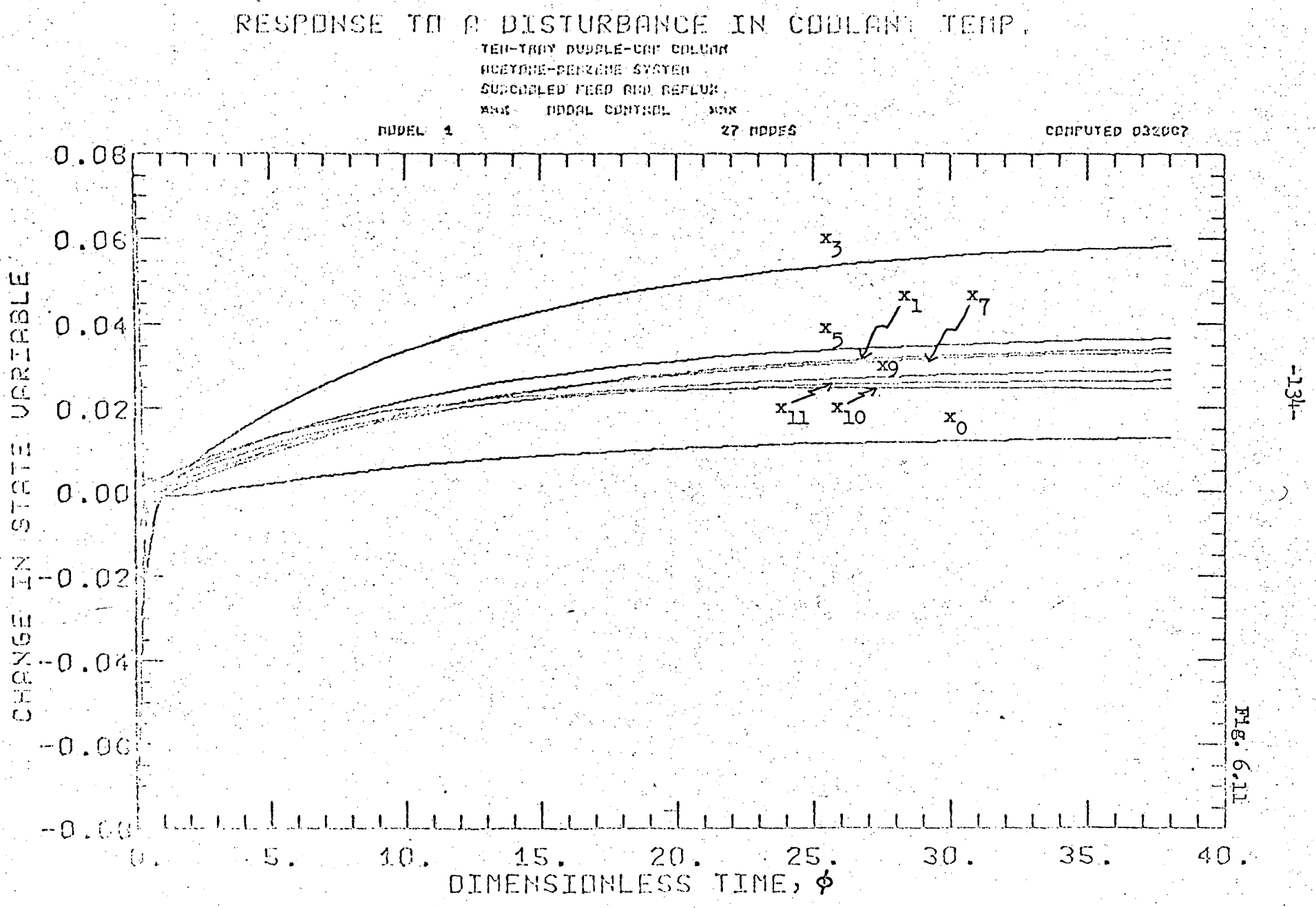

RESPONSE TO A DISTURBANCE IN COOLANT TEMP.
TEN-TRAY DOUBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 MODES
COMPUTED 032067
CHANGE IN STATE VARIABLE
0.08
0.06
0.04
0.02
0.00
-0.02
-0.04
-0.06
-0.08
x_3
x_1
x_7
x_5
x_9
x_{11}
x_{10}
x_0
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, ϕ

Fig. 6.11

faster by changes in column design. It has already been shown that the assumed manipulated inputs could not be used to build a controller for this mode, but calculations indicate that reduction of the amount of subcooling tends to reduce the activation of this mode. Consequently, design changes incorporating a heater in the reflux line and reduced accumulator holdup should significantly reduce the importance of the accumulator mode.

Even if the time constant of the first mode of the uncontrolled process were reduced until the accumulator mode was clearly dominant, the latter probably would not have a strong influence on the response, because its activation is not large. Thus, the inability to control the accumulator mode is not viewed as a serious limitation; it has little influence and can be made less significant by design changes. Moreover, for the column studied the dominant mode of the uncontrolled process can be made faster by a factor of 2.5 before the accumulator mode interferes with further improvement. If the second mode were not present, it would probably be possible to design a modal controller for the mode that was third in case A-10-1 by methods similar to those given. The latter mode is dominated by compositions, and the elements have only one alternation of sign. However, the state vector could not be driven in the directions of the composition modes faster than the third mode because of the many alternations in sign of the composition elements.

D. Feedforward Control

A feedforward control scheme, based on cancellation of the activations of the dominant modes when the disturbances can be measured, was described in Chapter II. The method has been applied to reduce the effect of feed flow rate and feed composition disturbances by manipulation of reflux rate, steam temperature, and coolant temperature. The feedforward controller developed in this section was used simultaneously with the 3X3 modal controller ($k_1 = 200$) that was specified in the previous section.

The equations that give the coefficients for the feedforward control matrix $\underline{\underline{M}}$ were determined from the table of activations, Table 6.3, according to the procedure described in Chapter II. For feed flow rate disturbances, a controller that cancels the activations of the first three modes can be found by solution of

$$\left\{\begin{array}{l} -0.01595\, m_1^{(1)} + 0.1395\, m_2^{(1)} - 0.1099\, m_3^{(1)} - 0.01243 = 0 \\ -0.04477\, m_1^{(1)} + 0.2971\, m_2^{(1)} - 0.3705\, m_3^{(1)} - 0.03624 = 0 \\ 0.01464\, m_1^{(1)} - 0.1019\, m_2^{(1)} + 0.1483\, m_3^{(1)} + 0.01306 = 0 \end{array}\right\} \qquad (6.5)$$

where $m_1^{(1)}$, $m_2^{(1)}$, and $m_3^{(1)}$ are the sizes of step changes that must be made in the manipulated variables ℓ_{11}, t_s, and t_{cw}, respectively, to achieve that cancellation for a step flow change of $f = 0.00940$. The solution to Equation (6.8) gives

$$\begin{aligned} m_1^{(1)} &= -0.370 \\ m_2^{(1)} &= 0.0135 \\ m_3^{(1)} &= -0.0423 \end{aligned} \qquad (6.6)$$

Thus the controller required

$$\begin{aligned} \ell_{11} &= -0.370\ (0.0100)\left(\frac{f}{0.00940}\right) \\ t_s &= 0.0135\ (0.0202)\left(\frac{f}{0.00940}\right) \\ t_{cw} &= -0.0423\ (0.0155)\left(\frac{f}{0.00940}\right) \end{aligned} \tag{6.7}$$

For feed composition disturbances the procedure was identical and yielded a new set of coefficients $(m_1^{(2)}, m_2^{(2)}, m_3^{(2)})$ such that

$$\begin{aligned} \ell_{11} &= -1.060\ (0.0100)\left(\frac{x_F}{0.0050}\right) \\ t_s &= -0.0187\ (0.0202)\left(\frac{x_F}{0.0050}\right) \\ t_{cw} &= 0.00144\ (0.0155)\left(\frac{x_F}{0.0050}\right) \end{aligned} \tag{6.8}$$

To test the method, control as specified by Equations (6.7) or (6.8) was applied concurrently with a step disturbance in feed flow rate or feed composition. The control was actually a set of step inputs in the manipulated variables, calculated according to Eq. (6.7) or (6.8). The activations of the first five modes are given in Table 6.4, where it can be seen that, for both cases, the first three activations were negligible. Even the fourth and fifth modes, which have time constants of 0.935 and 0.546 minutes respectively, did not contribute very significantly to the response. Therefore, the composition responses, as shown in Figures 6.12 and 6.13 for feed rate and feed composition changes respectively, reached a final steady state very rapidly, and also moved only a very small distance from the initial steady state.

The table below compares the final steady state compositions at the top and bottom of the column for the process with no control, modal control alone, and both modal and feedforward control. For both

Table 6.4. Activation of Modes by Step Changes of Inputs

Case A-10-1 with Control of Mode 1, $k_1 = 200$

Mode	$f = 0.00940$ + $\begin{cases} \ell_{11} = -0.00370 \\ t_s = 0.000273 \\ t_{cw} = -0.000656 \end{cases}$	$x_F = 0.0050$ + $\begin{cases} \ell_{11} = -0.0106 \\ t_s = -0.000378 \\ t_{cw} = 0.0000223 \end{cases}$
1-2 real	5.0×10^{-6}	-1.1×10^{-6}
1-2 imag.	9.9×10^{-7}	-4.5×10^{-6}
3	-4.7×10^{-6}	2.2×10^{-6}
4	-0.000123	0.00255
5	0.00411	0.000956

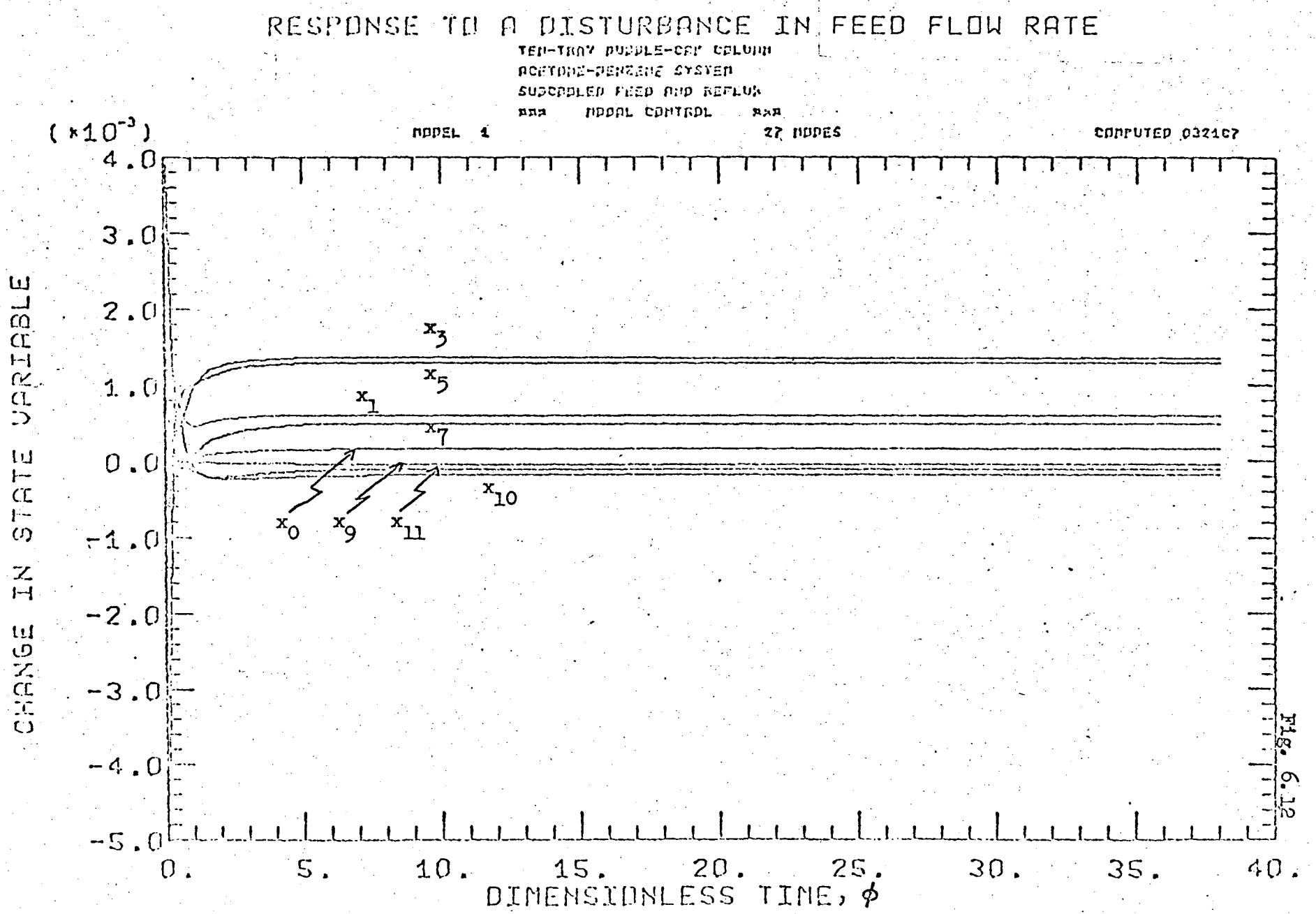

RESPONSE TO A DISTURBANCE IN FEED FLOW RATE
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 NODES
COMPUTED 032167
(×10⁻³)
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
CHANGE IN STATE VARIABLE
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, φ
x3
x5
x1
x7
x10
x0
x9
x11

Fig. 6.12

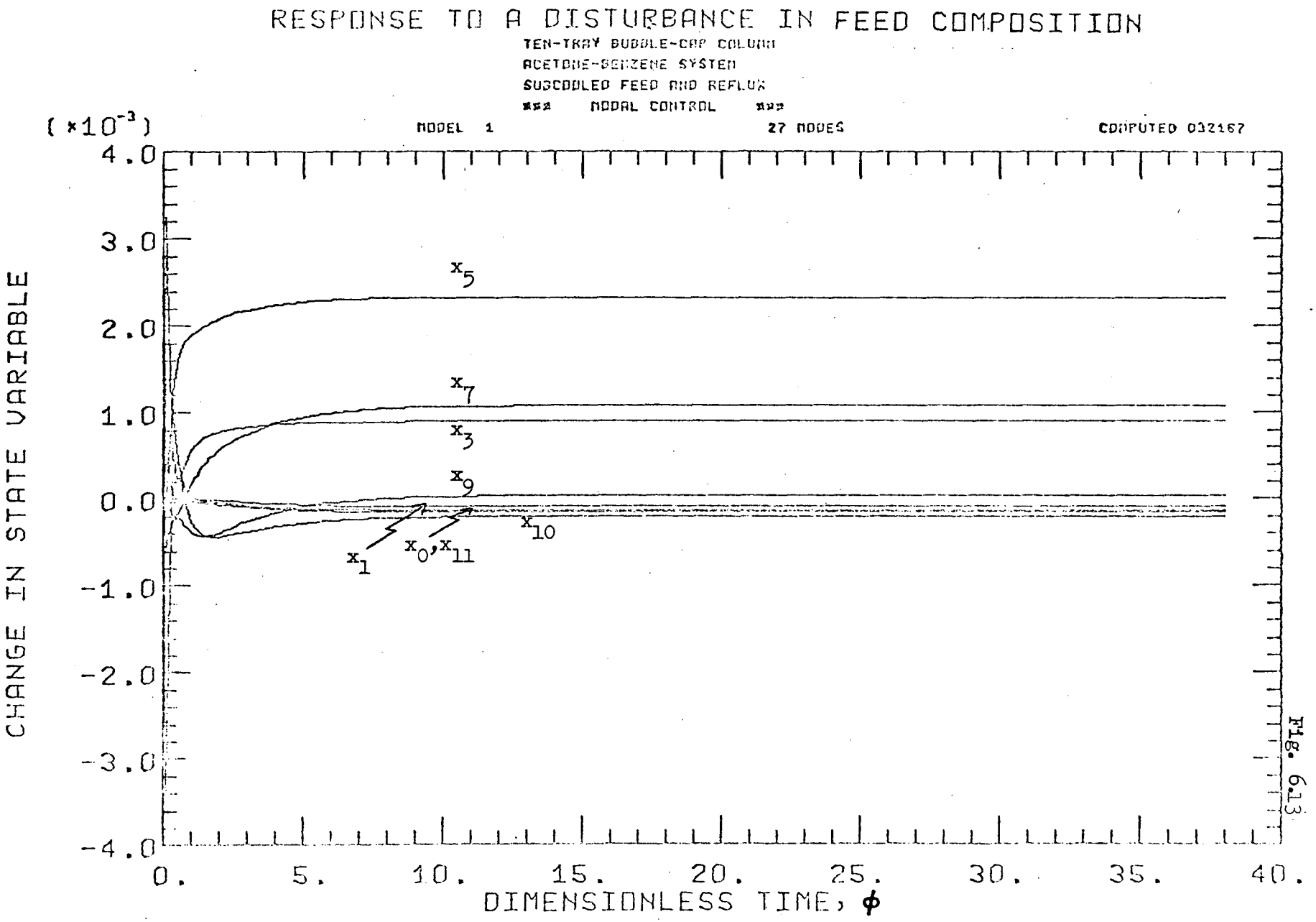

RESPONSE TO A DISTURBANCE IN FEED COMPOSITION
TEN-TRAY BUBBLE-CAP COLUMN
ACETONE-BENZENE SYSTEM
SUBCOOLED FEED AND REFLUX
*** MODAL CONTROL ***
MODEL 1
27 MODES
COMPUTED 032167
(×10⁻³)
CHANGE IN STATE VARIABLE
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
0.
5.
10.
15.
20.
25.
30.
35.
40.
DIMENSIONLESS TIME, φ
x5
x7
x3
x9
x10
x1
x0,x11

Fig. 6.13

Table 6.5

	f = 0.00940		x_F = 0.00500	
	$x_0(\infty)$	$x_{11}(\infty)$	$x_0(\infty)$	$x_{11}(\infty)$
No control	1.83×10^{-3}	4.12×10^{-3}	1.65×10^{-3}	5.16×10^{-3}
Modal control	1.42×10^{-3}	2.38×10^{-3}	1.18×10^{-3}	3.05×10^{-3}
Feedforward and modal control	1.68×10^{-4}	-3.92×10^{-5}	-1.36×10^{-4}	-1.59×10^{-4}

disturbances the deviations in product stream compositions were reduced to less than ten percent of the uncontrolled deviations. In addition, the transients disappeared in about two minutes, compared to more than twenty minutes for the uncontrolled process.

VII. CONCLUSION

The detailed study of the modes of a binary distillation column in this work has provided important background for the development of modal controllers. Analysis of the modes of Model 1, which is the most comprehensive of the three column models considered here, reveals characteristics that add to the understanding of distillation dynamics. One of the most significant findings is that the slowest mode involves compositions, rather than temperatures or holdups. Because this is the case, even Model 4, which includes only component balances, can be used to predict the slowest mode. Insight given by Model 3 confirms the findings of prior investigators[1] that the hydraulic phenomena tend to be decoupled from the accumulation of chemical species.

Despite its attractiveness, modal decomposition of processes suffers from a number of practical limitations. The formulation of accurate mathematical models and the evaluation of the parameters requires considerable effort. Also, the numerical computation required is extensive. It seems unlikely that modal decomposition will ever by used routinely in its present form. However, general studies of classes of processes may be feasible by this method.

An effective modal controller was designed by approximate methods for the slowest mode of the simulated distillation column. This controller was able to decrease the time required for the column to recover from disturbances by a factor of 2.5; furthermore it had no serious interaction with the other modes. The second slowest mode, which is associated with the accumulator, limited the improvement that could be achieved, because it was not possible to design a modal controller for

this mode. However, the influence of the second mode could be reduced by changes in the column design. It was found, in addition, that when disturbances were measurable, their effect on the process could be diminished by an order of magnitude. This was accomplished with a feed-forward controller designed to cancel the activations of the three most dominant modes.

The modal controllers developed here decrease the time required for the process to reach steady state. However, they did not appreciably reduce the magnitude of the response to step disturbances. In other words they permitted steady state error. This resulted from contributions of modes other than the controlled one, and from failure of the approximate controller to diminish the activation of the controlled mode.

The problems associated with lack of complete observability and controllability can cause considerable difficulty in the development of useful modal controllers for any real process. The discussion in Chapter II gives insight to these problems but does not offer solutions. Controllers were designed in this work without regard to the systematic solution of these problems.

The distillation modes observed in this work are probably typical of most binary columns. It can be expected that the composition effects are important, and therefore modal controllers similar to the one devised here should be useful for other binary distillation systems. However, a simple extension to multicomponent distillation cannot be made. The extra degrees of freedom are likely to result in more important temperature effects than are found in the binary case. In addition, a multicomponent column is more likely to have severe nonlinearities.

The development of realistic modal controllers for distributed parameter processes seems remote. A systematic procedure for controller design has not yet been devised even for lumped parameter processes. Furthermore, any distributed processes that may be purely convective (no diffusion) would suffer from the same limitation as cascades of identical tanks with unidirectional flow; for both cases independent modes do not exist, and the modal approach cannot be used.

The effective control of real multivariable chemical processes must be the ultimate objective of the modal approach. It is hoped that the concepts developed in this work provide a basis for the extensions and simplifications required to achieve this objective.

ACKNOWLEDGMENTS

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Nomenclature*

a	coefficient of state variables in Eqs. (2.15) and (2.16), parameter in physical property correlations (a_{RHO}, a_{CP}, a_{VH}), or parameter in exponent of vapor-liquid equilibrium correlation, °R
a_1-a_8	coefficients of state variables in Eq. (3.1)
A_{12}, A_{21}	parameters in Van Laar activity coefficient correlation
$\underline{\underline{A}}$	n×n state matrix of constant coefficients of the state variables
A_T, A_B	plate area, bubbling area, ft^2 (assume $A_T = A_B$)
b	parameter in physical property correlations (b_{RHO}, b_{CP}, b_{VH}), or parameter in exponent of the vapor-liquid equilibrium correlation
b_1-b_8	coefficients of state variables in Eq. (3.2).
$\underline{b}$	a vector in Eq. (C.2), Appendix C
B	flow rate of bottoms product, moles/sec
$\underline{\underline{B}}$	n×m input matrix of constant coefficients giving the effect of inputs on the rate of change of the state variables
c_1-c_8	coefficients of state variables in Eq. (3.3)
$\underline{\underline{C}}$	n×p input matrix for manipulated variables
D	flow rate of overhead product, moles/sec
$\underline{d}$	vector of process inputs (m-dimensional)
$\underline{\hat{d}}$	vector of disturbance inputs (q-dimensional)
$\underline{\underline{D}}$	n×q input matrix for disturbance variables
e	the base of the natural or Napierian system of logarithms

* Nomenclature for Appendices B and D follows Appendix B

E	Murphree plate efficiency based on the liquid phase
$\underline{e}^{(i)T}$	the i'th row of matrix $\underline{\underline{E}}$
$\underline{\underline{E}}$	$\ell \times r$ matrix of the modal controller. Each row specifies linear combinations of measurements.
f	dimensionless feed rate
F	feed rate, moles/sec
$\underline{\underline{F}}$	$p \times \ell$ matrix of the modal controller. Each column specifies linear combinations of manipulated inputs.
$\underline{f}^{(i)}$	the i'th column of matrix $\underline{\underline{F}}$
g_i	the i'th manipulable input
$\underline{g}$	vector of manipulable inputs (p-dimensional)
h	dimensionless holdup
H	liquid holdup, moles
H_w	residual holdup, moles (parameter in the hydraulic expression)
$\underline{\underline{H}}$	$r \times n$ measurement matrix
i,j	$= \sqrt{-1}$, identifies the imaginary part of complex numbers or variables
$\underline{\underline{I}}$	the identity matrix
k_i	the proportionality factor or gain for the i'th modal controller
$\underline{\underline{K}}$	$\ell \times \ell$ diagonal matrix of the modal controller, composed of controller proportionality factors or gains
ℓ	the number of modal controllers (number of modes controlled)
ℓ	dimensionless liquid flow rate
L	liquid flow rate, moles/sec
m	slope of vapor-liquid equilibrium curve
$m_j^{(i)}$	the j'th element of the i'th column of matrix $\underline{\underline{M}}$
$\underline{m}^{(i)}$	the i'th column of matrix $\underline{\underline{M}}$ (p-dimensional)

$\underline{\underline{M}}$	p×q matrix of the feedforward controller
n	the number of state variables
N	the number of plates in the distillation column
p	the number of manipulated inputs
p	dimensionless pressure
P	total pressure, atm.
q	the number of disturbance inputs
Q	rate of heat removal or addition, Btu/sec
$\underline{\underline{Q}}$	a submatrix of matrix $\underline{\underline{A}}$ defined in Appendix A.3, Eq. (A.3.1)
r	the number of measurements
$\underline{r}$	a vector defined in Appendix C, Eq. (C.7)
$\underline{\underline{R}}$	a submatrix of matrix $\underline{\underline{A}}$ defined in Appendix A.3, Eq. (A.3.1)
S	the sensitivity of an eigenvalue to the value of a parameter, defined by Eq. (2.18).
$\underline{\underline{S}}$	a submatrix of matrix $\underline{\underline{A}}$ defined in Appendix A.3, Eq. (A.3.1)
t	a dummy variable for time in Eq. (2.12)
t	dimensionless temperature
T	absolute temperature, °R
$\underline{u}^{(i)}$	a right eigenvector (or mode) of matrix $\underline{\underline{A}}$
$\underline{\underline{U}}$	the n×n matrix whose columns are the right eigenvectors of matrix $\underline{\underline{A}}$
v	dimensionless vapor flow rate
V	vapor flow rate, moles/sec
$\underline{v}^{(i)T}$	a left eigenvector of matrix $\underline{\underline{A}}$
$\underline{\underline{V}}^{T}$	the n×n matrix whose rows are the left eigenvectors of matrix $\underline{\underline{A}}$
w_i	the activation of mode i caused by an input (for real modes)
$\hat{w}_i$	the activation of mode i caused by an initial condition (for real modes)

W_i', W_i'' the activation of complex mode i caused by an initial condition. Defined by Eq. (A.1.8)

$\underline{w}^{(j)}$ an approximation to the j'th eigenvector of $\underline{\underline{A}}$ (Appendix C)

$\underline{\hat{w}}^{(j)}$ the j'th eigenvector of $(\underline{\underline{A}}-\lambda_j\underline{\underline{I}})^{-1}$ (Appendix C)

$\underline{w}_g^{(j)}$ vector of activations caused by the j'th manipulated input (n-dimensional)

$\underline{w}_{\hat{d}}^{(i)}$ vector of activations caused by the i'th disturbance input (n-dimensional)

$\underline{\underline{W}}$ the n×p matrix whose columns are the vectors $\underline{w}_g^{(j)}$

x mole fraction of light component (acetone) in the liquid phase

y mole fraction of light component in the vapor phase

$\underline{y}$ a vector defined in Appendix C, Eq. (C.8)

z_i state variable i (h, x, or t)

$\underline{z}$ the state vector (n-dimensional)

$\dot{\underline{z}}$ vector of time derivatives of the state variables

$\underline{z}^{(i)}$ the contribution of mode i to the state vector (Appendix A.1)

Greek Letters

α, α_i — The coefficient in the hydraulic expression, gal/min/in.; or a parameter of matrix $\underline{\underline{A}}$; or a coefficient in Eq. (2.17); or an unspecified coefficient (Appendix C)

β — the coefficient in the vapor flow equation, ft^2

δ — a small number used in Appendix A.2

δ_{ij} — the Kronecker delta, $\delta_{ij} \begin{cases} = 0, \text{ if } i \neq j \\ = 1, \text{ if } i = j \end{cases}$

ϵ — a small number used in Appendix A.2

θ — time, hr. (sometimes min. or sec.)

θ_o — the time at which a step change of the input is made (Eq.(2.13))

κ — coefficient that gives the influence of vapor rate on holdup, in H_2O/ft./sec.

λ_i — an eigenvalue of matrix $\underline{\underline{A}}$

$\underline{\underline{\Lambda}}$ — the nxn diagonal matrix of eigenvalues

$\underline{\xi}$ — vector of measured variables (r-dimensional)

τ — time constant

ϕ — dimensionless time

Subscripts

A — refers to the accumulator

C,c — refers to the condenser

CW,cw — refers to condenser coolant

F — refers to the feed stream

i (or j) — refers to plate i, any plate in the column other than the reboiler, feed plate or accumulator; or refers to the i'th mode, i'th measurement, etc.

jF — refers to the feed plate

N — refers to the top plate

q — refers to matrix $\underline{\underline{Q}}$ (Appendix A.3)

r refers to matrix $\underline{\underline{R}}$ (Appendix A.3)

R, r refers to the reboiler

S, s refers to steam (reboiler)

Plate numbering (subscripts)

0 reboiler

1,2,3,... any plate in column. The bottom plate is 1

N top plate

N + 1 accumulator (or condenser pressure)

Superscripts

i, j refers to the i'th or j'th vector (or eigenvector)

ℓ gives the number of iterations, Appendix C

q refers to matrix $\underline{\underline{Q}}$, Appendix A.3

r refers to matrix $\underline{\underline{R}}$, Appendix A.3

T denotes the transpose of a vector or matrix

* refers to equilibrium value

' refers to the real part of a complex number; or distinguishes a symbol

" refers to the imaginary part of a complex number; or distinguishes a symbol

Other marking

A. Above symbol

- denotes steady state value

~ denotes total time-dependent value; or an approximate value (Appendix C only)

B. Below symbol

- denotes a vector (usually a lower case symbol)

= denotes a matrix (usually an upper case symbol)

C. Arguments

(0) initial condition

(∞) final value (final steady state)

Variables in upper case are dimensional (H, L, V, P, T, F)

Variables in lower case are dimensionless (h, ℓ, v, p, t, f)

Appendix A

ADDITIONAL ASPECTS OF MODAL ANALYSIS

A.1 Response of Complex Modes

Consider the response of complex conjugate modes i and i+1, where

$$\left.\begin{aligned} \lambda_i &= \lambda_i' + j\lambda_i'' & \lambda_{i+1} &= \lambda_i' - j\lambda_i'' \\ \underline{u}^{(i)} &= \underline{u}^{(i)'} + j\underline{u}^{(i)''} & \underline{u}^{(i+1)} &= \underline{u}^{(i)'} - j\underline{u}^{(i)''} \\ \underline{v}^{(i)} &= \underline{v}^{(i)'} + j\underline{v}^{(i)''} & \underline{v}^{(i+1)} &= \underline{v}^{(i)'} - j\underline{v}^{(i)''} \end{aligned}\right\} \quad (A.1.1)$$

For step inputs the contributions of these modes, $\underline{z}^{(i)}$, are given by

$$\underline{z}^{(i)} = \frac{\left(\underline{v}^{(i)^T} \underline{\underline{B}}\, \underline{d}\right)}{-\lambda_i} \underline{u}^{(i)}\left(1-e^{\lambda_i \theta}\right) + \frac{\left(\underline{v}^{(i+1)^T} \underline{\underline{B}}\, \underline{d}\right)}{-\lambda_{i+1}} \underline{u}^{(i+1)}\left(1-e^{\lambda_{i+1} \theta}\right) \quad (A.1.2)$$

Here

$$\left(\underline{v}^{(i)^T} \underline{\underline{B}}\, \underline{d}\right) = \left[\left(\underline{v}^{(i)'}\right)^T \underline{\underline{B}}\, \underline{d}\right] + j\left[\left(\underline{v}^{(i)''}\right)^T \underline{\underline{B}}\, \underline{d}\right] \quad (A.1.3)$$

Define

$$\left.\begin{aligned} w_i' &= \left[\left(\underline{v}^{(i)'}\right)^T \underline{\underline{B}}\, \underline{d}\right] \\ w_i'' &= \left[\left(\underline{v}^{(i)''}\right)^T \underline{\underline{B}}\, \underline{d}\right] \end{aligned}\right\} \quad (A.1.4)$$

Thus

$$\underline{z}^{(i)} = \frac{\left(w_i' + jw_i''\right)\left(-\lambda_i' + j\lambda_i''\right)}{\lambda_i'^2 + \lambda_i''^2} \left(\underline{u}^{(i)'} + j\underline{u}^{(i)''}\right)\left(1-e^{\lambda_i' \theta}\, e^{+j\lambda_i'' \theta}\right)$$

$$+ \frac{\left(w_i' - jw_i''\right)\left(-\lambda_i' - j\lambda_i''\right)}{\lambda_i'^2 + \lambda_i''^2} \left(\underline{u}^{(i)'} - j\underline{u}^{(i)''}\right)\left(1-e^{\lambda_i' \theta}\, e^{-j\lambda_i'' \theta}\right) \quad (A.1.5)$$

Recall

$$\left.\begin{aligned} e^{j\lambda_i''\theta} &= \cos\lambda_i''\theta + j\sin\lambda_i''\theta \\ e^{-j\lambda_i''\theta} &= \cos\lambda_i''\theta - j\sin\lambda_i''\theta \end{aligned}\right\} \qquad (A.1.6)$$

Substitute (A.1.6) into (A.1.5), expand and rearrange

$$\begin{aligned} \underline{z}^{(i)} = &\left\{\left(-2\,\frac{w_i'\lambda_i' + w_i''\lambda_i''}{\lambda_i'^2+\lambda_i''^2}\right)\left(1-e^{\lambda_i'\theta}\cos\lambda_i''\theta\right)\right. \\ &\left. -\left(-2\,\frac{w_i''\lambda_i' - w_i'\lambda_i''}{\lambda_i'^2+\lambda_i''^2}\right)e^{\lambda_i'\theta}\sin\lambda_i''\theta\right\}\underline{u}^{(i)'} \\ + &\left\{-\left(-2\,\frac{w_i''\lambda_i' - w_i'\lambda_i''}{\lambda_i'^2+\lambda_i''^2}\right)\left(1-e^{\lambda_i'\theta}\cos\lambda_i''\theta\right)\right. \\ &\left. -\left(-2\,\frac{w_i'\lambda_i' + w_i''\lambda_i''}{\lambda_i'^2+\lambda_i''^2}\right)\sin\lambda_i''\theta\right\}\underline{u}^{(i)''} \end{aligned} \qquad (A.1.7)$$

Define

$$\begin{aligned} W_i' &= \frac{-2\left(w_i'\lambda_i' + w_i''\lambda_i''\right)}{\lambda_i'^2+\lambda_i''^2} \\ W_i'' &= \frac{-2\left(w_i''\lambda_i' - w_i'\lambda_i''\right)}{\lambda_i'^2+\lambda_i''^2} \end{aligned} \qquad (A.1.8)$$

Substitution into (A.1.7) gives

$$\begin{aligned} \underline{z}^{(i)} = &\left[W_i'\left(1-e^{\lambda_i'\theta}\cos\lambda_i''\theta\right) - W_i''\,e^{\lambda_i'\theta}\sin\lambda_i''\theta\right]\underline{u}^{(i)'} \\ + &\left[-W_i''\left(1-e^{\lambda_i'\theta}\cos\lambda_i''\theta\right) - W_i'\,e^{\lambda_i'\theta}\sin\lambda_i''\theta\right]\underline{u}^{(i)''} \end{aligned} \qquad (A.1.9)$$

Equation (A.1.9) demonstrates that the response of complex conjugate modes may be treated as the response of two real modes and should be compared with Eq. (2.12).

For decay following initial conditions a derivation similar to the one above gives the response contributed by a complex conjugate pair of modes as

$$\underline{z}^{(i)} = 2\left[\left(\underline{v}^{(i)'}\right)^T \underline{z}(0) \cos \lambda_i''\theta - \left(\underline{v}^{(i)''}\right)^T \underline{z}(0) \sin \lambda_i''\theta\right] e^{\lambda_i'\theta}\, \underline{u}^{(i)'}$$
$$+ 2\left[-\left(\underline{v}^{(i)''}\right)^T \underline{z}(0) \cos \lambda_i''\theta - \left(\underline{v}^{(i)'}\right)^T \underline{z}(0) \sin \lambda_i''\theta\right] e^{\lambda_i'\theta}\, \underline{u}^{(i)''} \qquad \text{(A.1.10)}$$

A.2 A Limiting Case for Modal Analysis

When a process is a simple cascade of identical stages with unidirectional flow such that no stage is influenced by those downstream, then the state space matrix takes the form shown by Eq. (2.15). Such a matrix has identical eigenvalues of multiplicity n and only one independent right eigenvector. Here a simple example is examined to reveal the nature of the modes when the degenerate situation is approached.

Consider the process obeying

$$\dot{\underline{z}} = \begin{bmatrix} -1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix} \underline{z} \qquad \text{(A.2.1)}$$

which has eigenvalues $\lambda_1 = \lambda_2 = \lambda_3 = -1$ and eigenvectors

$$\underline{u} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \underline{v} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \tag{A.2.2}$$

The right and left eigenvectors do not span the space, and therefore the usual modal representation does not apply. In addition the right and left eigenvectors are orthogonal ($\underline{u}^T\underline{v} = 0$). The response following an initial condition $\underline{z}(0)$ is given by

$$\left.\begin{aligned} z_1 &= z_1(0)e^{-\theta} + z_2(0)\theta e^{-\theta} + z_3(0)\theta^2 e^{-\theta} \\ z_2 &= z_2(0)e^{-\theta} + z_3(0)\theta e^{-\theta} \\ z_3 &= z_3(0)e^{-\theta} \end{aligned}\right\} \tag{A.2.3}$$

There is only one time constant, and the coefficients are time dependent.

A perturbed process that would result from making the stages slightly different from each other is

$$\dot{\underline{z}} = \begin{bmatrix} -1+\delta & 1-\epsilon & 0 \\ 0 & -1+\epsilon & 1 \\ 0 & 0 & -1 \end{bmatrix} \underline{z} \tag{A.2.4}$$

where δ and ϵ are small numbers.

The eigenvalues and eigenvectors are

$$\lambda_1 = -1 + \delta \qquad \underline{u}^{(1)} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \quad , \quad \underline{v}^{(1)} = \begin{bmatrix} 1 \\ \frac{1-\epsilon}{\delta-\epsilon} \\ \frac{1-\epsilon}{\delta(\delta-\epsilon)} \end{bmatrix} \tag{A.2.5}$$

$$\lambda_2 = -1 + \epsilon \qquad \underline{u}^{(2)} = \begin{bmatrix} 1 \\ \frac{\epsilon-\delta}{1-\epsilon} \\ 0 \end{bmatrix}, \quad \underline{v}^{(2)} = \begin{bmatrix} 0 \\ \frac{1-\epsilon}{\epsilon-\delta} \\ \frac{1-\epsilon}{\epsilon(\epsilon-\delta)} \end{bmatrix}$$

$$\lambda_3 = -1 \qquad \underline{u}^{(3)} = \begin{bmatrix} 1 \\ -\frac{\delta}{1-\epsilon} \\ \frac{\delta\epsilon}{1-\epsilon} \end{bmatrix}, \quad \underline{v}^{(3)} = \begin{bmatrix} 0 \\ 0 \\ \frac{1-\epsilon}{\delta\epsilon} \end{bmatrix} \qquad \text{(A.2.5)}$$

Wilkinson[64] analyzes perturbed matrices of this type in depth. Now consider the decay of the process following an initial condition, $\underline{z}(0)$, for which the activations of the modes, $\hat{w}_i = \underline{v}^{(i)T}\underline{z}(0)$, are

$$\left.\begin{aligned} \hat{w}_1 &= z_1(0) + z_2(0)\,\frac{(1-\epsilon)}{(\delta-\epsilon)} + z_3(0)\,\frac{(1-\epsilon)}{\delta(\delta-\epsilon)} \\ \hat{w}_2 &= z_2(0)\,\frac{(1-\epsilon)}{(\epsilon-\delta)} + z_3(0)\,\frac{(1-\epsilon)}{\epsilon(\epsilon-\delta)} \\ \hat{w}_3 &= z_3(0)\,\frac{(1-\epsilon)}{\delta\epsilon} \end{aligned}\right\} \qquad \text{(A.2.6)}$$

The state vector is given by

$$\underline{z} = \hat{w}_1 \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} e^{(-1+\delta)\theta} + \hat{w}_2 \begin{bmatrix} 1 \\ \frac{\epsilon-\delta}{1-\epsilon} \\ 0 \end{bmatrix} e^{(-1+\epsilon)\theta} + \hat{w}_3 \begin{bmatrix} 1 \\ -\frac{\delta}{1-\epsilon} \\ \frac{\delta\epsilon}{1-\epsilon} \end{bmatrix} e^{-\theta} \qquad \text{(A.2.7)}$$

Expansion of (A.2.7) gives

$$\left.\begin{aligned} z_1 &= z_1(0)e^{-(1-\delta)\theta} + z_2(0)\frac{(1-\epsilon)}{(\delta-\epsilon)}\left[e^{-(1-\delta)\theta} - e^{-(1-\epsilon)\theta}\right] \\ &\quad + z_3(0)\left[\frac{(1-\epsilon)(\delta-\epsilon) + \epsilon(1-\epsilon)e^{-(1-\delta)\theta} + \delta(1-\epsilon)e^{-(1-\epsilon)\theta}}{\delta\epsilon(\delta-\epsilon)}\right] \\ z_2 &= z_2(0)e^{-(1-\epsilon)\theta} + z_3(0)\left[\frac{e^{-(1-\epsilon)\theta} - e^{-\theta}}{\epsilon}\right] \\ z_3 &= z_3(0)e^{-\theta} \end{aligned}\right\} \quad (A.2.8)$$

The second terms of the expressions for both z_1 and z_2 show that the response involves a difference between two exponentials having nearly the same time constants and identical large activations. Thus the response calculation becomes very susceptible to errors when the degenerate situation is approached. Symptoms of this situation are closely spaced eigenvalues and nearly orthogonal right and left eigenvectors.

A.3 Eigenvalues and Eigenvectors for a Partially Decoupled Matrix (Model 3)

The character of the modes for a formulation such as Model 3 has been examined by Rosenbrock,[53] but the analysis is repeated here. This analysis applies to any matrix that may be partitioned as

$$\underline{\underline{A}} = \left[\begin{array}{c|c} \underline{\underline{Q}} & \underline{\underline{0}} \\ \hline \underline{\underline{S}} & \underline{\underline{R}} \end{array}\right] \quad (A.3.1)$$

Because $\det(\underline{\underline{A}}) = \det(\underline{\underline{Q}})\det(\underline{\underline{R}})$, the eigenvalues of $\underline{\underline{A}}$ must be either eigenvalues of $\underline{\underline{Q}}$, λ_i^q, or eigenvalues of $\underline{\underline{R}}$, λ_i^r. First consider eigenvalues of $\underline{\underline{Q}}$.

$$\underline{\underline{A}}\ \underline{u}_q^{(i)} = \lambda_i^q\ \underline{u}_q^{(i)} \qquad (A.3.2)$$

Partition $\underline{u}_q$ as

$$\underline{u}_q = \begin{bmatrix} \underline{u}_{q1} \\ - - - - \\ \underline{u}_{q2} \end{bmatrix} \qquad (A.3.3)$$

Now

$$\left[\begin{array}{c|c} \underline{\underline{Q}} - \lambda_i^q \underline{\underline{I}} & \underline{\underline{0}} \\ - - - - - - & - - - - - - \\ \underline{\underline{S}} & \underline{\underline{R}} - \lambda_i^q \underline{\underline{I}} \end{array}\right] \left[\begin{array}{c} \underline{u}_{q1}^{(i)} \\ - - - \\ \underline{u}_{q2}^{(i)} \end{array}\right] = \underline{0} \qquad (A.3.4)$$

Eq. (A.3.4) decomposes to

$$\left(\underline{\underline{Q}} - \lambda_i^q \underline{\underline{I}}\right) \underline{u}_{q1}^{(i)} = \underline{0} \qquad (A.3.5)$$

which defines $\underline{u}_{q1}^{(i)}$, and

$$\underline{\underline{S}}\ \underline{u}_{q1}^{(i)} + \left[\underline{\underline{R}} - \lambda_i^q \underline{\underline{I}}\right] \underline{u}_{q2}^{(i)} = \underline{0} \qquad (A.3.6)$$

so that

$$\underline{u}_{q2}^{(i)} = -\left[\underline{\underline{R}} - \lambda_i^q \underline{\underline{I}}\right]^{-1} \underline{\underline{S}}\ \underline{u}_{q1}^{(i)} \qquad (A.3.7)$$

Right eigenvectors corresponding to eigenvalues of $\underline{\underline{R}}$ are found by a similar procedure. In this case

$$\underline{u}_{r1}^{(i)} = \underline{0} \qquad (A.3.8)$$

and $\underline{u}_{r2}^{(i)}$ is defined by

$$\left[\underline{\underline{R}} - \lambda_i^r \underline{\underline{I}}\right] \underline{u}_{r2}^{(i)} = \underline{0} \qquad \text{(A.3.9)}$$

The left eigenvectors are determined in the same way.

In Model 3 submatrix $\underline{\underline{Q}}$ contains a representation of the column hydraulics, while $\underline{\underline{R}}$ describes the behavior of chemical species. Thus the modes associated with $\underline{\underline{Q}}$ are called hydraulic modes, and those associated with $\underline{\underline{R}}$ are called composition modes. The nature of the eigenvectors for each type are summarized as

hydraulic modes

$$\begin{aligned} \underline{u}_{q1} &= \text{right eigenvector of } \underline{\underline{Q}} \\ \underline{u}_{q2} &= \left[\lambda_i^q \underline{\underline{I}} - \underline{\underline{R}}\right]^{-1} \underline{\underline{S}}\, \underline{u}_{q1} \\ \underline{v}_{q1} &= \text{left eigenvector of } \underline{\underline{Q}} \\ \underline{v}_{q2} &= \underline{0} \end{aligned} \qquad \text{(A.3.10)}$$

composition modes

$$\begin{aligned} \underline{u}_{r1} &= \underline{0} \\ \underline{u}_{r2} &= \text{right eigenvector of } \underline{\underline{R}} \\ \underline{v}_{r1}^T &= \underline{v}_{r2}^T \underline{\underline{S}} \left(\lambda^r \underline{\underline{I}} - \underline{\underline{Q}}\right)^{-1} \\ \underline{v}_{r2} &= \text{left eigenvector of } \underline{\underline{R}} \end{aligned} \qquad \text{(A.3.11)}$$

A.4 Eigenvalue Sensitivities [61]

The sensitivity of an eigenvalue to changes in the value of any parameter, α, that affects matrix $\underline{\underline{A}}$ is derived in terms of the right and left eigenvectors by taking partial derivatives of both sides of Eq. (2.4) with respect to the parameter

$$\frac{\partial \underline{\underline{A}}}{\partial \alpha} \underline{u}^{(i)} + \underline{\underline{A}} \frac{\partial \underline{u}^{(i)}}{\partial \alpha} = \frac{\partial \lambda_i}{\partial \alpha} \underline{u}^{(i)} + \lambda_i \frac{\partial \underline{u}^{(i)}}{\partial \alpha} \qquad (A.4.1)$$

The scalar product of Eq. (A.4.1) with the left eigenvector $\underline{v}^{(i)}$ is formed. The eigenvectors are normalized so that

$$\underline{u}^{(i)T} \underline{v}^{(j)} = \delta_{ij} (\text{Kronecker delta}) \qquad (A.4.2)$$

and therefore

$$\left[\frac{\partial \underline{\underline{A}}}{\partial \alpha} \underline{u}^{(i)}\right]^T \underline{v}^{(i)} + \left[\underline{\underline{A}} \frac{\partial \underline{u}^{(i)}}{\partial \alpha}\right]^T \underline{v}^{(i)} = \frac{\partial \lambda_i}{\partial \alpha} + \left[\frac{\partial \underline{u}^{(i)}}{\partial \alpha}\right]^T \lambda_i \underline{v}^{(i)} \qquad (A.4.3)$$

Substitution of Eq. (2.10) leaves

$$\frac{\partial \lambda_i}{\partial \alpha} = \left[\frac{\partial \underline{\underline{A}}}{\partial \alpha} \underline{u}^{(i)}\right]^T \underline{v}^{(i)} \qquad (A.4.4)$$

A relative sensitivity, S, is given by

$$S = \frac{\alpha}{\lambda_i} \cdot \frac{\partial \lambda_i}{\partial \alpha} = \frac{\alpha}{\lambda_i} \left[\frac{\partial \underline{\underline{A}}}{\partial \alpha} \underline{u}^{(i)}\right]^T \underline{v}^{(i)} \qquad (A.4.5)$$

The cumulative effect of ℓ parameters is calculated by

$$S = \sum_{k=1}^{\ell} \frac{\alpha_k}{\lambda_i} \frac{\partial \lambda_i}{\partial \alpha_k} = \left[\sum_{k=1}^{\ell} \frac{\alpha_k}{\lambda_i} \frac{\partial \underline{\underline{A}}}{\partial \alpha_k} \underline{u}^{(i)}\right]^T \underline{v}^{(i)} \qquad (A.4.6)$$

When an eigenvalue is complex, the corresponding sensitivity also has a real part and an imaginary part.

Appendix B*

DISTILLATION COLUMN MODELS AND DATA

B.1 Model 1

Assumptions

1. Constant vapor holdup that is small compared to liquid holdup.
2. Perfect liquid mixing at every stage.
3. Adiabatic column.
4. Negligible dead time in downcomers and other piping.
5. Negligible holdup in condenser.
6. Constant liquid holdup in accumulator and reboiler.
7. Negligible thermal capacitance of column metal.
8. Stationary process described by linear differential equations for small perturbations from steady state.
9. Binary distillation, bubble-cap column, single feed stream, total condenser.

Equations for Plate i

(Numbering of plates is from bottom to top of column)

Mass balance for the liquid phase

$$\frac{d\tilde{H}_i}{d\theta} = \tilde{L}_{i+1} + \tilde{V}_{i-1} - \tilde{L}_i - \tilde{V}_i \qquad \text{(B.1.1)}$$

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* Some of the symbols and notation used in this appendix differ from usage elsewhere in this work. Consequently there is a separate table of nomenclature at the end of this section.

Light component balance for the liquid phase

$$\frac{d}{d\theta}\left(\tilde{x}_i\tilde{H}_i\right) = \tilde{L}_{i+1}\tilde{x}_{i+1} + \tilde{V}_{i-1}\tilde{y}_{i-1} - \tilde{L}_i\tilde{x}_i - \tilde{V}_i\tilde{y}_i \qquad (B.1.2)$$

Enthalpy balance for the liquid phase

$$c_i\frac{d}{d\theta}\left(\tilde{T}_i\tilde{H}_i\right) = c_{i+1}\tilde{L}_{i+1}\tilde{T}_{i+1} + \left(c_{i-1}\tilde{T}_{i-1} + \lambda_{i-1}\right)\tilde{V}_{i-1} - c_i\tilde{L}_i\tilde{T}_i - \left(c_i\tilde{T}_i + \lambda_i\right)\tilde{V}_i \qquad (B.1.3)$$

The balance equations are expressions for conservation of mass, chemical species, and enthalpy. In order to specify the system completely there are physical relationships among the variables that must be given.

Vapor-liquid equilibria[45d]

$$\frac{\tilde{y}_i}{\tilde{x}_i^*} = \frac{\gamma_i^{(1)}}{\tilde{P}_i}\exp\left(b_1 - a_1/\tilde{T}_i\right) \qquad (B.1.4)$$

$$\frac{1 - \tilde{y}_i}{1 - \tilde{x}_i^*} = \frac{\gamma_i^{(2)}}{\tilde{P}_i}\exp\left(b_2 - a_2/\tilde{T}_i\right) \qquad (B.1.5)$$

where the exponential terms account for the vapor pressure of the pure component and for deviations from the ideal gas law.

Activity coefficients (Van Laar)[45d]

$$\gamma_i^{(1)} = \exp\left[\frac{A_{12}}{\left(1 + \frac{A_{12}x_i}{A_{21}(1 - x_i)}\right)^2}\right]$$

$$\gamma_i^{(2)} = \exp\left[\frac{A_{21}}{\left(1 + \frac{A_{21}(1 - x_i)}{A_{12}x_i}\right)^2}\right] \qquad (B.1.6)$$

Murphree plate efficiency

$$E_i = \frac{\tilde{x}_{i+1} - \tilde{x}_i}{\tilde{x}_{i+1} - \tilde{x}_i^*} \qquad \text{(B.1.7)}$$

Vapor flow relationship

Vapor flow is determined by the pressure drop through the bubble-cap slots by an orifice-type equation[37,44a]

$$\tilde{V}_i \propto \left(\tilde{P}_i - \tilde{P}_{i+1} - \text{liquid head}\right)^{1/2}$$

$$\tilde{V}_i = \beta\left(\frac{\tilde{P}_i}{R\tilde{T}_i}\right)^{1/2}\left[\left(\tilde{P}_i - \tilde{P}_{i+1}\right)\frac{14.7 \times 144\ g_c}{M_V} - \frac{\tilde{H}_{i+1}}{A_T}\, g\, \frac{M_L}{M_V}\right]^{1/2}(14.7 \times 144)^{1/2} \qquad \text{(B.1.8)}$$

Plate hydraulics

Liquid flow rate depends on the height of liquid above the weir, but the holdup is influenced by vapor flow rate. A relationship among these variables can be expressed by one equation. Here it is given in linear form, and as a consequence can apply only over a limited range of operating conditions. A more general equation might incorporate the Francis weir formula.[25]

$$\tilde{H}_i - H_w = \alpha_i' \tilde{L}_i - \kappa_i' \tilde{V}_{i-1} \qquad \text{(B.1.9)}$$

where

$$\alpha_i' = \alpha A_T\left(\frac{60 \times 7.48}{12}\right) \text{ sec} \qquad \text{(B.1.10)}$$

and

$$\kappa_i' = \kappa\, \frac{A_T}{12\, A_B}\left(\frac{\rho_L}{\rho_V}\frac{M_V}{M_L}\right) \text{ sec}$$

α and κ are coefficients determined empirically.

Normalized Equations

The equations are put into dimensionless form, because it is usual practice and for two additional reasons. First the numerical procedures tend to be more stable when the matrix coefficients do not cover a wide range of magnitudes. Second, the eigenvector elements corresponding to variables whose dimensional values change the least during transients will tend to be insignificant so that these variables cannot be followed. The nondimensionalizing parameters are chosen to yield dimensionless values of order unity for the dependent steady state variables.

The parameters used for nondimensionalization of the variables are the steady state reflux rate $\bar{L}_{N+1}$, and the residual holdup H_w, which is approximately the steady state holdup on a plate. Also used are the vapor pressure $P_N^{o(1)}$, the heat capacity c^o, and the heat of vaporization λ^o, all evaluated for the light component at the steady state temperature of the top plate. Time is made dimensionless by the approximate time for change of inventory on a plate at steady state, $\frac{H_w}{\bar{L}_{N+1}}$. Temperature is divided by λ^o/c^o, which is the temperature rise for one mole of the light component that corresponds to the same enthalpy increase as the vaporization of one mole. The dimensionless heat transfer resistances are the dimensional resistances divided by the resistance to convective transport of heat down the column, $c^o\bar{L}_{N+1}$. The dimensionless variables and properties are summarized as follows:

$$\text{time} \qquad \phi = \theta \frac{\bar{L}_{N+1}}{H_w}$$

$$\text{flow} \qquad \tilde{\ell} = \frac{\tilde{L}}{\bar{L}_{N+1}}$$

$$\text{temperature} \qquad \tilde{t} = \frac{\tilde{T}c^o}{\lambda^o}$$

pressure $\tilde{p} = \dfrac{\tilde{P}}{P_N^{O(1)}}$

holdup $\tilde{h} = \tilde{H}/H_w$

heat capacity $c' = c/c^O$

heat of vaporization $\lambda' = \lambda/\lambda^O$

heat transfer resistance $U' = UA/c^O\bar{L}_{N+1}$

The dimensionless equations then are

$$\frac{d\tilde{h}_i}{d\phi} = \tilde{\ell}_i + \tilde{v}_{i-1} - \tilde{\ell}_i - \tilde{v}_i \qquad \text{(B.1.1-a)}$$

$$\frac{d}{d\phi}\left(\tilde{x}_i\tilde{h}_i\right) = \tilde{\ell}_{i+1}\tilde{x}_{i+1} + \tilde{v}_{i-1}\tilde{y}_{i-1} - \tilde{\ell}_i\tilde{x}_i - \tilde{v}_i\tilde{y}_i \qquad \text{(B.1.2-a)}$$

$$c_i' \frac{d}{d\phi}\left(\tilde{t}_i\tilde{h}_i\right) = c_{i+1}'\tilde{\ell}_{i+1}\tilde{t}_{i+1} + \left(c_{i-1}'\tilde{t}_{i-1} + \lambda_{i-1}'\right)\tilde{v}_{i-1} - c_i'\tilde{\ell}_i\tilde{t}_i - \left(c_i'\tilde{t}_i + \lambda_i'\right)\tilde{v}_i \qquad \text{(B.1.3-a)}$$

$$\frac{\tilde{y}_i}{\tilde{x}_i^*} = \frac{\gamma_i^{(1)}}{\tilde{p}_i}\frac{\exp\left(b_1 - a_1'/\tilde{t}_i\right)}{P_N^{O(1)}} \qquad \text{(B.1.4-a)}$$

$$\frac{1 - \tilde{y}_i}{1 - \tilde{x}_i^*} = \frac{\gamma_i^{(2)}}{\tilde{p}_i}\frac{\exp\left(b_2 - a_2'/\tilde{t}_i\right)}{P_N^{O(1)}} \qquad \text{(B.1.5-a)}$$

$$\tilde{v}_i = \beta_i'\left[\frac{\tilde{p}_i}{\tilde{t}_i}\left(\tilde{p}_i - \tilde{p}_{i+1} - \nu_i'\tilde{h}_{i+1}\right)\right]^{1/2} \qquad \text{(B.1.8-a)}$$

$$\tilde{h}_i = 1 + \alpha_i''\tilde{\ell}_i - \kappa_i''\tilde{v}_{i-1} \qquad \text{(B.1.9-a)}$$

The coefficients in the dimensionless equations are

$$\alpha_i'' = \alpha_i' \frac{\bar{L}_{N+1}}{H_w} \qquad \text{(B.1.10-a)}$$

$$\kappa_i'' = \kappa_i' \frac{\bar{L}_{N+1}}{H_w} \qquad \text{(B.1.11-a)}$$

$$\beta_i' = \beta \frac{P_N^{0(1)}}{\bar{L}_{N+1}} \left(\frac{c^0 g_c}{\lambda^0 R M_V} \right)^{1/2} \times 14.7 \times 144 \qquad \text{(B.1.12)}$$

$$\nu_i' = \frac{M_L}{P_N^{0(1)}} \frac{g}{g_c} \frac{H_w}{A_T} \frac{1}{14.7 \times 144} \qquad \text{(B.1.13)}$$

Linearization of the equations is carried out with all time dependent variables taken as the sum of a steady state component and a deviation component; for example

$$\tilde{\ell}_i = \bar{\ell}_i + \ell_i$$

Then products involving the deviation variables are assumed to be negligible. When the balance equations (B.1.1-3) are decomposed in this way, the corresponding steady state equations may be subtracted. The component and enthalpy balance equations involve the time derivative of holdup, which is eliminated by use of the total mass balance, Eqn. B.1.1. The resulting simplified, linear balances are:

$$\frac{dh_i}{d\phi} = \ell_{i+1} + v_{i-1} - \ell_i - v_i \qquad \text{(B.1.14)}$$

$$\bar{h}_i \frac{dx_i}{d\phi} = \bar{\ell}_{i+1} x_{i+1} + \left(\bar{x}_{i+1} - \bar{x}_i \right) \ell_{i+1} + \bar{v}_{i-1} y_{i-1} + \left(\bar{y}_{i-1} - \bar{x}_i \right) v_{i-1} - \bar{\ell}_i x_i - \bar{v}_i y_i - \left(\bar{y}_i - \bar{x}_i \right) v_i \qquad \text{(B.1.15)}$$

$$c_i' \bar{h}_i \frac{dt_i}{d\phi} = c_{i+1}' \bar{\ell}_{i+1} t_{i+1} + \left(c_{i+1}' \bar{t}_{i+1} - c_i' \bar{t}_i\right) \ell_{i+1}$$
$$+ \left(c_{i-1}' \bar{t}_{i-1} - c_i' \bar{t}_i\right) v_{i-1} + c_{i-1}' \bar{v}_{i-1} t_{i-1}$$
$$+ \lambda_{i-1}' v_{i-1} - \left(c_i' \bar{\ell}_i + c_i' \bar{v}_i\right) t_i - \lambda_i' v_i \qquad \text{(B.1.16)}$$

The remaining relationships are linearized by use of Taylor series expansions about the steady state in which terms containing derivatives of higher order than first are eliminated. The steady state relationships are subtracted to give equations in the deviation variables. For example, Eq. (B.1.4) is linearized by

$$y_i = \left(\frac{\partial \tilde{y}_i}{\partial \tilde{x}_i^*}\right)_{ss} x_i^* + \left(\frac{\partial \tilde{y}_i}{\partial \tilde{p}_i}\right)_{ss} p_i + \left(\frac{\partial \tilde{y}_i}{\partial \tilde{t}_i}\right)_{ss} t_i$$

and the result is

$$y_i = \left[\gamma_i(1) \frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{\bar{p}_i \, P_N^{O(1)}}\right] x_i^* + \left[-\gamma_i(1)_{\bar{x}_i^*} \frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{\bar{p}_i^2 \, P_N^{O(1)}}\right] p_i$$
$$+ \left[\frac{a_1'}{\bar{t}_i^2} \gamma_i(1)_{x_i^*} \frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{\bar{p}_i \, P_N^{O(1)}}\right] t_i \qquad \text{(B.1.17)}$$

where x_i^* is related to x_i through the Murphree efficiency relation

$$x_i^* = \frac{x_i}{E_i} - x_{i+1} \frac{\left(1 - E_i\right)}{E_i} \qquad \text{(B.1.18)}$$

Eq. (B.1.8-a) is linearized to give

$$v_i = \left[\frac{1}{2}\frac{\beta_i'^2}{\bar{v}_i}\left(2\frac{\bar{p}_i}{\bar{t}_i} - \frac{\bar{p}_{i+1}}{\bar{t}_i} - \frac{\nu_i'\bar{h}_{i+1}}{\bar{t}_i}\right)\right]p_i + \left[\frac{1}{2}\frac{\beta_i'^2}{\bar{v}_i}\left(-\frac{\bar{p}_i}{\bar{t}_i}\right)\right]p_{i+1} - \left[\frac{1}{2}\frac{\bar{v}_i}{\bar{t}_i}\right]t_i + \left[\frac{1}{2}\frac{\beta_i'^2}{\bar{v}_i}\left(-\nu_i'\frac{\bar{p}_i}{\bar{t}_i}\right)\right]h_{i+1} \tag{B.1.19}$$

and Eq. (B.1.9-a) becomes

$$\ell_i = G_i\left(h_i + \kappa_i'' v_{i-1}\right) \tag{B.1.20}$$

$$\text{where} \quad G_i = \frac{1}{\alpha_i''}$$

An expression for total pressure is found by summation of the partial pressures which may be obtained from Eqs. (B.1.4) and (B.1.5).

$$\tilde{p}_i = \tilde{p}_i\tilde{y}_i + \tilde{p}_i\left(1 - \tilde{y}_i\right)$$

After linearization

$$p_i = \eta_i x_i^* + \psi_i t_i \tag{B.1.21}$$

where

$$\eta_i = \frac{\gamma_i^{(1)}}{P_N^{0(1)}}\exp\left(b_1 - a_1'/\bar{t}_i\right) - \frac{\gamma_i^{(2)}}{P_N^{0(1)}}\exp\left(b_2 - a_2'/\bar{t}_i\right) \tag{B.1.22}$$

$$\psi_i = \frac{1}{\bar{t}_i^2}\left[a_1'\gamma_i^{(1)}\bar{x}_i^*\frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{P_N^{0(1)}} + a_2'\gamma_i^{(2)}\left(1 - \bar{x}_i^*\right)\frac{\exp\left(b_2 - a_2'/\bar{t}_i\right)}{P_N^{0(1)}}\right] \tag{B.1.23}$$

Now the linear formulation is embodied in Eqs. (B.1.14) through (B.1.21), and the variables for each plate are h_i, x_i, t_i, ℓ_i, v_i, p_i, y_i, x_i^*. The balance equations (B.1.14-16) may be expressed in terms of any three of these; the ones chosen are h_i, x_i, and t_i. Thus explicit

expressions for ℓ_i, v_i, p_i, x_i^*, and y_i in terms of the other three are required. Straightforward manipulation of the preceding equations yields these expressions

$$y_i = \frac{\zeta_i}{E_i} x_i - \zeta_i \frac{\left(1 - E_i\right)}{E_i} x_{i+1} + \mu_i t_i \qquad \text{(B.1.24-a)}$$

where

$$\zeta_i = \left[\gamma_i(1) \frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{\bar{p}_i \, P_N^{O(1)}}\right]\left(1 - \frac{\bar{x}_i^*}{\bar{p}_i} \eta_i\right) \qquad \text{(B.1.24-b)}$$

$$\mu_i = \left[\gamma_i(1)\bar{x}_i^* \frac{\exp\left(b_1 - a_1'/\bar{t}_i\right)}{\bar{p}_i \, P_N^{O(1)}}\right]\left(\frac{a_1'}{\bar{t}_i^2} - \frac{\psi_i}{\bar{p}_i}\right) \qquad \text{(B.1.24-c)}$$

$$p_i = \frac{\eta_i}{E_i} x_i - \frac{\eta_i}{E_i}\left(1 - E_i\right)x_{i+1} + \psi_i t_i \qquad \text{(B.1.25)}$$

$$v_i = \xi_i h_{i+1} + \tau_i x_i + \sigma_i x_{i+1} + \hat{\sigma}_i x_{i+2} + \delta_i t_i + \epsilon_i t_{i+1} \qquad \text{(B.1.26)}$$

where

$$\xi_i = -\frac{1}{2} \frac{\beta_i'^2}{\bar{v}_i} \frac{\bar{p}_i}{\bar{t}_i} \nu_i' \qquad \text{(B.1.27)}$$

$$\tau_i = \frac{1}{2} \frac{\beta_i'^2}{\bar{v}_i} \frac{\eta_i}{E_i}\left(2\bar{p}_i - \bar{p}_{i+1} - \nu_i'\bar{h}_{i+1}\right)/\bar{t}_i \qquad \text{(B.1.28)}$$

$$\sigma_i = -\tau_i\left(1 - E_i\right) + \xi_i \frac{\eta_{i+1}}{E_{i+1}\nu_i'} \qquad \text{(B.1.29)}$$

$$\hat{\sigma}_i = -\xi_i \frac{\eta_{i+1}}{\nu_i'} \frac{\left(1 - E_{i+1}\right)}{E_{i+1}} \qquad \text{(B.1.30)}$$

$$\delta_i = \tau_i \frac{\psi_i E_i}{\eta_i} - \frac{1}{2} \frac{\bar{v}_i}{\bar{t}_i} \qquad \text{(B.1.31)}$$

$$\epsilon_i = \xi_i \frac{\psi_{i+1}}{\nu_i} \qquad \text{(B.1.32)}$$

In terms of holdups, compositions and temperatures only, the balance equations for plate i are

$$\begin{aligned}
\frac{dh_i}{d\phi} &= \left[\xi_{i-1}\left(1 - G_i K_i''\right) - G_i\right] h_i + \left[G_i + \xi_i\left(G_{i+1} K_{i+1}'' - 1\right)\right] h_{i+1} \\
&+ \left[\tau_{i-1}\left(1 - G_i K_i''\right)\right] x_{i-1} + \left[\tau_i\left(G_{i+1} K_{i+1}'' - 1\right) + \sigma_{i-1}\left(1 - G_i K_i''\right)\right] x_i \\
&+ \left[\sigma_i\left(G_{i+1} K_{i+1}'' - 1\right) + \hat{\sigma}_{i-1}\left(1 - G_i K_i''\right)\right] x_{i+1} + \left[\hat{\sigma}_i\left(G_{i+1} K_{i+1}'' - 1\right)\right] x_{i+2} \\
&+ \left[\delta_{i-1}\left(1 - G_i K_i''\right)\right] t_{i-1} + \left[\delta_i\left(G_{i+1} K_{i+1}'' - 1\right) + \epsilon_{i-1}\left(1 - G_i K_i''\right)\right] t_i \\
&+ \left[\epsilon_i\left(G_{i+1} K_{i+1}'' - 1\right)\right] t_{i+1} \qquad \text{(B.1.33)}
\end{aligned}$$

$$\begin{aligned}
\bar{h}_i \frac{dx_i}{d\phi} &= \left[\xi_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right)\right] h_i \\
&+ \left[\left(\bar{x}_{i+1} - \bar{x}_i\right) G_{i+1} + \xi_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right) G_{i+1} K_{i+1}'' - \bar{y}_i + \bar{x}_i\right\}\right] h_{i+1} \\
&+ \left[\tau_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right) + \frac{\zeta_{i-1}}{E_{i-1}} \bar{v}_{i-1}\right] x_{i-1} \\
&+ \left[-\zeta_{i-1} \bar{v}_{i-1} \frac{\left(1 - E_{i-1}\right)}{E_{i-1}} - \bar{\ell}_i - \bar{v}_i \frac{\zeta_i}{E_i} + \tau_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right) G_{i+1} K_{i+1}'' \right.\right. \\
&\qquad \left.\left. - \bar{y}_i + \bar{x}_i\right\} + \sigma_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right)\right] x_i \\
&+ \left[\bar{\ell}_{i+1} + \zeta_i \bar{v}_i \frac{\left(1 - E_i\right)}{E_i} + \sigma_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right) G_{i+1} K_{i+1}'' - \bar{y}_i + \bar{x}_i\right\} \right. \\
&\qquad \left. + \hat{\sigma}_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right)\right] x_{i+1}
\end{aligned}$$

$$+ \left[\hat{\sigma}_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right)G_{i+1}\kappa''_{i+1} - \bar{y}_i + \bar{x}_i\right\}\right]x_{i+2}$$

$$+ \left[\mu_{i-1}\bar{v}_{i-1} + \delta_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right)\right]t_i$$

$$+ \left[-\mu_i\bar{v}_i + \delta_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right)G_{i+1}\kappa''_{i+1} - \bar{y}_i + \bar{x}_i\right\} + \epsilon_{i-1}\left(\bar{y}_{i-1} - \bar{x}_i\right)\right]t_i$$

$$+ \left[\epsilon_i\left\{\left(\bar{x}_{i+1} - \bar{x}_i\right)G_{i+1}\kappa''_{i+1} - \bar{y}_i + \bar{x}_i\right\}\right]t_{i+1} \qquad \text{(B.1.34)}$$

$$c'_i\bar{h}_i\frac{dt_i}{d\phi} = \left[\xi_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right)\right]h_i$$

$$+ \left[G_{i+1}\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right) + \xi_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\}\right]h_{i+1}$$

$$+ \left[\tau_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right)\right]x_{i-1}$$

$$+ \left[\tau_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\} + \sigma_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right)\right]x_i$$

$$+ \left[\sigma_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\} + \hat{\sigma}_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right)\right]x_{i+1}$$

$$+ \left[\hat{\sigma}_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\}\right]x_{i+2}$$

$$+ \left[\delta_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right) + c'_{i-1}\bar{v}_{i-1}\right]t_{i-1}$$

$$+ \left[\delta_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\} + \epsilon_{i-1}\left(c'_{i-1}\bar{t}_{i-1} - c'_i\bar{t}_i + \lambda'_{i-1}\right)\right.$$

$$\left. - \left(c'_i\bar{\ell}_i + c'_i\bar{v}_i\right)\right]t_i$$

$$+ \left[\epsilon_i\left\{\left(c'_{i+1}\bar{t}_{i+1} - c'_i\bar{t}_i\right)G_{i+1}\kappa''_{i+1} - \lambda'_i\right\} + c'_{i+1}\bar{\ell}_{i+1}\right]t_{i+1}$$

(B.1.35)

Equations for the Feed Plate

The feed is assumed to be entirely liquid, which may be subcooled. The balance equations are modified for the feed plate (plate j) as follows

$$\frac{dh_j}{d\phi} = \left[\text{R.H.S. Eq. (B.1.33)}\right] + f \qquad \text{(B.1.36)}$$

$$\bar{h}_j \frac{dx_j}{d\phi} = \left[\text{R.H.S. Eq. (B.1.34)}\right] + \bar{f}x_F + \bar{x}_F f \qquad \text{(B.1.37)}$$

$$c'_j \bar{h}_j \frac{dt_j}{d\phi} = \left[\text{R.H.S. Eq. (B.1.35)}\right] + c'_F \bar{f} t_F + c'_F \bar{t}_F f \qquad \text{(B.1.38)}$$

where the notation R.H.S. means the right-hand side of the equation specified.

Equations for the Top Plate

Equations for plate N differ from those for the other plates because the reflux enters at the top and the vapor flow expression depends on the pressure drop in the overhead piping. When i = N,

$$\left.\begin{aligned} \xi_N = \epsilon_N = \sigma_N = 0 \\ \text{and} \qquad \zeta_{N+1} = \mu_{N+1} = G_{N+1} = 0 \\ E_{N+1} = 1 \end{aligned}\right\} \qquad \text{(B.1.39)}$$

The expression for the overhead vapor flow rate is derived in the next section (Eq. (B.1.48)). Its use along with Eq. (B.1.39) results in modified balance equations as follows

$$\frac{dh_N}{d\phi} = \left[\text{R.H.S. Eq. (B.1.33)}\right] + \ell_{n+1} + \psi_{n+1} Dt_{cw} \qquad \text{(B.1.40)}$$

$$\bar{h}_N \frac{dx_N}{d\phi} = \left[\text{R.H.S. Eq. (B.1.34)}\right] + \left(\bar{x}_{N+1} - \bar{x}_N\right)\ell_{N+1} + \left(\bar{y}_N - \bar{x}_N\right)\psi_{N+1}Dt_{cw} \tag{B.1.41}$$

$$c'_N\bar{h}_N \frac{dt_N}{d\phi} = \left[\text{R.H.S. Eq. (B.1.35)}\right] + \left(c'_{N+1}\bar{t}_{N+1} - c'_N\bar{t}_N\right)\ell_{N+1} + \lambda'_N\psi_{N+1}Dt_{cw} \tag{B.1.42}$$

Equations for the Condensing System

The condenser is divided into two sections, as shown in Figure B.1.1. The first condenses the vapor to give saturated liquid at temperature T_c, and the second subcools the liquid to temperature T_{sc}. Both the condensing and cooling sections are exposed to coolant at average temperature T_{cw}, but there is a different heat transfer resistance and driving force for each. The condenser efficiency, E_{N+1}, is taken as unity.

The heat balances for the condenser and cooler are

$$\tilde{V}_N\left(c_N\tilde{T}_c + \lambda_N\right) - \tilde{V}_N c_N\tilde{T}_c = h_c A_c\left(\tilde{T}_c - \tilde{T}_{cw}\right) \tag{B.1.43}$$

and

$$\tilde{V}_N c_N\left(\tilde{T}_c - \tilde{T}_{sc}\right) = h_{sc}A_{sc}\left(\frac{\tilde{T}_c + \tilde{T}_{sc}}{2} - \tilde{T}_{cw}\right) \tag{B.1.44}$$

where an average driving force has been used in the cooler.

The heat transfer resistances are calculated from steady state conditions as

$$\left.\begin{aligned} h_c A_c &= \frac{\bar{V}_N\lambda_N}{\bar{T}_c - \bar{T}_{cw}} \\ h_{sc}A_{sc} &= \frac{\bar{V}_N c_N\left(\bar{T}_c - \bar{T}_{sc}\right)}{\frac{1}{2}\left(\bar{T}_c + \bar{T}_{sc}\right) - \bar{T}_{cw}} \end{aligned}\right\} \tag{B.1.45}$$

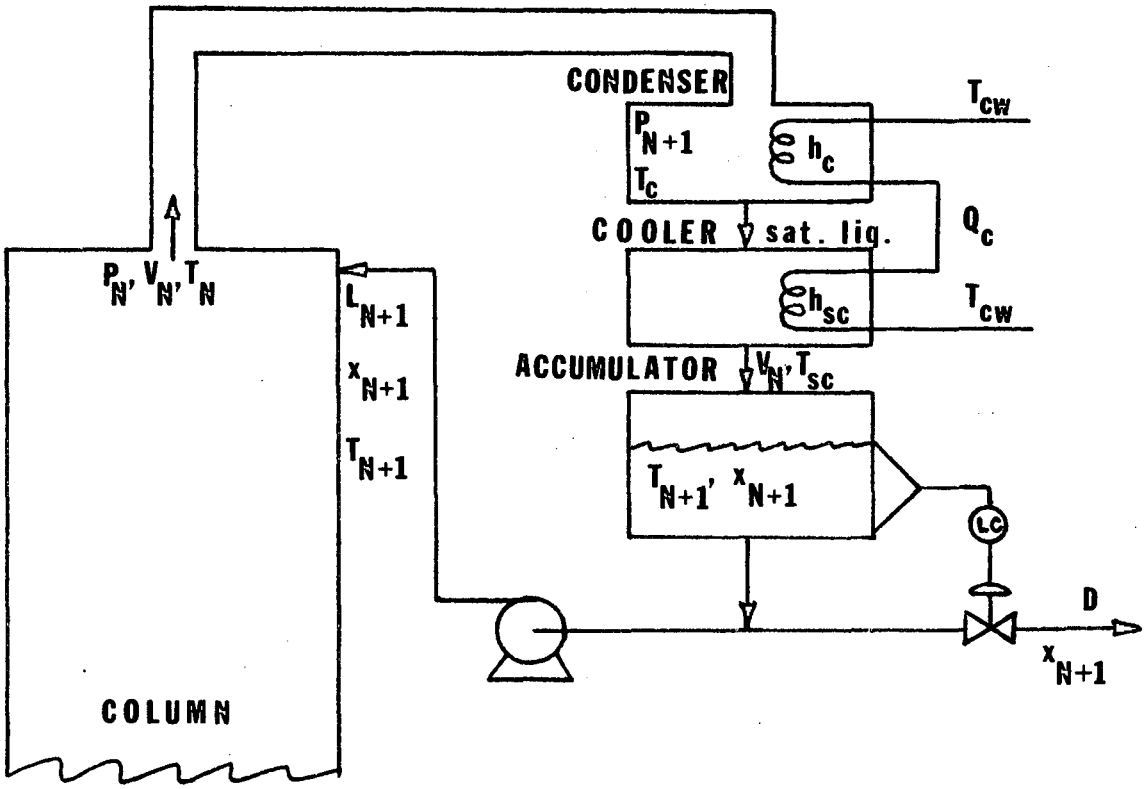

Fig. B.1.1 Schematic diagram of condensing system.

The condenser pressure is less than that on the top plate by an amount equal to the pressure drop in the overhead piping. This pressure drop determines the overhead vapor flow rate. Thus

$$\tilde{V}_N = \beta_N \left(\frac{\tilde{P}_N}{R\tilde{T}_N} \times 14.7 \times 144 \right)^{1/2} \left[\left(\tilde{P}_N - \tilde{P}_{N+1} \right) \frac{g_c}{M_V} \times 14.7 \times 144 \right]^{1/2} \qquad (B.1.46)$$

where β_N is evaluated by integration of the energy equation for compressible pipe flow, as shown in Appendix B.4. The result is

$$\beta_N = \left(\frac{2 D_p 5}{64 f_p Z} \right)^{1/2} \qquad (B.1.47)$$

The previous equations plus a dew pressure relation (from Eqns. (B.1.4-5)) serve to determine $\tilde{V}_N$, $\tilde{T}_c$, $\tilde{P}_{N+1}$ and $\tilde{T}_{sc}$. The expressions are made dimensionless and are linearized. Then substitution of some of the relations that were derived previously yields the final relations

$$v_N = \tau_N x_N + \sigma_N x_{N+1} + \delta_N t_N - \psi_{N+1} Dt_{cw} \qquad (B.1.48)$$

where

$$\tau_N = \frac{\frac{1}{2} \beta_N'^2 \left(\frac{1}{\bar{t}_N \bar{v}_N E_N} \right) \left[\eta_N \left(2\bar{p}_N - \bar{p}_{N+1} \right) - \bar{p}_N \eta_{N+1} \zeta_N \right]}{1 + \frac{1}{2} \beta_N'^2 \frac{\lambda_N'}{U_c'} \frac{\bar{p}_N \psi_{N+1}}{\bar{t}_N \bar{v}_N}} \qquad (B.1.49)$$

$$\sigma_N = \tau_N \left(1 - E_N \right) \qquad (B.1.50)$$

$$\delta_N = \frac{\frac{1}{2} \beta_N'^2 \left(\frac{1}{\bar{t}_N \bar{v}_N} \right) \left[\psi_N \left(2\bar{p}_N - \bar{p}_{N+1} \right) - \bar{p}_N \eta_{N+1} \mu_N \right] - \frac{1}{2} \frac{\bar{v}_N}{\bar{t}_N}}{1 + \frac{1}{2} \beta_N'^2 \frac{\lambda_N'}{U_c'} \psi_{N+1} \frac{\bar{p}_N}{\bar{t}_N \bar{v}_N}} \qquad (B.1.51)$$

$$D = \left(\frac{1}{2}\beta_N'^2 \frac{\bar{p}_N}{\bar{t}_N\bar{v}_N}\right) \Bigg/ \left(1 + \frac{1}{2}\frac{\lambda_N'}{U_c'}\psi_{N+1}\beta_N'^2 \frac{\bar{p}_N}{\bar{t}_N\bar{v}_N}\right) \tag{B.1.52}$$

Also

$$t_c = \tau_N \frac{\lambda_N'}{U_c'} x_N + \sigma_N \frac{\lambda_N'}{U_c'} x_{N+1} + \delta_N \frac{\lambda_N'}{U_c'} t_N + \left(1 - \frac{\lambda_N'\psi_{N+1}D}{U_c'}\right) t_{cw} \tag{B.1.53}$$

$$p_{N+1} = \left[\eta_{N+1}\frac{\zeta_N}{E_N} + \psi_{N+1}\tau_N\frac{\lambda_N'}{U_c'}\right] x_N + \left[-\eta_{N+1}\zeta_N\frac{(1 - E_N)}{E_N} + \psi_{N+1}\sigma_N\frac{\lambda_N'}{U_c'}\right] x_{N+1}$$
$$+ \left[\eta_{N+1}\mu_N + \psi_{N+1}\delta_N\frac{\lambda_N'}{U_c'}\right] t_N + \left[\frac{\psi_{N+1}}{1 + \frac{1}{2}\psi_{N+1}\frac{\lambda_N'}{U_c'}\beta_N'^2\frac{\bar{p}_N}{\bar{t}_N\bar{v}_N}}\right] t_{cw} \tag{B.1.54}$$

and finally

$$t_{sc} = (sc1)x_N + (sc2)x_{N+1} + (sc3)t_N + (sc4)t_{cw} \tag{B.1.55}$$

where

$$sc1 = \tau_N\left[\frac{\lambda_N'}{U_c'}\left(\bar{v}_N c_N' - \frac{U_{sc}'}{2}\right) + c_N'\left(\bar{t}_c - \bar{t}_{sc}\right)\right] \Bigg/ \left(\bar{v}_N c_N' + \frac{U_{sc}'}{2}\right) \tag{B.1.56}$$

$$sc2 = -sc1\left(1 - E_N\right) \tag{B.1.57}$$

$$sc3 = (sc1)\delta_N/\tau_N \tag{B.1.58}$$

$$sc4 = \frac{\left[U_{sc}' + \left(\bar{v}_N c_N' - \frac{1}{2}U_{sc}'\right)\left(1 - \frac{\lambda_N'\psi_{N+1}D}{U_c'}\right) - \psi_{N+1}Dc_N'\left(\bar{t}_c - \bar{t}_{sc}\right)\right]}{\bar{v}_N c_N' + \frac{1}{2}U_{sc}'} \tag{B.1.59}$$

and

$$\left.\begin{aligned} U_c' &= \frac{h_c A_c}{c^O \bar{L}_{N+1}} \\ U_{sc}' &= \frac{h_{sc} A_{sc}}{c^O \bar{L}_{N+1}} \end{aligned}\right\} \tag{B.1.60}$$

The balance equations for the accumulator are now derived in a straightforward manner (recall that the mass holdup is constant). The dimensionless component balance is

$$\bar{h}_{N+1} \frac{d\tilde{x}_{N+1}}{d\phi} = \tilde{v}_N \tilde{y}_N - \tilde{x}_{N+1} \tilde{v}_N \qquad \text{(B.1.61)}$$

When this equation is linearized and simplified by use of $\bar{y}_N = \bar{x}_{N+1}$ and previous relations, there results

$$\frac{dx_{N+1}}{d\phi} = \frac{\bar{v}_N}{\bar{h}_{N+1}} \left[\frac{\zeta_N}{E_N} x_N - \left(1 + \frac{1 - E_N}{E_N} \zeta_N \right) x_{N+1} + \mu_N t_N \right] \qquad \text{(B.1.62)}$$

The dimensionless enthalpy balance is

$$c'_{N+1} \bar{h}_{N+1} \frac{dt_{N+1}}{d\phi} = \tilde{v}_N \left[c'_{N+1} \tilde{t}_{sc} - c'_{N+1} \tilde{t}_{N+1} \right] \qquad \text{(B.1.63)}$$

When this equation is linearized and t_{sc} is eliminated by Eq. (B.1.48) it becomes

$$\frac{dt_{N+1}}{d\phi} = \frac{\bar{v}_N}{\bar{h}_{N+1}} \left[(sc1)x_N + (sc2)x_{N+1} + (sc3)t_N - t_{N+1} + (sc4)t_{cw} \right] \qquad \text{(B.1.64)}$$

Equations for the Reboiler

The reboiler behaves much as a plate except that the holdup is constant and heat is transferred to the liquid from steam. The bottom product stream is taken from the reboiler. The three balance equations in dimensionless form are

$$\ell_1 - \ell_0 - v_0 = 0 \qquad \text{(B.1.65)}$$

$$\bar{h}_0 \frac{dx_0}{d\phi} = \ell_1 x_1 - \ell_0 x_0 - v_0 y_0 \qquad \text{(B.1.66)}$$

$$c_0' \bar{h}_0 \frac{dt_0}{d\phi} = c_1' t_1 \ell_1 - c_0' t_0 \ell_0 - \left(c_0' t_0 + \lambda_0'\right) v_0 + U_r' \left(t_s - t_0\right) \qquad \text{(B.1.67)}$$

$$\text{where} \qquad U_r' = \frac{h_r A_r}{c^0 \bar{L}_{N+1}} \qquad \text{(B.1.68-a)}$$

The heat transfer coefficient is evaluated from steady state conditions by

$$h_r A_r = \frac{Q_r}{\bar{T}_s - \bar{T}_0} \qquad \text{(B.1.68-b)}$$

When the equations are linearized and expressed in terms of state variables by a procedure similar to that for a plate, they take the form

$$\begin{aligned}
\bar{h}_0 \frac{dx_0}{d\phi} &= \left[G_1\left(\bar{x}_1 - \bar{x}_0\right)\left(1 + \kappa_1'' \xi_0\right) + \xi_0\left(\bar{x}_0 - \bar{y}_0\right)\right] h_1 \\
&+ \left[-\bar{\ell}_0 - \bar{v}_0 \frac{\zeta_0}{E_0} + \left(\bar{x}_1 - \bar{x}_0\right) G_1 \kappa_1'' \tau_0 + \left(\bar{x}_0 - \bar{y}_0\right) \tau_0\right] x_0 \\
&+ \left[\bar{\ell}_1 + \zeta_0 \frac{1 - E_0}{E_0} \bar{v}_0 + \left(\bar{x}_1 - \bar{x}_0\right) G_1 \kappa_1'' \sigma_0 + \left(\bar{x}_0 - \bar{y}_0\right) \sigma_0\right] x_1 \\
&+ \left[\left(\bar{x}_1 - \bar{x}_0\right) G_1 \kappa_1'' \hat{\sigma}_0 + \left(\bar{x}_0 - \bar{y}_0\right) \hat{\sigma}_0\right] x_2 \\
&+ \left[-\mu_0 \bar{v}_0 + \left(\bar{x}_1 - \bar{x}_0\right) G_1 \kappa_1'' \delta_0 + \left(\bar{x}_0 - \bar{y}_0\right) \delta_0\right] t_0 \\
&+ \left[\left(\bar{x}_1 - \bar{x}_0\right) G_1 \kappa_1'' \epsilon_0 + \left(\bar{x}_0 - \bar{y}_0\right) \epsilon_0\right] t_1
\end{aligned} \qquad \text{(B.1.69)}$$

$$\begin{aligned}
c_0' \bar{h}_0 \frac{dt_0}{d\phi} &= \left[\left(c_1' \bar{t}_1 - c_0' \bar{t}_0\right) G_1 \left(1 + \kappa_1'' \xi_0\right) - \lambda_0' \xi_0\right] h_1 \\
&+ \left[\left(c_1' \bar{t}_1 - c_0' \bar{t}_0\right) G_1 \kappa_1'' \tau_0 - \lambda_0' \tau_0\right] x_0
\end{aligned}$$

$$+ \left[\left(c_1'\bar{t}_1 - c_0'\bar{t}_0\right)G_1\kappa_1''\sigma_0 - \lambda_0'\sigma_0\right]x_1$$

$$+ \left[\left(c_1'\bar{t}_1 - c_0'\bar{t}_0\right)G_1\kappa_1''\hat{\sigma}_0 - \lambda_0'\hat{\sigma}_0\right]x_2$$

$$+ \left[\left(c_1'\bar{t}_1 - c_0'\bar{t}_0\right)G_1\kappa_1''\delta_0 - \lambda_0'\delta_0 - \left(c_0'\bar{\ell}_0 + c_0'\bar{v}_0 + U_r'\right)\right]t_0$$

$$+ \left[\left(c_1'\bar{t}_1 - c_0'\bar{t}_0\right)G_1\kappa_1''\epsilon_0 - \lambda_0'\epsilon_0 + c_1'\bar{\ell}_1\right]t_1$$

$$+ U_r't_s \qquad \text{(B.1.70)}$$

The reboiler efficiency, E_0, is assumed to be unity.

Modification for Pressure Control

Condenser pressure may be controlled by manipulation of coolant temperature in proportion to pressure

$$t_{cw} = -k_{pc}p_{N+1} + t_{cw_e} \qquad \text{(B.1.71)}$$

where k_{pc} is the controller proportionality factor or gain and t_{cw_e} is an additional external input. Pressure may be eliminated from Eq. (B.1.71) by substitution of Eq. (B.1.47) to give

$$t_{cw} = (pc1)t_{cw_e} - (pc2)x_N - (pc3)x_{N+1} - (pc4)t_N \qquad \text{(B.1.72)}$$

where

$$pc1 = \left\{1 + k_{pc}\left[\frac{\psi_{N+1}}{1 + \frac{1}{2}\psi_{N+1}\frac{\lambda_N'}{U_c'}\beta_N'^2\frac{\bar{p}_N}{\bar{t}_N\bar{v}_N}}\right]\right\}^{-1} \qquad \text{(B.1.73)}$$

$$pc2 = k_{pc}\left[\eta_{N+1}\zeta_N/E_N + \psi_{N+1}\tau_N \frac{\lambda'_N}{U'_c}\right]\Big/ pc1 \qquad (B.1.74)$$

$$pc3 = k_{pc}\left[-\eta_{N+1}\zeta_N \frac{1 - E_N}{E_N} + \psi_{N+1}\sigma_N \frac{\lambda'_N}{U'_c}\right]\Big/ pc1 \qquad (B.1.75)$$

$$pc4 = k_{pc}\left[\eta_{N+1}\mu_N + \psi_{N+1}\delta_N \frac{\lambda'_N}{U'_c}\right]\Big/ pc1 \qquad (B.1.76)$$

The balance equations are then those for the accumulator and top plate with Eq. (B.1.72) substituted for t_{cw}.

B.2 Model 3

Model 3 invokes the assumptions used in Model 1 plus the assumption that there is neither accumulation of enthalpy on any plate nor exchange of enthalpy between liquid and vapor streams. The only exceptions are thermal effects at the feed plate and the top plate due to introduction of subcooled liquid streams. These are accounted for by enthalpy balances on those plates.

Equations for a Plate

Equations for vapor-liquid equilibria, efficiency, hydraulics and vapor flow are the same as those used in Model 1.

Mass balance

$$\frac{d\tilde{H}_i}{d\theta} = \tilde{L}_{i+1} + \tilde{V}_{i-1} - \tilde{L}_i - \tilde{V}_i \qquad (B.2.1)$$

Component balance

$$\frac{d}{d\theta}\left(\tilde{x}_i\tilde{H}_i\right) = \tilde{L}_{i+1}\tilde{x}_{i+1} - \tilde{L}_i\tilde{x}_i + \tilde{V}_{i-1}\tilde{y}_{i-1} - \tilde{V}_i\tilde{y}_i \qquad (B.2.2)$$

Because there is no vapor holdup and no enthalpy change across plate i

$$\tilde{V}_i = \tilde{V}_{i-1} \tag{B.2.3}$$

and thus

$$\frac{d\tilde{H}_i}{d\theta} = \tilde{L}_{i+1} - \tilde{L}_i \tag{B.2.4}$$

In this derivation it is <u>not</u> assumed that $\bar{L}_{i+1} = \bar{L}_i$ and $\bar{V}_{i-1} = \bar{V}_i$; the steady state flows may all be different.

The linearized dimensionless balance equations are

$$\frac{dh_i}{d\phi} = \ell_{i+1} - \ell_i \tag{B.2.5}$$

$$\bar{h}_i \frac{dx_i}{d\phi} = \left(\bar{x}_{i+1} - \bar{x}_i\right)\ell_{i+1} + \left(\bar{y}_{i-1} - \bar{y}_i\right)v_i + \bar{\ell}_{i+1}x_{i+1} - \bar{\ell}_i x_i + \bar{v}_{i-1}y_{i-1} - \bar{v}_i y_i \tag{B.2.6}$$

As in Model 1 (with $\mu_i = 0$)

$$y_i = \frac{\zeta_i}{E_i} x_i - \zeta_i \frac{1 - E_i}{E_i} x_{i+1} \tag{B.1.24-a}$$

$$\ell_i = G_i\left(h_i + \kappa_i'' v_{i-1}\right) \tag{B.1.20}$$

The vapor flow rates are unchanged between the reboiler and the feed plate, and between the feed plate and the top plate. At the feed plate vapor is condensed by the subcooled feed. The amount condensed, $\tilde{v}_{cF}$, is determined by a heat balance on the feed plate (plate j)

$$\tilde{v}_{cF}\lambda_j' = c_j'\left(\tilde{t}_j - \tilde{t}_F\right)\tilde{f} \tag{B.2.7}$$

In linearized form (with $\tilde{t}_j = \bar{t}_j$)

$$v_{cF} = \frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)f - \left(\frac{c'_j}{\lambda'_j}\bar{f}\right)t_F \qquad (B.2.8)$$

This amount is added to the liquid rate entering the feed plate, that is $\ell_j = \ell_{j+1} + v_{cF}$.

At the top plate there is a similar enthalpy balance that gives the amount of vapor condensed

$$v_{cN} = \frac{c'_N}{\lambda'_N}\left(\bar{t}_N - \bar{t}_{N+1}\right)\ell_{N+1} \qquad (B.2.9)$$

There is no term for t_{N+1} because it is assumed to be constant.

Now the vapor flow rate in various sections of the column may be summarized

Below the feed plate

$$v_i = v_0 \qquad (B.2.10)$$

Above the feed plate

$$v_i = v_0 - \frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)f + \left(\frac{c'_j}{\lambda'_j}\bar{f}\right)t_F \qquad (B.2.11)$$

Above the top plate

$$v_N = v_0 - \frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)f + \left(\frac{c'_j}{\lambda'_j}\bar{f}\right)t_F - \frac{c'_N}{\lambda'_N}\left(\bar{t}_N - \bar{t}_{N+1}\right)\ell_{N+1} \qquad (B.2.12)$$

The boilup rate, v_0, is considered as an input variable.

The mass and component balances may be written in terms of the state variables (holdups and compositions). The appropriate expression for vapor rate must be substituted according to the location of the plate. For all but the feed plate and top plate the equations are

$$\frac{dh_i}{d\phi} = -G_i h_i + G_{i+1} h_{i+1} + \left[-G_i K''_i + G_{i+1} K''_{i+1}\right] v_i \qquad \text{(B.2.13)}$$

$$\begin{aligned}\bar{h}_i \frac{dx_i}{d\phi} = {} & \left[G_{i+1}\left(\bar{x}_{i+1} - \bar{x}_i\right)\right] h_{i+1} + \left[\bar{v}_{i-1} \frac{\zeta_{i-1}}{E_{i-1}}\right] x_{i-1} \\ & + \left[-\bar{\ell}_i - \bar{v}_{i-1}\zeta_{i-1} \frac{1 - E_{i-1}}{E_{i-1}} - \bar{v}_i \frac{\zeta_i}{E_i}\right] x_i \\ & + \left[\bar{\ell}_{i+1} + \bar{v}_i \zeta_i \frac{1 - E_i}{E_i}\right] x_{i+1} \\ & + \left[\bar{y}_{i-1} - \bar{y}_i + \left(\bar{x}_{i+1} - \bar{x}_i\right) G_{i+1} K''_{i+1}\right] v_i \end{aligned} \qquad \text{(B.2.14)}$$

where $\psi_i = \mu_i = \delta_i = \epsilon_i = 0$ for $i = 0, N+1$.

For the feed plate (plate j) the flow rate of liquid is changed by the heat balance to give

$$\begin{aligned}\frac{dh_j}{d\phi} = {} & -G_j h_j + G_{j+1} h_{j+1} + \left[-G_j K''_j + G_{j+1} K''_{j+1}\right] v_0 \\ & + \left[\frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)\left(1 - G_{j+1} K''_{j+1}\right)\right] f \\ & - \left[\bar{f} \frac{c'_j}{\lambda'_j}\left(1 - G_{j+1} K''_{j+1}\right)\right] t_F \end{aligned} \qquad \text{(B.2.15)}$$

$$\begin{aligned}\bar{h}_j \frac{dx_j}{d\phi} = {} & \left[\text{Eqn. (B.2.14) except } v_i \text{ term}\right] \\ & + \left[\left(\bar{x}_{j+1} - \bar{x}_j\right) G_{j+1} K''_{j+1} - \bar{y}_j + \bar{y}_{j-1}\right] v_0 \\ & + \left[\frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)\left\{\bar{y}_{j-1} + \bar{y}_j - \bar{x}_j - \left(\bar{x}_{j+1} - \bar{x}_j\right) G_{j+1} K''_{j+1}\right\} + \bar{x}_F\right] f \\ & + \left[\bar{f} \frac{c'_j}{\lambda'_j}\left\{\bar{x}_j - \bar{y}_{j-1} - \bar{y}_j + \left(\bar{x}_{j+1} - \bar{x}_j\right) G_{j+1} K''_{j+1}\right\}\right] t_F \end{aligned}$$

$$+ \left[\bar{f}\right] x_F \qquad \text{(B.2.16)}$$

In a similar way the top plate equations are

$$\frac{dh_N}{d\phi} = -G_N h_N + \left[1 + \frac{c'_N}{\lambda'_N}\left(\bar{t}_N - \bar{t}_{N+1}\right)\right]\ell_{N+1} - \left[G_N K''_N\right]v_O + \left[G_N K''_N \frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)\right]f - \left[G_N K''_N \frac{c'_j}{\lambda'_j}\bar{f}\right]t_F \qquad \text{(B.2.17)}$$

$$\bar{h}_N \frac{dx_N}{d\phi} = \left[\bar{v}_{N-1}\frac{\zeta_{N-1}}{E_{N-1}}\right]x_{N-1} + \left[-\bar{\ell}_N - \bar{v}_{N-1}\zeta_{N-1}\frac{1 - E_{N-1}}{E_{N-1}} - \bar{v}_N\frac{\zeta_N}{E_N}\right]x_N + \left[\bar{\ell}_{N+1} + \bar{v}_N\zeta_N\frac{1 - E_N}{E_N}\right]x_{N+1} + \left[\frac{c'_N}{\lambda'_N}\left(\bar{t}_N - \bar{t}_{N+1}\right)\left(\bar{y}_N - \bar{x}_N\right) + \bar{x}_{N+1} - \bar{x}_N\right]\ell_{N+1} + \left[\bar{y}_{N-1} - \bar{y}_N\right]v_O - \left[\left(\bar{y}_{N-1} - \bar{y}_N\right)\frac{c'_j}{\lambda'_j}\left(\bar{t}_j - \bar{t}_F\right)\right]f + \left[\left(\bar{y}_{N-1} - \bar{y}_N\right)\frac{c'_j}{\lambda'_j}\bar{f}\right]t_F \qquad \text{(B.2.18)}$$

Accumulator Equations

There is only a component balance equation because accumulator hold-up is constant

$$\bar{h}_{N+1}\frac{dx_{N+1}}{d\phi} = \bar{v}_N\left(y_N - x_{N+1}\right)$$

In terms of state variables

$$\bar{h}_{N+1}\frac{dx_{N+1}}{d\phi} = \left[\bar{v}_N\frac{\zeta_N}{E_N}\right]x_N - \left[\bar{v}_N\left(1 + \zeta_N\frac{1 - E_N}{E_N}\right)\right]x_{N+1} \qquad \text{(B.2.19)}$$

Reboiler Equations

Again the reboiler holdup is constant so that

$$\ell_1 - \ell_0 - v_0 = 0$$

The component balance equation becomes

$$\bar{h}_0 \frac{dx_0}{d\phi} = \left[G_1\left(\bar{x}_1 - \bar{x}_0\right)\right]h_1 + \left[-\bar{\ell}_0 - \zeta_0\bar{v}_0\right]x_0 + \left[\bar{\ell}_1\right]x_1 + \left[\bar{x}_0 - \bar{y}_0 + G_1\kappa_1''\left(\bar{x}_1 - \bar{x}_0\right)\right]v_0 \qquad (B.2.20)$$

with $E_0 = 1$. It should be noted that there are five input variables for Model 3: f, t_F, x_F, ℓ_{N+1}, and v_0.

B.3 Model 4

The assumptions required for Model 4 in addition to those invoked for Model 1 are

1. Enthalpy of all streams remains constant
2. Constant holdup on all plates
3. All flow rates remain constant

The only time dependent effect remaining is transfer and accumulation of chemical species which satisfy the following balance.

$$\bar{H}_i \frac{d\tilde{x}_i}{d\theta} = \bar{L}_{i+1}\tilde{x}_{i+1} + \bar{V}_{i-1}\tilde{y}_{i-1} - \bar{L}_i\tilde{x}_i - \bar{V}_i\tilde{y}_i \qquad (B.3.1)$$

The linearized equilibrium expression is the same as for Model 1

$$y_i = \frac{\zeta_i}{E_i}x_i - \zeta_i\frac{\left(1 - E_i\right)}{E_i}x_{i+1} \qquad (B.3.2)$$

The linearized balance equation for plate i is

$$\bar{h}_i \frac{dx_i}{d\phi} = \left[\bar{v}_{i-1} \frac{\zeta_{i-1}}{E_{i-1}}\right] x_{i-1} + \left[-\bar{\ell}_i - \zeta_{i-1}\bar{v}_{i-1} \frac{1 - E_{i-1}}{E_{i-1}} - \bar{v}_i \frac{\zeta_i}{E_i}\right] x_i + \left[\bar{\ell}_{i+1} + \bar{v}_i \zeta_i \frac{1 - E_i}{E_i}\right] x_{i+1} \qquad (B.3.3)$$

For the reboiler

$$\bar{h}_0 \frac{dx_0}{d\phi} = \left[-\bar{\ell}_0 - \bar{v}_0 \zeta_0\right] x_0 + \left[\bar{\ell}_1\right] x_1 \qquad (B.3.4)$$

because $E_0 = 1$

For the accumulator

$$\bar{h}_{N+1} \frac{dx_{N+1}}{d\phi} = \left[\bar{v}_N \frac{\zeta_N}{E_N}\right] x_N - \left[\bar{v}_N \left(1 + \zeta_N \frac{1 - E_N}{E_N}\right)\right] x_{N+1} \qquad (B.3.5)$$

At the feed plate

$$\bar{h}_j \frac{dx_j}{d\phi} = \left[\text{R.H.S. Eqn. (B.3.3)}\right] + \bar{f} x_F \qquad (B.3.6)$$

In this formulation the only input variable is x_F.

B.4 Coefficient for Vapor Flow in Overhead Piping

The energy equation for compressible pipe flow is[35]

$$\frac{dP}{\rho_v} + \frac{V^2}{2a_p g_c} \left(\frac{4}{\pi D_p^2} M_v\right)^2 d\left(\frac{1}{\rho_v^2}\right) + \frac{2V^2 f_p}{\rho_v^2 g_c D_p} \left(\frac{4}{\pi D_p^2} M_v\right)^2 ds = 0 \qquad (B.4.1)$$

where

$\rho_v = M_v \rho_M$ (ρ_M is molar density of vapor)

D_p is the pipe diameter

s is a distance variable

and a_p is a velocity profile correction factor ≈ 1

This equation may be integrated over the length of the pipe to give

$$14.7 \times 144\left(P_N - P_{N+1}\right) = \frac{V_N^2}{M_v g_c}\left(\frac{4}{\pi D_p^2} M_v\right)^2 \left\{ \frac{1}{2a_p} \int_{\rho_1}^{\rho_2} \rho_M \, d\left(\frac{1}{\rho_M^2}\right) + \frac{2f_p}{D_p} \int_0^Z \frac{dL}{\rho_M} \right\} \qquad (B.4.2)$$

Assume that an average density, $\bar{\rho}_M$, serves to characterize the vapor density for the purposes of the second integration

$$14.7 \times 144\left(P_N - P_{N+1}\right) = V_N^2 \left(\frac{16 M_v}{\pi^2 D_p^4 g_c}\right) \left\{ \frac{1}{2a_p} \left[\frac{2}{\rho_M}\right]_{\rho_1}^{\rho_2} + \frac{2f_p}{D_p} \frac{Z}{\bar{\rho}_M} \right\} \qquad (B.4.3)$$

Assume $\bar{\rho}_M = \dfrac{RT_N}{P_N}$ and solve (B.4.3) for V_N^2

$$V_N^2 = \left(P_N - P_{N+1}\right)\left(\frac{\pi^2 D_p^4 g_c \times 144 \times 14.7}{16 M_v}\right)\left[\frac{144 \times 14.7}{\frac{1}{a_p}\left(\frac{RT_{N+1}}{P_{N+1}} - \frac{RT_N}{P_N}\right) + \frac{4f_p Z}{D_p\left(\frac{RT_N}{P_N}\right)}}\right] \qquad (B.4.4)$$

It is assumed also that $\dfrac{1}{a_p}\left(\dfrac{RT_{N+1}}{P_{N+1}} - \dfrac{RT_N}{P_N}\right)$ is much smaller than $\left(4f_p Z \Big/ RT_N/P_N\right)$, and thus

$$V_N = \left[\frac{\pi^2 D_p^5}{64 f_p Z}\right]^{1/2} \left[\frac{P_N}{RT_N} \frac{g_c}{M_v} \left(P_N - P_{N+1}\right)\right]^{1/2} \times (14.7 \times 144) \qquad \text{(B.4.5)}$$

By comparison with Eqn. (B.1.36), the vapor flow coefficient is

$$\beta_N = \left(\frac{\pi^2 D_p^5}{64 f_p Z}\right)^{1/2} \qquad \text{(B.4.6)}$$

B.5 Time Constants for Reboiler and Accumulator Metal

The large mass of metal in the walls and tubes of the reboiler and condenser might be expected to contribute significant thermal lags. This possibility is investigated here by a simple calculation.

Although the reboiler was modeled here as if it were a kettle type, the actual reboiler used for the experimental column was a thermosiphon with the process fluid boiling inside vertical tubes.[6] The most important lag due to the metal would probably be the one encountered when steam pressure is changed in the shell. In this case both shell and tubes provide thermal capacity. A time constant is calculated from data given by Bonnet and Gerster.[6]

Tubes: 163 tubes, 14 BWG, Admiralty metal
3/4 in. O.D., 121.9 inches long

mass = 1070 lb. = 16.6 moles
outside area = 314 ft^2

Shell: 17 in. I.D., 1/2-inch wall thickness
118-1/4 inches long, steel

mass = 920 lb. = 16.5 moles
inside area = 44 ft^2

Tube sheets are neglected because they contribute less than 10 percent of

the total mass. A time constant for the thermal capacitance of the metal, τ_{MR}, is estimated by

$$\tau_{MR} = \frac{c_{MR} M_{MR}}{h_{MR} A_{MR}}$$

where

thermal capacity = c_{MR} = 5.8 Btu/mole°F

heat transfer area = A_{MR} = 44 + 314 = 358 ft^2

total mass = M_{MR} = 16.5 + 16.6 = 33.1 lb. moles

heat transfer coefficient = h_{MR} = 1000 Btu/ft^2 hr°F (estimated)

Then

$$\tau_{MR} = 1.9 \text{ sec}$$

This time constant is sufficiently small that it is probably safe to ignore the effect of the metal thermal capacity. Moreover, the condenser contains roughly one-third as much metal as the reboiler, so that even if the heat transfer coefficient on the shell side were only 100 Btu/ft^2 hr°F the associated time constant would be about 6 sec.

Nomenclature for Appendix B

a_p	Velocity profile correction factor, Eqn. (B.4.1)
a	Parameter in exponent of vapor-liquid equilibrium correlation, °R
A_{12}, A_{21}	Parameters in Van Laar activity coefficient correlation
A_T, A_B	Plate area, bubbling area, ft^2 (assume $A_T = A_B$)
A_c, A_{MR}, A_r, A_{sc}	Heat transfer areas, ft^2
b	Parameter in exponent of vapor-liquid equilibrium correlation
B	Flow rate of bottoms product, moles/sec
c	Molar heat capacity, Btu/lb. mole, °F
D	Coefficient defined by Eqn. (B.1.52), or flow rate of overhead product, moles/sec
D_p	Pipe diameter, feet
E	Murphree plate efficiency based on the liquid phase
E_{MV}	Murphree plate efficiency based on the vapor phase
F	Feed rate, moles/sec
f_p	Fanning friction factor
g	Gravitational acceleration, ft/sec^2
g_c	Conversion factor, $\frac{\text{lb.(mass)}}{\text{lb.(force)}} \frac{\text{ft}}{\text{sec}^2}$
G	Coefficient defined by Eqn. (B.1.20)
H	Liquid holdup, moles
H_L, H_V	Enthalpy of liquid or vapor phase, Btu/lb. mole
H_w	Residual holdup, moles (parameter in the hydraulics expression)
h_c, h_{MR}, h_{sc}	Heat transfer coefficients, Btu/ft^2 hr °F
k_{pc}	Proportionality factor or gain for pressure control
K	K value, y/x

L	Liquid flow rate, moles/sec
M_L, M_V	Average molecular weight of liquid or vapor phase
M_{MR}	Mass of reboiler metal, lb. or lb. moles
m	Slope of vapor-liquid equilibrium curve
P	Total pressure, atm
P^0	Vapor pressure of pure component
pc1-pc4	Coefficients defined by Equations (B.1.73)-(B.1.76)
Q	Rate of heat removal or addition, Btu/sec
R	Gas constant, 1544 ft-lb. (force)/lb.mole °F
sc1-sc4	Coefficients defined by Equations (B.1.56)-(B.1.59)
s	Distance variable (Appendix B.4)
T	Absolute temperature, °R
U'	Dimensionless heat transfer resistance
V	Vapor flow rate, moles/sec
x	Mole fraction of light component (acetone) in the liquid phase
y	Mole fraction of light component in the vapor phase
z	State variable (h, x or t)
Z	Length of pipe for overhead vapor

Greek Letters

α	Coefficient in hydraulic expression, gal/min/in.; α' defined by Eqn. (B.1.10)
β	Coefficient in vapor flow equation, ft^2; β' defined by Eqn. (B.1.12)
β_N	Coefficient for overhead vapor flow, ft^2; defined by Eqn. (B.4.6)
γ	Activity coefficient
δ	Coefficient defined by Eqn. (B.1.31)
ϵ	Coefficient defined by Eqn. (B.1.32)

ζ	Coefficient defined by Eqn. (B.1.24-b)
η	Coefficient defined by Eqn. (B.1.22)
θ	Time, hr (sometimes min or sec)
κ	Coefficient that gives the influence of vapor rate on holdup, in $H_2O/ft/sec$; κ' defined by Eqn. (B.1.11)
λ	Molar heat of vaporization, Btu/lb. mole
μ	Coefficient defined by Eqn. (B.1.24-c)
ν'	Coefficient defined by Eqn. (B.1.13)
ξ	Coefficient defined by Eqn. (B.1.27)
π	The number 3.14159....
ρ_M	Molar density, lb. moles/ft^3
ρ_L, ρ_v	Density of liquid or vapor phase, lb./ft^3
σ	Coefficient defined by Eqn. (B.1.29)
$\hat{\sigma}$	Coefficient defined by Eqn. (B.1.30)
τ	Coefficient defined by Eqn. (B.1.28)
τ_{MR}	Time constant for the thermal capacity of the reboiler metal
ϕ	Dimensionless time
ψ	Coefficient defined by Eqn. (B.1.23)

Subscripts

C,c	Refers to condenser
CW,cw	Refers to condenser coolant
e	Refers to external input variable (not manipulated)
F	Refers to feed stream
i	Refers to plate i, any plate in the column other than the reboiler, feed plate or accumulator
j	Refers to the feed plate

L	Refers to liquid phase property
MR	Refers to reboiler metal
N	Refers to the top plate
p	Refers to pipe
R,r	Refers to the reboiler
S,s	Refers to steam (reboiler)
sc	Refers to subcooled reflux entering the accumulator
ss	Refers to derivative evaluated at steady state conditions
w	Refers to residual liquid holdup on a plate (H_w)
1,2	Refers to Component 1 (light component) or 2 (heavy) when used with correlation parameters

Plate Numbering (subscripts)

0	Reboiler
1,2,3...	Any plate in column. The bottom plate is 1.
N	Top plate
N+1	Accumulator (or condenser pressure)

Superscripts

(1),(2)	Refers to Component 1 (light component) or 2 (heavy), when used with component properties
0	Refers to physical property evaluated at the reference state, which is the steady state temperature of plate N; or vapor pressure of pure component evaluated at the temperature of the plate indicated by the subscript
' and "	Dimensionless quantity (physical property or parameter made dimensionless) or used to distinguish a derived coefficient
*	Refers to equilibrium value

$\hat{}$ Used only as $\hat{\sigma}$ to distinguish a new coefficient

Other Markings

$\sim$ Above variables. Denotes total time-dependent value.

$-$ Above variables. Denotes steady state value.

. No mark above variables denotes deviation from steady state value.

Variables in upper case are dimensional (H, L, V, P, T, F)

Variables in lower case are dimensionless (h, ℓ, v, p, t, f)

Appendix C

CALCULATION OF EIGENVECTORS BY INVERSE ITERATION[64,65]

An eigenvector $\underline{u}^{(j)}$ of matrix $\underline{\underline{A}}$ is defined by the relationship

$$(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})\, \underline{u}^{(j)} = \underline{0} \tag{C.1}$$

By definition the n×n matrix $(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})$ is singular. Therefore, a common procedure for the computation of $\underline{u}^{(j)}$ is to arbitrarily choose one element of $\underline{u}^{(j)}$ as unity and then solve for the rest of the elements using n-1 of Equations (C.1).

In actual computations $(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})$ is not quite singular because the eigenvalue is not known exactly. Consequently, the use of only n-1 of the n equations can cause errors in the computed eigenvectors. A scheme that avoids these errors is derived by consideration of the set of equations

$$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})\, \underline{w}^{(j)} = \underline{b} \tag{C.2}$$

where $\tilde{\lambda}_j$ is an approximation to the j'th eigenvalue of $\underline{\underline{A}}$ (λ_j)

$\underline{w}^{(j)}$ is an approximation to the j'th eigenvector of $\underline{\underline{A}}$ $(\underline{u}^{(j)})$

and $\underline{b}$ is an arbitrary vector

Express $\underline{b}$ as a linear combination of the true eigenvectors. This can be done because the eigenvectors span the space.

$$\underline{b} = \sum_{i=1}^{n} \alpha_i \underline{u}^{(i)} \tag{C.3}$$

Thus

$$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})\, \underline{w}^{(j)} = \sum_{i=1}^{n} \alpha_i \underline{u}^{(i)}$$

or

$$\underline{w}^{(j)} = (\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})^{-1} \sum_{i=1}^{n} \alpha_i \underline{u}^{(i)}$$

which may be rearranged as

$$\underline{w}^{(j)} = \sum_{i=1}^{n} \alpha_i (\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})^{-1} \underline{u}^{(i)} \tag{C.4}$$

$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})$ may be inverted because it is not quite singular.

Since the eigenvalues of $(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})$ are $(\lambda_i - \tilde{\lambda}_j)$, the eigenvalues of $(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})^{-1}$ are $(\lambda_i - \tilde{\lambda}_j)^{-1}$. Thus if $\hat{\underline{w}}^{(j)}$ is the j'th eigenvector of $(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})^{-1}$

$$\left[(\underline{\underline{A}} - \lambda_j \underline{\underline{I}})^{-1} - (\lambda_j - \tilde{\lambda}_j)^{-1} \underline{\underline{I}} \right] \hat{\underline{w}}^{(j)} = \underline{0}$$

which yields

$$(\lambda_j - \tilde{\lambda}_j) \hat{\underline{w}}^{(j)} = (\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}}) \hat{\underline{w}}^{(j)}$$

or

$$\lambda_j \hat{\underline{w}}^{(j)} = \underline{\underline{A}} \hat{\underline{w}}^{(j)}$$

Thus

$$\hat{\underline{w}}^{(j)} \equiv \underline{u}^{(j)},$$

the eigenvectors of $\underline{\underline{A}}$ and $(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})^{-1}$ are identical.

The equation that defines eigenvector i of $(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})^{-1}$ is

$$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})^{-1} \underline{u}^{(i)} = \left(\frac{1}{\lambda_i - \tilde{\lambda}_j} \right) \underline{u}^{(i)} \tag{C.5}$$

and Eq. (C.4) becomes

$$\underline{w}^{(j)} = \sum_{i=1}^{n} \alpha_i \left(\frac{1}{\lambda_i - \tilde{\lambda}_j} \right) \underline{u}^{(i)} \tag{C.6}$$

If $\tilde{\lambda}_j$ is a reasonably good approximation to eigenvalue λ_j, then only the term in $\underline{u}^{(j)}$ will be important in the sum. Thus the solution of Eq. (C.2) yields a vector that is strongly reinforced in the direction of $\underline{u}^{(j)}$ so long as the arbitrary initial vector $\underline{b}$ is chosen such that its elements are not deficient in that direction.

There is usually no priori knowledge regarding the largest component of vector $\underline{u}^{(j)}$. In practice it has been found by Wilkinson that the new vector on the right hand side that is generated by triangularization of the set of equations (C.1) gives satisfactory results when it is chosen to have all its elements unity. Consequently, all manipulation of the equations in triangularization may be carried out without regard for the right-hand side (vector $\underline{b}$).

The preceding gives a computational procedure for a first estimate to $\underline{u}^{(j)}$, which is denoted $^{(1)}\underline{w}^{(j)}$. This estimate may be improved by the substitution $\underline{b} = {}^{(1)}\underline{w}^{(j)}$ in Eq. (C.2) followed by the solution of Eq. (C.2) to find $^{(2)}\underline{w}^{(j)}$. This procedure is repeated ℓ times until there is reasonable agreement between the successive estimates $^{(\ell-1)}\underline{w}^{(j)}$ and $^{(\ell)}\underline{w}^{(j)}$ (where both have been normalized in the same way).

The last estimate of the eigenvector may be further improved by another iterative procedure. The vector $\underline{r}$, which is small compared to $^{(\ell-1)}\underline{w}^{(j)}$, is formed by

$$\underline{r} = {}^{(\ell-1)}\underline{w}^{(j)} - (\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})\ {}^{(\ell)}\underline{w}^{(j)}. \tag{C.7}$$

Now $\underline{r}$ is used in place of $\underline{b}$ in Eq. (C.2) to find $\underline{y}$

$$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})\ \underline{y} = \underline{r} \tag{C.8}$$

Substitution of Eq. (C.8) into Eq. (C.7) gives

$$(\underline{\underline{A}} - \tilde{\lambda}_j \underline{\underline{I}})\ (\underline{y} + {}^{(\ell)}\underline{w}(j)) \;=\; {}^{(\ell-1)}\underline{w}(j) \qquad \text{(C.9)}$$

A more accurate eigenvector ${}^{(\ell+1)}\underline{w}(j)$ is the sum

$${}^{(\ell+1)}\underline{w}(j) \;=\; \underline{y} + {}^{(\ell)}\underline{w}(j) \qquad \text{(C.10)}$$

This procedure is repeated until full convergence is achieved.

Appendix D

PARAMETER VALUES, PHYSICAL PROPERTIES, AND CORRELATIONS*

Parameters and correlations have been chosen to duplicate as closely as possible the behavior of the distillation column at the University of Delaware that has been studied by Gerster et al.[2,3,33,56] The kinds of data required may be subdivided as properties of the system being fractionated (acetone-benzene) and basic distillation column parameters or correlations.

The parameters and correlations chosen to describe the properties of the acetone-benzene system are summarized in Table D.1. The vapor-liquid equilibrium data used are those of Tallmadege and Canjar[58] because data in other sources[9,19,59] are either incomplete or not thermodynamically consistant. The rest of the correlations shown in Table D.1 give approximate matching of data[26,27,45,58] over the range of interest.

A correlation for Murphree efficiencies was derived from data in the University of Delaware report to the A.I.Ch.E. on tray efficiencies.[19] With many approximations, the vapor phase Murphree efficiencies, E_{MV_i}, may be estimated by

$$E_{MV_i} = 1.095 - \exp\left[-1.353 + 0.389\ \bar{V}_i\ \frac{M_V}{A_T\sqrt{\rho_V}} - 6.537\ \bar{L}_i\ \frac{M_L}{\rho_L}\right] \qquad (D.1)$$

over the range of variables used here. The liquid phase Murphree efficiencies used in this work are related to the vapor phase efficiencies by[19]

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* For identification of symbols refer to the nomenclature section of Appendix B.

Table D.1. Properties of Acetone-Benzene System

Vapor-Liquid Equilibrium[58]

$$K_1 = \frac{y}{x} = \frac{\gamma^{(1)}}{P} \exp\left[- \frac{7660}{T} + 12.79 \right]$$

$$K_2 = \frac{1-y}{1-x} = \frac{\gamma^{(2)}}{P} \exp\left[- \frac{6160}{T} + 9.79 \right]$$

Activity Coefficients (see Eq. B.1.6)[45d]

Van Laar constants: $A_{12} = A_{21} = 0.268$

Heat of Vaporization of Mixture[58,45a]

$\lambda = x(2.16\times10^4 - 14.5T) + (1-x)(2.215\times10^4 - 14.07T)$ Btu/lb. mole

Heat Capacity of Liquid Mixture[26,45b]

$c = x(17.26+0.0247T) + (1-x)(9.37+0.0421T)$ Btu/lb. mole, °R

Liquid Enthalpies[26]

Acetone $H_L = 11,480 + 17.26T + 0.01237T^2$ Btu/lb. mole

Benzene $H_L = 9710 + 9.38T + 0.02105T^2$ Btu/lb. mole

Vapor Enthalpies[45a,26]

Acetone $H_V = 33,080 + 2.76T + 0.01237T^2$ Btu/lb. mole

Benzene $H_V = 31,860 - 4.69T + 0.02105T^2$ Btu/lb. mole

Vapor Pressure[45c]

Acetone $P^{o(1)} = 1.19\times10^5 \exp(-6950/T)$ atm.

Benzene $P^{o(2)} = 5.55\times10^4 \exp(-6950/T)$ atm.

Molecular Weight

Acetone 58.08

Benzene 78.11

Density of Liquid[27]

Acetone $\rho_L = 73.40 - 0.0451T$ lb/ft^3

Benzene $\rho_L = 77.50 - 0.0416T$ lb/ft^3

$$E_i = \frac{1}{(1/E_{MV_i} - 1)} \qquad (D.2)$$
$$1 + \frac{}{m_i \bar{V}_i/\bar{L}_i}$$

where m_i is the slope of the vapor-liquid equilibrium curve at plate i $(d\bar{y}_i/d\bar{x}_i^*)$. The slope may be evaluated from equations (B.1.4) and (B.1.5) by

$$m_i = \frac{\partial \bar{y}_i}{\partial \bar{x}_i^*} + \frac{\partial \bar{y}_i}{\partial \bar{T}_i} \frac{d\bar{T}_i}{d\bar{x}_i^*} \qquad (D.3)$$

which applies at constant pressure. The result is

$$m_i = \frac{\bar{y}_i}{\bar{x}_i^*} \left[1 + \frac{\bar{x}_i^* a_1 \left(\frac{1 - \bar{y}_i}{1 - \bar{x}_i^*} - \frac{\bar{y}_i}{\bar{x}_i^*} \right)^2}{a_2 \left(\frac{1 - \bar{y}_i}{1 - \bar{x}_i^*} \right) \left(1 - \frac{\bar{y}_i}{\bar{x}_i^*} \right) - a_1 \frac{\bar{y}_i}{\bar{x}_i^*} \left(1 - \frac{1 - \bar{y}_i}{1 - \bar{x}_i^*} \right)} \right] \qquad (D.4)$$

The efficiencies are used in the steady state calculation to give a modified K-value (y/x)

$$K_i = K_i^* \left[\frac{1}{E_i} - \frac{x_{i+1}}{x_i} \left(\frac{1 - E_i}{E_i} \right) \right] \qquad (D.5)$$

where K_i^* is the K-value corresponding to 100 percent plate efficiency.

Plate hydraulics also are estimated from the University of Delaware report on tray efficiencies,[19] by extrapolation of Fig. V-3, p. 72. A correlation for height of liquid on a plate is converted to one that gives holdup in moles in terms of liquid and vapor flow rates (Eq. B.1.9-11) and includes the downcomer holdup of 1.20 gal. Luyben, Verneuil and

Gerster[33] indicated that it is reasonable to lump the downcomer and the tray holdups in this way. A so-called residual holdup, H_w, that corresponds to 0.407 moles or 2.77 inches of clear liquid is introduced. The other parameters in Eqs. (B.1.10 and B.1.11) are

$$\alpha = 0.030$$

and $$\kappa = 0.40$$

For all but the top plate the vapor flow coefficient, β, is estimated from average conditions for the variables in Eq. (B.1.8). An inter-stage pressure drop of 6 in. water is assumed. The coefficient that results

$$\beta = 0.159 \text{ sq. ft.}$$

has the units of area because it includes as a factor the cross-sectional area for vapor flow. At the top plate Eq. (B.4.6) is used to calculate the coefficient for flow through the overhead piping, where Z = 15 ft. and D_p = 6 in., with the result

$$\beta_N = 0.30 \text{ sq. ft.}$$

For typical operating conditions this value of β_N gives a pressure drop of 0.002 atm. in the overhead piping.

The plate area, A_T, is taken to be the same as the bubbling area, A_B, and

$$A_T = A_B = 2.45 \text{ sq. ft.}$$

Appendix E

ADDITIONAL STEADY STATE DATA

Steady state conditions for cases A-5 and A-3 are given in Tables E.1 and E.2. The McCabe-Thiele diagrams are shown in Figs. E.1 and E.2. These cases are based on five-plate and three-plate columns respectively.

Table E.1

Steady State A-5

Plate No.	Temperature, °R	Pressure, Atm.	Liquid Flow Rate, moles/sec.	Liquid Composition, mole fraction	Murphree Efficiency	Dimensionless Holdup[4]
0	680.3	2.799	0.0100[2]	0.131	1.00	13.882
1	669.7	2.781	0.0506	0.303	0.75	0.951
2	662.7	2.763	0.0508	0.424	0.72	0.942
3	659.3	2.746	0.0511	0.506	0.71	0.934
4	656.7	2.733	0.0196	0.579	0.78	0.781
5	654.5	2.722	0.0197	0.663	0.78	0.775
6	562.4[1]	2.720	0.0160[3]	0.746	1.00	18.010
						36.275 = Total

Feed rate = 0.0250 moles/sec on plate 3

Distillate flow rate = 0.0150 moles/sec.

Condenser heat load = 704.7 Btu/sec.

Reboiler heat load = 518.9 Btu/sec.

1. Reflux temperature
2. Bottom product flow rate
3. Reflux flow rate
4. Holdup relative to residual holdup, H_w (H_w = 0.407 moles)

Table E.2

Steady State A-3

Plate No.	Temperature, °R	Pressure, atm.	Liquid Flow Rate, moles/sec.	Liquid Composition, mole fraction	Murphree efficiency	Dimensionless Holdup(4)
0	673.4	2.779	0.0100(2)	0.200	1.00	13.882
1	664.5	2.762	0.0508	0.392	0.73	0.943
2	659.9	2.744	0.0511	0.495	0.71	0.934
3	656.6	2.732	0.0197	0.591	0.78	0.780
4	563.3(1)	2.730	0.0160(3)	0.700	1.00	18.010
						34.549 = Total

Feed Rate = 0.0250 moles/sec. on plate 2.

Distillate flow rate = 0.0150 moles/sec.

Condenser heat load = 707.3 Btu/sec.

Reboiler heat load = 518.5 Btu/sec.

1. Reflux temperature
2. Bottom product flow rate
3. Reflux flow rate
4. Holdup relative to residual holdup, H_w (H_w = 0.407 moles)

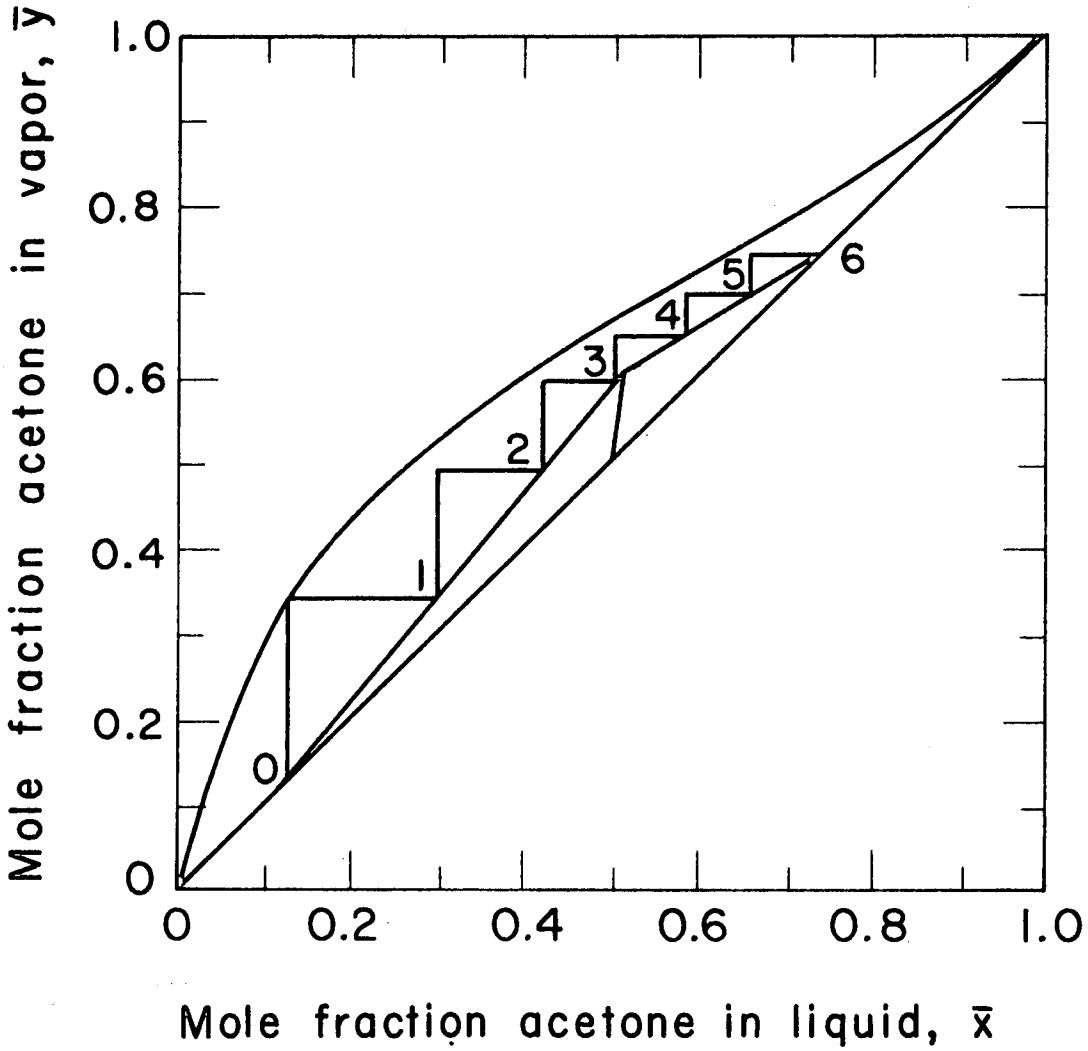

Fig. E.1 McCabe-Thiele diagram for case A-5

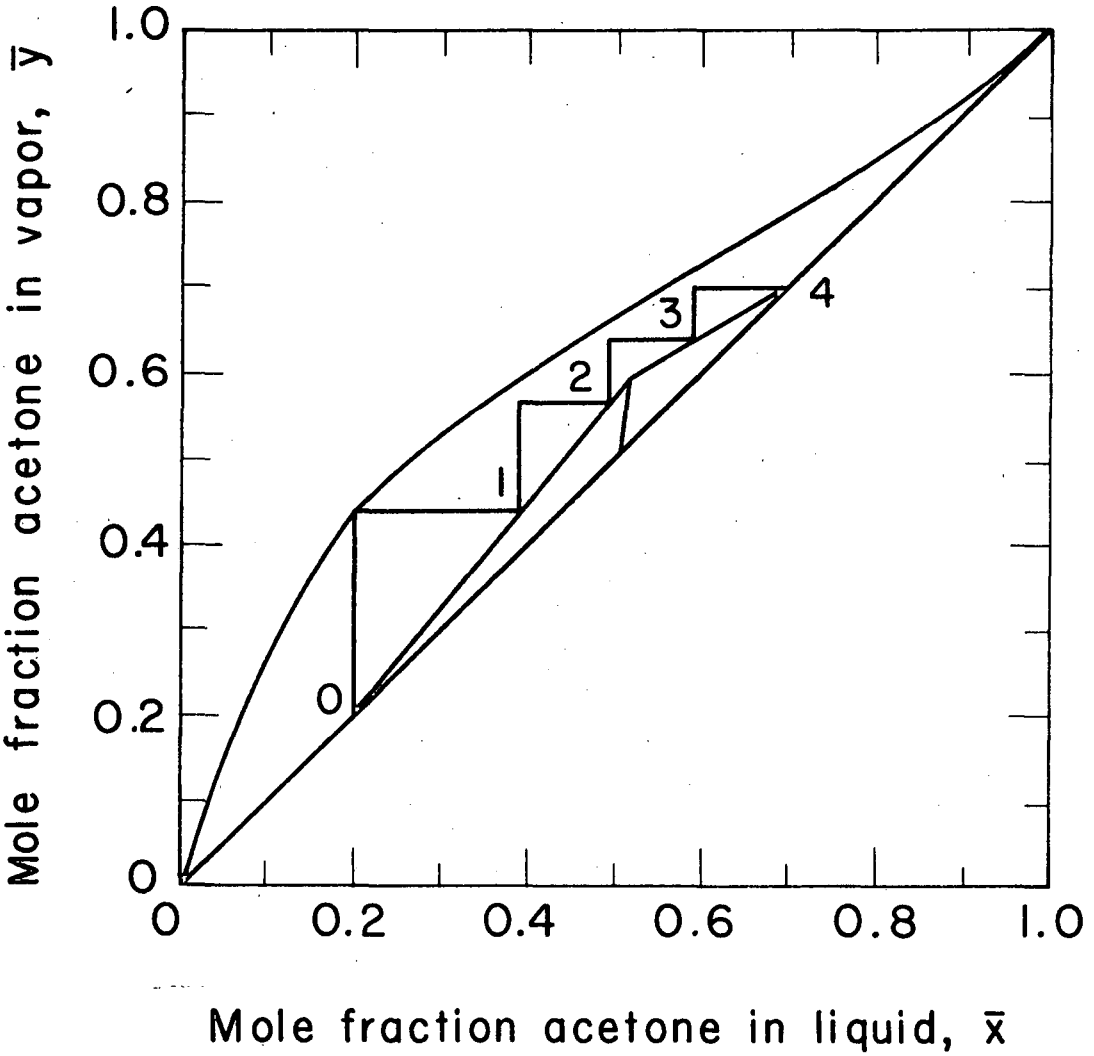

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Fig. E.2 McCabe-Thiele diagram for case A-3

Appendix F

NUMERICAL EXAMPLES OF MATRICES, EIGENVALUES, AND EIGENVECTORS

The numerical values of the coefficients that comprise the state matrix $\underline{\underline{A}}$ and the input matrix $\underline{\underline{B}}$ are shown in Tables F.1 and F.2 for case A-10-1, and in Table F.3 for case A-10-4. The eigenvalues of the matrix given in Table F.1 are listed in Table F.4. The right and left eigenvectors for the first six modes of this case (A-10-1) are in Table F.5.

Table F.1 COEFFICIENTS OF STATE SPACE MATRIX

HOLDUP EQUATIONS

ROW 2

-9.0390E 00	9.0196E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	-2.8036E 02	5.2594E 02	-2.9255E 02	4.5229E 01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-4.8618E 02	1.0837E 03
-6.0423E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 3

0.0000E-39	-9.0196E 00	8.9998E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	+2.7734E 02	4.7890E 02	-2.6700E 02	4.5194E 01	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-5.7231E 02
1.2825E 03	-7.0507E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 4

0.0000E-39	0.0000E-39	-8.9998E 00	8.9839E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-2.2842E 02	4.1037E 02	-2.4689E 02	4.3850E 01
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-6.7841E 02	1.4825E 03	-7.9332E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 5

0.0000E-39	0.0000E-39	0.0000E-39	-8.9839E 00	8.9725E 00	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.8859E 02	3.6486E 02	-2.3097E 02
4.1138E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	-7.7741E 02	1.6454E 03	-8.5741E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 6

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.9725E 00	8.9091E 00	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.6316E 02	3.6220E 02
-2.3321E 02	3.6939E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	-8.5207E 02	1.9294E 03	-1.0764E 03	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 7

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.9091E 00	8.8983E 00	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.7509E 02
3.3947E 02	-1.9238E 02	2.8785E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	-1.0720E 03	2.2043E 03	-1.1323E 03	0.0000E-39	0.0000E-39

Table F.1 (continued)

0.0000E-39	0.0000E-39						
ROW 8							
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.8983E 00	8.8875E 00
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-1.4739E 02	2.9682E 02	-1.7647E 02	2.6334E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.1279E 03	2.3201E 03	-1.1917E 03	0.0000E-39
0.0000E-39	0.0000E-39						
ROW 9							
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.8875E 00
8.8749E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	-1.3538E 02	2.7092E 02	-1.5956E 02	2.3572E 01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.1878E 03	2.4405E 03	-1.2522E 03
0.0000E-39	0.0000E-39						
ROW 10							
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-8.8769E 00	8.8663E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	-1.2314E 02	2.4387E 02	-1.4133E 02	2.0427E 01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.2488E 03	2.5635E 03
-1.3147E 03	0.0000E-39						
ROW 11							
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	-8.8663E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	-1.1064E 02	1.1763E 02	-2.0400E 01	-0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-1.3113E 03
1.3095E 03	-0.0000E-39						

COMPOSITION EQUATIONS

ROW 1 REBOILER

5.5564E-02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	-6.4396E-02	-2.8537E-01	8.7495E-02	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	9.9555E-01	-1.0637E 00
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						
ROW 2							
-1.2276E-02	1.0942E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	2.4700E 01	-2.7184E 01	9.1996E 00	-4.1499E-01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	2.8166E 01	-3.5113E 01
5.5449E 03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

Table F.1 (continued)

ROW 3

0.0000E-39	-2.9965E-02	1.1736E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	4.2710E 01	-5.6858E 01	2.4904E 01	-2.9884E 00	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	7.3875E 01
-1.2297E 02	4.6622E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 4

0.0000E-39	0.0000E-39	-4.8946E-02	9.3002E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.9247E 01	-7.7129E 01	4.0699E 01	-5.9907E 00
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
1.3155E 02	-2.4294E 02	1.0838E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 5

0.0000E-39	0.0000E-39	0.0000E-39	-6.3402E-02	6.3196E-01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.8483E 01	-8.7183E 01	5.1026E 01
-7.9760E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	1.8354E 02	-3.5246E 02	1.6624E 02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 6

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-7.2524E-02	5.0408E-01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.5786E 01	-8.9923E 01
5.0364E 01	-6.0564E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	2.2059E 02	-4.3166E 02	2.1072E 02	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 7

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-9.9896E-02	6.6137E-01	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	5.4232E 01
-8.4518E 01	3.6647E 01	-4.5392E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	3.1153E 02	-4.9065E 02	1.7855E 02	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 8

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-7.9739E-02	6.3923E-01
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
3.6110E 01	-5.4563E 01	2.3027E 01	-2.5566E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	2.5379E 02	-3.7005E 02	1.1570E 02	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 9

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-5.9771E-02
6.1556E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	2.5084E 01	-3.4325E 01	1.1989E 01	-9.6398E-01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.9461E 02	-2.4628E 02	5.1211E 01
0.0000E-39	0.0000E-39						

Table F.1 (continued)

ROW 10

0.0010E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-4.4072E-02	6.0377E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	1.6951E 01	-1.7885E 01	3.1966E 00	2.7117E-01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.3349E 02	-1.1640E 02
-1.7452E 01	0.0000E-39						

ROW 11

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	-2.0341E-02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	8.7553E 00	-1.1075E 01	2.9520E 00	-0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	6.9478E 01
-6.9881E 01	-0.0000E-39						

ROW 12 CONDENSER

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.1154E-01	-1.3206E-01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
2.1453E-02	0.0000E-39						

TEMPERATURE EQUATIONS

ROW 1 REBOILER

-2.7487E-03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	-5.2752E 01	4.6697E 01	-7.9150E 00	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-9.2725E 01	9.6447E 01
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 2

-5.7839E-01	-7.9755E-02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	7.5519E 02	-1.3944E 03	7.7006E 02	-1.1859E 02	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.3122E 03	-2.8840E 03
1.5874E 03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 3

0.0000E-39	-6.1421E-01	5.6682E-02	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	7.2758E 02	-1.2229E 03	6.6799E 02	-1.1195E 02	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.5040E 03
-3.2713E 03	1.7497E 03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

Table F.1 (continued)

ROW 4

0.0000E-39	0.0000E-39	-6.3131E-01	2.5397E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	5.6793E 02	-9.9187E 02	5.8345E 02	-1.0241E 02
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
1.A892E 03	-3.5747E 03	1.8561E 03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 5

0.0000E-39	0.0000E-39	0.0000E-39	-6.3295E-01	4.0714E-01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.4251E 02	-8.3712E 02	5.2018E 02
-9.1741E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	1.92CAE C3	-3.7677E 03	1.9155E 03	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 6

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-6.2965E-01	5.9378E-01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	3.5539E 02	-7.9849E 02
5.CB48E 02	-6.7050E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	1.9109E 03	-4.2490E 03	2.3341E 03	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 7

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.8970E-01	7.0332E-01	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.5204E 02
-8.6614E 02	4.8542E 02	-7.2305E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	2.7704E 03	-5.6167E 03	2.8459E 03	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 8

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-8.9635E-01	7.1637E-01
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
3.7170E 02	-7.3488E 02	4.3450E 02	-6.4531E 01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	2.8472E 03	-5.7705E 03	2.9219E 03	0.0000E-39
0.0000E-39	0.0000E-39						

ROW 9

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	-9.0093E-01
7.2884E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	3.2418E 02	-6.5960E 02	3.8356E 02	-5.6400E 01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	2.9252E 03	-5.9245E 03	2.9978E 03
0.0000E-39	0.0000E-39						

ROW 10

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-9.6514E-01	7.3827E-01	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	2.9588E 02	-5.7873E 02	3.8193E 02	-4.7757E 01	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	3.0029E 03	-6.0785E 03
3.0791E 03	0.0000E-39						

ROW 11

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	-9.0942E-01	-0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	2.5973E 02	-2.7659E 01	4.7990E 01	-0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	3.0812E 03
-3.0975E 03	1.1949E 00						

ROW 12 CONDENSER

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.1164E-03	-2.4504E-04	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
4.0563E-02	-1.0758E-01						

Table F.2 COEFFICIENTS OF INPUT MATRIX B

COLUMN VECTOR FOR FEED RATE

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.0000E 00	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	5.3376E-01
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	1.4898E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

COLUMN VECTOR FOR FEED TEMP

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	1.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	1.5129E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

COLUMN VECTOR FOR FEED COMP

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.6680E 00
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

COLUMN VECTOR FOR REFLUX RATE

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	1.0000E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	6.8037E-02	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
-4.8669E-01	0.0000E-39						

COLUMN VECTOR FOR REBOILER DUTY

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	1.0182E 00	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39						

COLUMN VECTOR FOR CONDENSER WATER TEMP

0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	7.0479E 00	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	4.7952E-01	0.0000E-39	0.0000E-39	0.0000E-39
0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39	0.0000E-39
9.1066E 00	5.5179E-02						

Table F.3.

Coefficients of State Matrix, $\underline{\underline{A}}$, and Input Matrix, $\underline{\underline{B}}$, for Model 4

Case A-10-4, No Control

Main Diagonal	Upper Diagonal	Lower Diagonal	$\underline{\underline{B}}$ (1 vector)
-72.099	0.22985	9.7279	0
-12.329	4.8108	9.0785	0
-12.115	4.9185	7.3363	0
-11.121	4.9695	6.2105	0
-10.587	4.9892	5.6138	0
- 9.4214	2.5901	5.2502	1.668
- 7.6184	2.5503	4.5529	0
- 6.9241	2.5416	4.3844	0
- 6.7681	2.5281	4.2362	0
- 6.6247	2.5101	4.1060	0
- 6.0526	2.0774	0.15032	0
- 0.14058			0

NOTE: Matrix $\underline{\underline{B}}$ is (N×1). The vector operates on the single input, feed composition.

Table F.4

EIGENVALUES

ROOT NO.	REAL	IMAGINARY
1	-4.53312E-02	
2	-1.07553E-01	
3	-1.30132E-01	
4	-4.77476E-01	
5	-7.82485E-01	
6	-1.06143E 00	
7	-2.11171E 00	
8	-3.96372E 00	1.04466E 00
9	-3.96372E 00	-1.04466E 00
10	-4.91641E 00	2.05194E 00
11	-4.91641E 00	-2.05194E 00
12	-6.9916CE 00	3.91976E 00
13	-6.99160E 00	-3.91976E 00
14	-8.69703E 00	
15	-8.92631E 00	-1.13714E 00
16	-8.92631E 00	1.13714E 00
17	-9.64561E 00	-4.29334E 00
18	-9.64561E 00	4.29334E 00
19	-1.20992E 01	-3.20262E 00
20	-1.20992E 01	3.20262E 00
21	-1.22207E 01	
22	-1.34378E 01	9.47926E-01
23	-1.34378E 01	-9.47926E-01
24	-1.72214E 01	
25	-7.03351E 01	
26	-4.57013E 02	
27	-1.17445E 03	
28	-2.21042E 03	
29	-3.35445E 03	
30	-4.62913E 03	
31	-5.91804E 03	
32	-6.95002E 03	
33	-8.99976E 03	
34	-1.10305E 04	

SUM OF ROOTS = -4.4956966E 04
PROD OF ROOTS = 4.0455645E 21 X 1.E 25

BEGIN EIGVEC TIME 1072.93

Table F.5

EIGENVALUES WITH CORRESPONDING EIGENVECTORS

EIGENVALUE	EIGENVECTOR COMPONENTS						
-4.53312E-02	EIGENVECTOR OF MATRIX A						
	H 2	H 3	H 4	H 5	H 6	H 7	H 8
	-9.8868E-04	-2.0645E-03	-3.7301E-03	-4.5216E-03	-5.2437E-03	-3.0935E-03	-3.3071E-03
	H 9	H10	H11	X 1	X 2	X 3	X 4
	-3.4935E-03	-3.6804E-03	-3.8473E-03	4.3235E-02	1.1303E-01	1.7728E-01	2.0087E-01
	X 5	X 6	X 7	X 8	X 9	X10	X11
	1.8198E-01	1.4639E-01	1.8859E-01	2.4220E-01	3.0243E-01	3.7057E-01	4.4921E-01
	X12	T 1	T 2	T 3	T 4	T 5	T 6
	5.7701E-01	-9.0041E-04	-1.7287E-02	-2.2935E-02	-1.6164E-02	-6.2570E-03	5.4705E-03
	T 7	T 8	T 9	T10	T11	T12	
	2.5657E-03	2.5749E-04	-1.5259E-03	-2.7577E-03	-2.8408E-03	3.6346E-03	
	EIGENVECTOR OF MATRIX A TRANSPOSED						
	H 2	H 3	H 4	H 5	H 6	H 7	H 8
	4.8706E-03	1.2697E-02	2.1428E-02	2.8499E-02	3.3332E-02	3.7200E-02	4.1948E-02
	H 9	H10	H11	X 1	X 2	X 3	X 4
	4.6848E-02	5.1771E-02	5.6701E-02	6.6915E-01	5.8175E-02	6.3056E-02	6.6696E-02
	X 5	X 6	X 7	X 8	X 9	X10	X11
	7.0071E-02	7.3588E-02	6.5918E-02	6.8187E-02	6.8743E-02	6.7994E-02	6.6254E-02
	X12	T 1	T 2	T 3	T 4	T 5	T 6
	1.4086E 00	-1.6899E-01	-1.1882E-02	-1.1891E-02	-1.1949E-02	-1.2133E-02	-1.2450E-02
	T 7	T 8	T 9	T10	T11	T12	
	-1.0856E-02	-1.0955E-02	-1.0868E-02	-1.0692E-02	-1.0489E-02	-2.0704E-01	
-1.97553E-01	EIGENVECTOR OF MATRIX A						
	H 2	H 3	H 4	H 5	H 6	H 7	H 8
	2.4883E-02	2.7921E-02	3.2308E-02	3.5157E-02	3.7111E-02	3.7362E-02	3.8247E-02
	H 9	H10	H11	X 1	X 2	X 3	X 4
	3.9054E-02	3.9749E-02	4.0326E-02	-8.2580E-02	-1.9334E-01	-2.8572E-01	-3.0498E-01
	X 5	X 6	X 7	X 8	X 9	X10	X11
	-2.5612E-01	-1.8462E-01	-1.9042E-01	-1.7403E-01	-1.3063E-01	-5.7257E-02	4.8861E-02
	X12	T 1	T 2	T 3	T 4	T 5	T 6
	2.2272E-01	4.4481E-02	6.7533E-02	7.1197E-02	5.5814E-02	3.7470E-02	2.0015E-02

Table F.5 (continued)

T 7	T 8	T 9	T10	T11	T12	
1.9171E-02	1.6090E-02	1.1472E-02	5.8829E-03	4.0375E-04	7.1597E-01	

EIGENVECTOR OF MATRIX A TRANSPOSED

H 2	H 3	H 4	H 5	H 6	H 7	H 8
3.0867E-03	7.2321E-03	1.1505E-02	1.4701E-02	1.6689E-02	1.8071E-02	1.9288E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
2.0160E-02	2.0749E-02	2.1111E-02	4.6423E-01	3.2169E-02	3.1424E-02	2.9988E-02

X 5	X 6	X 7	X 8	X 9	X10	X11
2.7628E-02	2.3983E-02	1.4748E-02	9.5414E-03	5.2347E-03	1.7334E-03	-1.0282E-03

X12	T 1	T 2	T 3	T 4	T 5	T 6
-9.5353E-02	-5.1173E-02	-3.5073E-03	-3.3798E-03	-3.1692E-03	-2.8432E-03	-2.3415E-03

T 7	T 8	T 9	T10	T11	T12	
-1.2852E-03	-7.4002E-04	-3.6763E-04	-1.2202E-04	3.3517E-05	1.5338E 00	

-1.30132E-01

EIGENVECTOR OF MATRIX A

H 2	H 3	H 4	H 5	H 6	H 7	H 8
-3.6099E-02	-3.9766E-02	-4.4721E-02	-4.7242E-02	-4.8723E-02	-4.4620E-02	-4.4944E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
-4.5143E-02	-4.5263E-02	-4.5290E-02	1.2864E-01	2.9568E-01	4.3538E-01	4.6421E-01

X 5	X 6	X 7	X 8	X 9	X10	X11
3.8848E-01	2.7719E-01	2.7542E-01	2.4782E-01	1.9159E-01	1.0547E-01	-1.1114E-02

X12	T 1	T 2	T 3	T 4	T 5	T 6
-1.9163E-01	-1.9425E-02	-5.5445E-02	-6.2686E-02	-4.0560E-02	-1.3047E-02	1.3466E-02

T 7	T 8	T 9	T10	T11	T12	
1.6337E-02	2.1522E-02	2.8052E-02	3.5247E-02	4.1917E-02	-8.8014E-02	

EIGENVECTOR OF MATRIX A TRANSPOSED

H 2	H 3	H 4	H 5	H 6	H 7	H 8
2.5650E-02	6.1905E-02	9.9925E-02	1.2893E-01	1.4745E-01	1.6073E-01	1.7302E-01

H 9	H10	H11	X 1	X 2	X 3	X 4
1.8250E-01	1.8955E-01	1.9461E-01	3.5289E 00	2.6291E-01	2.6466E-01	2.5845E-01

X 5	X 6	X 7	X 8	X 9	X10	X11
2.4331E-01	2.1552E-01	1.3961E-01	9.6760E-02	5.9801E-02	2.8658E-02	3.3138E-03

X12	T 1	T 2	T 3	T 4	T 5	T 6
-7.5141E-01	-8.3491E-01	-5.7704E-02	-5.6393E-02	-5.4404E-02	-5.1605E-02	-4.7457E-02

T 7	T 8	T 9	T10	T11	T12	
-3.4258E-02	-2.9418E-02	-2.5873E-02	-2.3346E-02	-2.1581E-02	1.1603E 00	

-4.77476E-01

EIGENVECTOR OF MATRIX A

Table F.5 (continued)

H 2	H 3	H 4	H 5	H 6	H 7	H 8
7.2048E-02	7.2648E-02	7.1850E-02	7.0119E-02	6.7355E-02	6.2580E-02	6.0609E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
5.9167E-02	5.8306E-02	5.8058E-02	-1.0641E-01	-9.5820E-02	-2.7207E-02	7.5847E-02

X 5	X 6	X 7	X 8	X 9	X10	X11
1.5369E-01	1.8502E-01	3.2787E-01	4.5160E-01	4.9816E-01	4.3723E-01	2.5766E-01

X12	T 1	T 2	T 3	T 4	T 5	T 6
-7.8985E-02	3.5984E-04	-1.3784E-02	-3.9985E-02	-6.1169E-02	-7.0631E-02	-6.5465E-02

T 7	T 8	T 9	T10	T11	T12
-8.0536E-02	-8.9177E-02	-8.9553E-02	-8.1875E-02	-6.9049E-02	7.8364E-03

EIGENVECTOR OF MATRIX A TRANSPOSED

H 2	H 3	H 4	H 5	H 6	H 7	H 8
-2.3043E-02	-3.0405E-02	-2.5339E-02	-1.2715E-02	1.0030E-03	1.5578E-02	3.7214E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
5.9914E-02	8.0328E-02	9.6568E-02	-3.7787E 00	-6.1627E-02	3.8706E-02	1.2432E-01

X 5	X 6	X 7	X 8	X 9	X10	X11
2.0399E-01	2.7517E-01	2.9690E-01	2.8693E-01	2.3911E-01	1.6226E-01	7.5733E-02

X12	T 1	T 2	T 3	T 4	T 5	T 6
-4.0272E-01	-2.1622E-01	-1.9577E-02	-2.4645E-02	-3.1316E-02	-3.9200E-02	-4.7179E-02

T 7	T 8	T 9	T10	T11	T12
-4.5490E-02	-4.4475E-02	-3.9761E-02	-3.4340E-02	-2.9993E-02	9.7299E-02

-7.82485E-01

EIGENVECTOR OF MATRIX A

H 2	H 3	H 4	H 5	H 6	H 7	H 8
-1.8485E-01	-1.7779E-01	-1.7003E-01	-1.6299E-01	-1.5724E-01	-1.3926E-01	-1.3400E-01

H 9	H10	H11	X 1	X 2	X 3	X 4
-1.2934E-01	-1.2492E-01	-1.2055E-01	6.8495E-02	1.9764E-02	-3.5322E-02	-5.0112E-02

X 5	X 6	X 7	X 8	X 9	X10	X11
-1.2116E-02	4.6766E-02	1.7097E-01	3.2262E-01	4.2483E-01	4.1904E-01	2.7423E-01

X12	T 1	T 2	T 3	T 4	T 5	T 6
-5.0986E-02	1.2610E-01	1.4522E-01	1.5761E-01	1.5516E-01	1.4570E-01	1.4031E-01

T 7	T 8	T 9	T10	T11	T12
1.2601E-01	1.1243E-01	1.0514E-01	1.0697E-01	1.1635E-01	-8.5090E-03

EIGENVECTOR OF MATRIX A TRANSPOSED

H 2	H 3	H 4	H 5	H 6	H 7	H 8
-1.5974E-02	-4.5054E-02	-7.6121E-02	-1.0143E-01	-1.1940E-01	-1.3406E-01	-1.4453E-01

H 9	H10	H11	X 1	X 2	X 3	X 4
-1.5284E-01	-1.6082E-01	-1.7130E-01	1.7814E-01	-6.7526E-02	-8.6530E-02	-8.1657E-02

Table F.5 (continued)

X 5	X 6	X 7	X 8	X 9	X10	X11
-5.3820E-02	-2.5586E-03	7.0427E-02	1.1602E-01	1.2348E-01	9.7573E-02	5.2817E-02

X12	T 1	T 2	T 3	T 4	T 5	T 6
-1.4790E-01	3.3617E 00	2.3093E-01	2.2428E-01	2.1543E-01	2.0463E-01	1.9161E-01

T 7	T 8	T 9	T10	T11	T12
1.4715E-01	1.3638E-01	1.2900E-01	1.2291E-01	1.1616E-01	-2.1094E-01

-1.06143E 00

EIGENVECTOR OF MATRIX A

H 2	H 3	H 4	H 5	H 6	H 7	H 8
9.4159E-02	8.5217E-02	7.9009E-02	7.2786E-02	6.5877E-02	5.7597E-02	5.1608E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
4.6292E-02	4.2130E-02	3.9409E-02	2.8954E-02	-8.0007E-02	-2.4171E-01	-3.5387E-01

X 5	X 6	X 7	X 8	X 9	X10	X11
-3.3145E-01	-2.0829E-01	-5.8829E-02	1.8962E-01	4.1612E-01	5.0010E-01	3.6373E-01

X12	T 1	T 2	T 3	T 4	T 5	T 6
-4.2560E-02	-4.5635E-02	-8.7054E-03	2.8717E-02	3.9407E-02	2.7305E-02	6.7643E-03

T 7	T 8	T 9	T10	T11	T12
-1.1149E-02	-3.5171E-02	-5.3977E-02	-5.9209E-02	-5.0139E-02	1.9663E-03

EIGENVECTOR OF MATRIX A TRANSPOSED

H 2	H 3	H 4	H 5	H 6	H 7	H 8
3.7487E-02	3.6991E-02	6.9094E-03	-3.1119E-02	-6.0666E-02	-8.1389E-02	-8.8524E-02

H 9	H10	H11	X 1	X 2	X 3	X 4
-8.1013E-02	-6.6949E-02	-5.4573E-02	3.2256E 00	-1.6060E-01	-3.3276E-01	-4.2464E-01

X 5	X 6	X 7	X 8	X 9	X10	X11
-4.2170E-01	-3.0096E-01	-7.7981E-03	1.9995E-01	2.7824E-01	2.3058E-01	1.0450E-01

X12	T 1	T 2	T 3	T 4	T 5	T 6
-2.3212E-01	-2.9312E 00	-1.8984E-01	-1.7398E-01	-1.6094E-01	-1.5839E-01	-1.7221E-01

T 7	T 8	T 9	T10	T11	T12
-1.7414E-01	-1.9416E-01	-2.0047E-01	-1.9878E-01	-1.9575E-01	2.4607E-01

Appendix G

COMPUTER PROGRAMS: DESCRIPTION AND USE

All of the calculations described in the text are accomplished by a set of integrated FORTRAN IV programs that run on an IBM 7094 computer with IBSYS Version 13. In addition, calculated response data can be stored on a magnetic tape and processed subsequently by a separate plot preparation program. The mode calculation and the plotting subroutines are described in this appendix.

G.1 Input/Output

Tape Unit Usage

Binary scratch units: 4, 34, 41

BCD scratch unit: 5

Input unit: 2 (or referenced by READ statements)

Output unit: 3 (or referenced by PRINT statements)

Storage of response data for plotting: 6 (binary) (When this unit is used a tape reel must be supplied to receive the data)

The unit numbers above are those used in the FORTRAN programs.

Tape Unit References

Unit 4 EXEC., DERIV., EIGMA., SENTY., RESPN.

Unit 34 EXEC., AUXOU., DERIV., MOD1., M234., EIGMA., ALOC., XZERO., INPUB., EIVEC., VECIO., SENTY.

Unit 41 EXEC., SAVE., MOD1., RESPN.

Unit 5 EIGMA.

Unit 6 SKIP., RESPN.

Input Data: Sequence and Format

The following list gives the sequence for the input data and the corresponding format. The FORTRAN variables are grouped according to cards, although in some cases the input format makes the number of cards indefinite. Only the data required for the options selected should be provided.

EXEC.

```
KCALC, MODEL, NWDS, NINCR, NOTFSS, VTST,
 I4     I4     I4    I4      I4     E8.4

    NSEN, JOPT, IRSET
     I4    I4    I4

(LABELS (I), I = 1, NWDS)                    If NWDS > 0
    12A6, 4 cards max.
```

DISTM.

```
NC, NS, NF, JCOTYP, KTYP, NIT, NDRAW,
    (IN(I), I = 1,5), NPROB

(AK(I), BK(I), CK(I), DK(I), AHL(I), BHL(I),
    CHL(I), AHV(I), BHV(I), CHV(I), I = 1, NC)

(AL(J), J = 1, NS)

(T(J), J = 1, NS)

J (feed stage)                          } DO loop
HF(J), (FX(I,J), I = 1, NC)             } for K = 1, NF

JD (draw stage)                         } DO loop
SL(JD), SV(JD)                          } for K = 1, NDRAW

SUMERR, HETERR, SUBCOL, DTLIM, (SPECS(I), I = 1,4),
    CHECK
```

Integers are all I4; floating point numbers are all E8.4

Used only when KCALC = 1,2,3, or 5

EQUIL.

I4 and E8.4

(P(J), J = 1, NS)

(WT(J), DENS(J), ADENS(J), J = 1, NC) — only when IN(2) = 2

AT, RHLDUP, ALPHA, BETA, PERR, BETAN, CAP — only when IN(2) = 2

(ACTCON(I), I = 1,4), — only when KTYP = 1

((XX(I,J), I = 1, NC), J = 1, NS) — only when KTYP = 1

Used only when KCALC = 1,2,3, or 5

DISTM.

9E8.4 (3 cards)

APO, BPO, APOP, BPOP, ACP, BCP, CCP, DCP,
AVH, BVH, CVH, DVH, HLDUPA, HLDUPB,
TF, FJF, DELTR, DELTC, DUMMY — only when IN(3) = 2

Used only if KCALC = 4 or 6

Read by EIGMA. and INPUT. if KCALC = 4

Read by DERIV. if KCALC = 6

FORM, N, K, VTST, NSEN, JOPT
F10.2 I10 I10 F10.2 I10 I10

(VECT(I), I = 1, N)
15A4 (per card)

(A(I), I = 1, N), (B(I), I = 1, N),

(BP(I), I = 1, N)
7F10.5 (per card) — If FORM = 0

((AA(I,J), J = 1, N), I = 1, N)
7F10.5 (per card) — If FORM = 1

(AA(I,J), J = 1, N) DO loop for I = 1, N
6E12.5 — If FORM = 5

DUMMY, (AA(I,J), J = 1, N) DO loop for I = 1, N — If FORM = 2 or 3

(AA(J,N+I), J = 1, N) DO loop for I = 1,K
7F10.5 (per card) or 6E12.5 if FORM=5 — If K > 0 and FORM ≠ 2

DUMMY, (AA(J,N+I), J = 1, N) DO loop for I = 1, K
6E12.5 — If K > 0 and FORM = 2

DERIV.

- (If KCALC = 6, see listing for DERIV.)
- (NPAR(I), MULT(I), I = 1, NSEN) 12(I4,I2) per card — Only when NSEN ≠ 0; Repeat cards for each model selected.

SKIP. These cards are used to skip past NP sets of response data on the plot data tape.

- IX, IH, IT, IDIF, NV, JFR, JTR (NV ≠ 0) 7I2 plotting control card
- Plot data card No. 1 } cards punched in previous response calculations
- Plot data card No. NP }
- Blank card

Controlled by DEBUG at RESPN. 800 with NPLOT = 3. Call to SKIP can occur no more than once.

RESPN.

- (NRESP(J), J = 1, 10) 10I2
- (D(I), I = 1, K) 9E8.4 (per card) — Repeat for each nonzero element of NRESP.

Only when KCALC = 5; Repeat cards for each model selected.

G.2 Program Control Parameters

Values Specified by Normal Input Data*

KCALC indicates type of calculation desired

- = 1 Distillation calculation only
- = 2 Distillation and mode calculation
- = 3 Autonomous distillation response (2 or 3 steady states required)
- = 4 Mode calculation only; supply state matrix on cards
- = 5 Forced response (distillation)
- = 6 Mode calculation and forced response only; supply state matrix on cards

---

* In order of their appearance.

MODEL indicates distillation models to be used

= 1 Model 1

= 2 Model 2

= 4 Model 3

= 8 Model 4

= Appropriate sum of above for a combination of models.

NWDS Number of words (6 characters) for LABELS

NINCR Number of times at which response is calculated

= 20 if input value is zero

NOTFSS controls the autonomous response calculation

= 0 if response calculation is based on final steady state

= 1 if final steady state is not to be used for parameter evaluation; a third steady state is provided for this purpose.

VTST determines number of eigenvectors calculated. Only those having eigenvalues no greater than VTST times the smallest eigenvalue are evaluated.

NSEN The number of parameter sensitivity calculations

JOPT Unused input parameter (internal use when KCALC = 6)

IRSET = 0 to hold reboiler steam temperature constant during autonomous response

= 1 to hold boilup rate constant during autonomous response

LABELS provides up to 4 cards of BCD information for title

NC Number of components

NS Number of stages, including reboiler and condenser

NF Number of feed streams

JCOTYP = 0 for partial condenser

= 2 for total condenser

KTYP = 0 for exponential equilibrium expression

= 1 for nonideal vapor-liquid equilibrium, used only when IN(2) = 2

= 2 for power series equilibrium expression

NIT Maximum number of overall iterations in the distillation calculation. Normally use 30.

NDRAW Number of side stream draws

IN(1) > 25 yields intermediate iteration printout for the distillation calculation

IN(2) = 0 for distillation calculation without pressures

= 2 for distillation calculation with pressures

IN(3) ≠ 0 for distillation calculation only

= 2 for calculation of state matrix

IN(4) = 0 for inclusion of Murphree efficiency calculation

= 1 for calculation with Murphree efficiencies = 0.70

If IN(4) = 0, must also have KTYP = 1 and IN(2) = 2

IN(5) controls printing of convergence information for pressure, efficiency, activity and reboiler criterion (subroutine SPEC.)

= 0 for no printing

= 1 for printing

NPROB For identification of distillation calculation

FORM controls input format for matrix read from cards

= 0 for tridiagonal matrix

= 1 for general matrix (format 7F10.5)

= 2, 3 or 4 Do not use

= 5 for general matrix (format GE12.5)

N is the number of state variables

K is the number of input variables (inputs to the simulated process)

Values Specified by DEBUG

KCON set at MOD1. 9000 to modify state matrix

= 1 normally (no modifications)

= 2 for condenser pressure control

= 3 for overhead flow disturbances transmitted to column (instead of to overhead product)

= 4 for modal control

manipulate ℓ_{N+1}, t_s, t_{cw}; measure t_o, t_{N+1}, x_{N+1}, x_o, t_{jF}

= 5 for options 2 and 4 combined

AA1-AA5
BB1-BB5
CC1-CC5
} set at CNTRL. 400 for modal control where:

$$\ell_{N+1} = AA1t_o + AA2t_{N+1} + AA3x_{N+1} + AA4x_o + AA5t_{jF}$$

$$t_s = BB1t_o + BB2t_{N+1} + BB3x_{N+1} + BB4x_o + BB5t_{jF}$$

$$t_{cw} = CC1t_o + CC2t_{N+1} + CC3x_{N+1} + CC4x_o + CC5t_{jF}$$

KPLOT set at RESPN. 800 to control plotting

= 0 normally (no plotting)

= 1 for transient response

= 2 for frequency response
= 3 for options 1 and 2
} must also set NOFR = 2 at RESPN. 800

NPLOT set at RESPN. 800 to control plot data tape

= 1 rewinds data tape (unit 6). Use no more than once.

= 2 normally. Data tape not shifted.

= 3 causes tape to space past all previous data. Must provide plot control card and data cards punched in prior response calculations (see input data sequence).

NPR set at QREIG. 10 to control printing in QR calculation

= 1 normally. Extra information printed by QR subroutines

= 0 to eliminate all printing by QR subroutines

G.3 Identification of Input Variables

Input for the Distillation Calculation (DISTM. and EQUIL.)

AK, BK, CK, DK are parameters in the vapor-liquid equilibrium expressions

$$\frac{y_i}{x_i} = AK(I) + BK(I) \times T + CK(I) \times T^2 + DK(I) \times T^3$$

when KTYP = 2

$$\frac{y_i}{x_i} = \exp\left\{\frac{AK(I)}{T + DK(I)} + BK(I) + CK(I)\left[T + DK(I)\right]\right\}$$

when KTYP = 0

$$\frac{y_i}{x_i^*} = \frac{\gamma_i}{P} \exp\left\{\frac{AK(I)}{T + DK(I)} + BK(I) + CK(I)\left[T + DK(I)\right]\right\}$$

when KTYP = 1

AHL, BHL, CHL are parameters in an enthalpy correlation for liquid streams (per mole)

$$\text{enthalpy} = \sum_{i=1}^{NC} x_i\left[AHL(I) + BHL(I) \times T + CHL(I) \times T^2\right]$$

AHV, BHV, CHV are parameters in an enthalpy correlation for vapor streams (per mole)

$$\text{enthalpy} = \sum_{i=1}^{NC} y_i\left[AHV(I) + BHV(I) \times T + CHV(I) \times T^2\right]$$

AL are flow rates of the liquid streams leaving each plate. The bottom product flow rate AL(1) and reflux flow rate AL(NS) are fixed by the input. All other flow rates are estimates.

T are estimated temperatures for each plate.

J is the feed plate.

HF is the total enthalpy of the feed (not on mass basis)

FX is the feed rate

JD is a plate at which there is a side stream draw

SL, SV are the flow rates of the liquid and vapor drawn from the plate

SUMERR is the error limit on the sum of mole fractions. The sum of mole fractions can differ from unity by no more than SUMERR. Usually SUMERR = 0.001.

HETERR is the error limit for the heat balance. For convergence the proposed fractional change in flow rates must be less than HETERR. Usually HETERR = 0.001.

SUBCOL is the subcooling of reflux (degrees below bubble point) for total condenser

DTLIM is a limit on the temperature correction, in degrees. Usually DTLIM = 10.0

SPECS not used

CHECK = 11.111, verifies correct input sequence

P are estimated pressures for each plate; P(N+1) fixes the condenser pressure

WT are molecular weights for each component

DENS, ADENS are parameters in the molar density correlation

$$\rho = \sum_{i=1}^{NC} x_i \Big(\text{DENS(I)} + \text{ADENS(I)} \times T\Big)/\text{WT(I)}$$

AT is the plate area, ft^2

RHLDUP = H_w, residual holdup, in moles

ALPHA = α, coefficient in the hydraulic expression, in. H_2O/gpm

BETA = β, coefficient in the vapor flow expression, ft^2

PERR is the convergence criterion for pressure. The pressure correction must be less than PERR, in atm

BETAN = β_N, coefficient for vapor flow overhead, ft^2

CAP = κ, coefficient that gives the influence of vapor rate on holdup, in H_2O/ft/sec

ACTCON are the constants for the Van Laar activity coefficient correlation

$$\text{ACTCON}(1) = A_{12}$$
$$\text{ACTCON}(2) = A_{21}$$
$$\text{ACTCON}(3) = A_{12}$$

Thus

$$\gamma_i = \exp\left\{\frac{\text{ACTCON(I)}}{1+\left[\frac{x_i \times \text{ACTCON(I)}}{(1-x_i)\times \text{ACTCON(I+1)}}\right]^2}\right\}$$

for a binary system only.

XX are estimated compositions on each plate for both components, used for initial estimates of activity coefficients.

APO, BPO are parameters for calculation of the vapor pressure of the light component

$$P^{o(1)} = \text{APO} \times \exp(-\text{BPO}/T)$$

APOP, BPOP are parameters for calculation of the vapor pressure of the heavy component

$$P^{o(2)} = \text{APOP} \times \exp(-\text{BPOP}/T)$$

ACP, BCP, CCP, DCP are parameters for calculation of liquid heat capacity by

$$c = x(ACP + BCP \times T) + (1-x)(CCP + DCP \times T)$$

AVH, BVH, CVH, DVH are parameters for calculation of heat of vaporization by

$$\lambda = x(AVH - BVH \times T) + (1-x)(CVH - DVH \times T)$$

HLDUPA is the accumulator holdup in moles

HLDUPB is the reboiler holdup in moles

TF is the temperature of the feed stream

FJF is the feed plate in floating point format

DELTR is the temperature driving force for the reboiler

DELTC is the average temperature driving force for the condenser.

Input for the Mode Calculation
(DERIV.,or EIGMA., and INPUT.)

VECT is a vector of BCD labels for the state variables

A, B, BP are the main diagonal, upper diagonal and lower diagonal coefficients, respectively, for a tridiagonal state matrix

AA is the NXN state matrix $\underline{\underline{A}}$ arranged by rows. If FORM = 5, each row must start on a new card.

AA(J,N+I), where I = 1,K, is the input matrix $\underline{\underline{B}}$ arranged by columns. If FORM = 0 or 5, each column must start on a new card.

Input for the Sensitivity Calculation
(DERIV.)

NPAR is the index number of the parameter for which sensitivity is to be calculated. The index number is the sequence in the labeled common /DCOM/, which is given in a following section.

MULT is the number of sequential parameters to be included in the calculation of a summed sensitivity.

Input for Response Calculations
(RESPN.)

NRESP is a vector that identifies the type of response calculation to be performed. If NRESP(1) = 0, no calculations are performed. A maximum of 10 responses may be calculated for disturbances in:

= 1 feed flow rate
= 2 feed temperature
= 3 feed composition
= 4 reflux flow rate
= 5 reboiler steam temperature
= 6 condenser coolant temperature
= 7 two or more inputs

D is the vector of input variables d

G.4 Overlay Structure

The programs are too extensive to reside in the IBM 7094 core storage at one time. Consequently they are grouped in links, as shown in Figure G.4.1, and the FORTRAN IV overlay feature is used. The letters A through F in the figure refer to the origins for the links. The main program, which always resides in core storage, is EXEC.

G.5 COMMON Usage

Communication among the subroutines is carried out by subroutine arguments and by labeled COMMON. The COMMON names and the subroutines that use them are listed below.

/CEIG/	EXEC., EIGMA., SKIP., SENTY., RESPN.
/CDIST/	EXEC., DISTM., SPEC., DERIV.
/DCOM/	SAVE., RHOMW., DISTM., SPEC., OUTPU., EQUIL., AUXOU., DERIV., MOD1., CNTRL., M234.

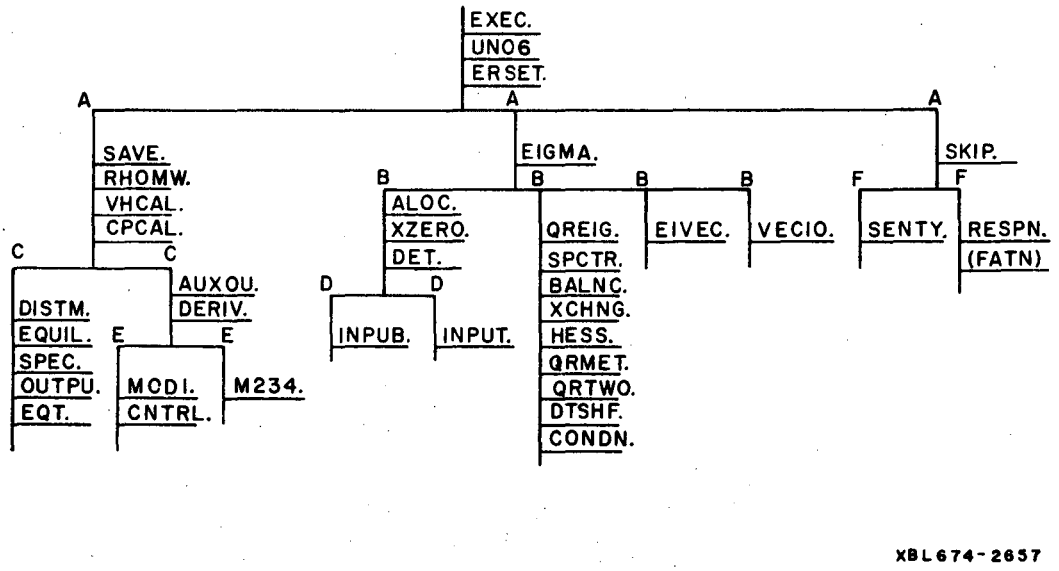


Fig. G.4.1 Overlay structure

/AUX/ AUXOU., DERIV., MODl., CNTRL., M234.

/EIGCOM/ EIGMA., INPUB., INPUT., EIVEC., VECIO.

/CCHAR/ EIGMA., INPUB., INPUT.

/CXZERO/ EIGMA., XZERO., VECIO.

/CRESP/ SKIP., SENTY., RESPN.

The labeled COMMON /DCOM/ is especially important because it contains all of the distillation parameters. Any of these parameters in /DCOM/ may be used for eigenvalue sensitivity calculations. They are referred to by their sequence numbers as shown below.

COMMON /DCOM/

Parameter	Sequence No., NPAR	Dimension	Parameter	Sequence No., NPAR	Dimension
AK	0001	10	AL	1524	70
BK	0011	10	ERR	1594	70
CK	0021	10	V	1664	70
DK	0031	10	SL,A,GAM	1734	70
KTYP	0041	1	SV,B,DELT	1804	70
EQ	0042	700	NS	1874	1
T	0742	70	NF	1875	1
X	0812	700	NDRAW	1876	1
NC	1512	1	JCOTYP	1877	1
N	1513	1	IN	1878	5
QC	1514	1	SPECS	1883	4
QR	1515	1	F	1887	70
QNET	1516	1	HF	1957	70
CHECK	1517	1	FX	2027	700
DL	1518	1	DTLIM	2727	1
OK	1519	1	SUMERR	2728	1
ITERAT	1520	1	HETERR	2729	1
ITHEAT	1521	1	SUBCOL	2730	1
ITTEMP	1522	1	NPROB	2731	1
NIT	1523	1	HL	2732	70

Parameter	Sequence No., NPAR	Dimension	Parameter	Sequence No., NPAR	Dimension
HV	2802	70	CVH	3355	1
OLDDL,XI	2872	70	DVH	3356	1
QERR,EPS,BP	2942	70	HLDUPA	3357	1
JF	3012	1	HLDUPB	3358	1
P	3013	70	TF	3359	1
HLDUP	3083	70	FJF	3360	1
WT	3153	10	DELTR	3361	1
DENS	3163	10	DELTC	3362	1
ADENS	3173	10	CAP	3363	1
ACTCON	3183	10	TS	3364	1
PERR	3193	1	UA	3365	1
SW	3194	1	VR	3366	1
AT	3195	1	QRERR	3367	1
ALPHA	3196	1	BETAN	3368	1
BETA	3197	1	WC*	3369	1
RHLDUP	3198	1	AHL	3370	10
PTOP	3199	1	BHL	3380	10
XX	3200	140	CHL	3390	10
NIN	3340	1	AHV	3400	10
APO	3341	1	BHV	3410	10
BPO	3342	1	CHV	3420	10
APOP	3343	1	CMC*	3430	1
BPOP	3344	1	CMR*	3431	1
A1	3345	1	WMC*	3432	1
B1	3346	1	WMR*	3433	1
A2	3347	1	AMC*	3434	1
B2	3348	1	AMR*	3435	1
ACP	3349	1	USCP	3436	1
BCP	3350	1	UCP	3437	1
CCP	3351	1	UMRP	3438	1
DCP	3352	1	URP*	3439	1
AVH	3353	1	FILL*	3440	11
BVH	3354	1	Total	3450	

* Disregard these parameters. They are not used.

G.6 Identification of Program Variables for Distillation Calculations*

AA	=	$\underline{\underline{A}}$	EPS	=	ϵ
ACT 1,ACT 2	=	$\gamma^{(1)},\gamma^{(2)}$	EQ	=	$y/x^* = K$
ACTCON	=	A_{12} or A_{21}	ETA	=	η
AL	=	$\bar{L}$ or $\bar{\ell}$	F	=	$\bar{F}$ or $\bar{f}$
ALPHA	=	α	GAM	=	γ
ALPHP	=	α'	GAMC	=	$G = 1/\gamma'$
AT	=	A_T	HLDUP	=	$\bar{H}$ or $\bar{h}$
BETA	=	β	HLDUPA	=	$\bar{H}_{N+1} = \bar{h}_{N+1}$
BETAN	=	β_N	HLDUPB	=	$\bar{H}_O = \bar{h}_O$
BETAP	=	β'	HL	=	liquid enthalpy
CAP	=	κ	HV	=	vapor enthalpy
CAPA	=	κ''	L(-1)**	=	N
CP	=	c	N	=	n
CPF	=	c_F	NS(-1)**	=	N+1
CPO	=	c^O	P	=	$\bar{P}$ or $\bar{p}$
DEE	=	D	PC1-PC4	=	pc1-pc4
DELT	=	δ	PNU	=	ν'
DELTC	=	$\bar{T}_{N+1} - T_{cw}$	PSI	=	ψ
DELTR	=	$\bar{T}_s - \bar{T}_O$	PTOP	=	$\bar{P}_N = \bar{p}_N$
E	=	E	QC	=	Q_c

* These variables are defined in the Nomenclature section that follows Appendix B.

** The index for plate numbers begins with the reboiler as plate 1 in the FORTRAN programs.

QR	=	Q_r	UMR	=	U_r
RHLDUP	=	H_w	UMRP	=	U'_r
RHO	=	ρ_L	USC	=	U_{sc}
RHOV	=	ρ_v	USCP	=	U'_{sc}
SC1-SC4	=	sc1-sc4	V	=	$\bar{V}$ or $\bar{v}$
SIG	=	σ	VAPHT	=	λ
SIGHT	=	$\hat{\sigma}$	VAPHTO	=	λ^0
SUBCOL	=	$\bar{T}_c - \bar{T}_{N+1}$	VMW	=	M_v (mixture)
T	=	$\bar{T}$ or $\bar{t}$	VPTOP	=	$P_N^{0(1)}$
TAU	=	τ	WT	=	M (molecular wt.)
TAUL3		not used	X	=	$\bar{x}$
TC	=	T_c or t_c	XEQ	=	$\bar{x}^*$
TCW	=	T_{cw} or t_{cw}	XF	=	$\bar{x}_F$
TF	=	T_F or t_F	XI	=	ξ
TS	=	T_s or t_s	XMU	=	μ
UC	=	U_c	Y	=	$\bar{y}$
UCP	=	U'_c	ZETA	=	ζ

G.7 Subroutine Descriptions

EXEC is the executive program (main program for the mode and response calculation). It reads and prints control parameters and titles, controls the calculations performed, and prints timing information.

ERRSET overrides error traps as follows:

1. Eliminates job termination after ten error messages,
2. eliminates field width error message,
3. allows truncated numbers to be printed, and
4. causes termination after 100 overflows and divide checks.

SAVE stores and retrieves steady state distillation information (from COMMON/DCOM/) using unit 41.

RHOMW calculates average molecular weight of the vapor or average molar density of the liquid.

VHCALC evaluates the latent heat of vaporization.

CPCALC evaluates the heat capacity of a binary mixture.

DSTMAN controls the steady state distillation calculation. This program and the subroutines called by it are basically the same as those written by J. S. Newman.[42] The method is of the Thiele-Geddes type with temperature correction accomplished by a Newton-Raphson iteration.

EQUIL calculates bubble points and vapor-liquid equilibrium constants. Correlations may be of the power series or exponential type. If the latter, activity coefficients, pressure dependence, and Murphree efficiencies may be included.

SPEC superimposes on outer loop (iteration) on the entire distillation calculation. It provides for the evaluation of pressures, Murphree efficiencies, activities, and for constant reboiler conditions at more than one steady state.

OUTPUT prints distillation steady state results.

EQT evaluates derivatives of the vapor-liquid equilibrium constants.

DERIV calculates the derivative of matrix $\underline{\underline{A}}$ with respect to any parameter in /DCOM/ and stores it on unit 4. A forward difference approximation to the derivative is determined (step size one percent of the parameter).

AUXOUT evaluates the coefficients of the linearized differential equations for all three distillation models.

MOD1 determines matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ for Model 1.

CNTRL modifies the coefficients of matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ according to the control equations. It is used primarily for modal control or pressure control calculations.

M 234 determines matrices $\underline{\underline{A}}$ and $\underline{\underline{B}}$ for Models 3 and 4.

EIGMAN controls the calculation of eigenvalues and eigenvectors. It also pairs up complex conjugate modes, orders the modes, calculates the sum and product of the eigenvalues, and prints timing information.

ALOC positions unit 34 so that the data from the distillation calculation are ready for use in the mode calculation.

XZERO calculates a nonzero initial condition determined by the difference between two steady states.

DET calculates the determinant of a matrix without destroying the matrix.

INPUTB reads the $\underline{\underline{A}}$ and $\underline{\underline{B}}$ matrices from unit 34, and calculates the trace and determinant of $\underline{\underline{A}}$.

INPUT is like INPUTB but uses card input.

QREIG controls the calculation of eigenvalues by the QR method program written by B. Parlett.[44] The following subroutines are subordinate: SPECTRM, BALANC, XCHANG, SUBDIA, QRMETH, QQR2, DTSHIF, CONDIT.

EIGVEC calculates eigenvectors by inverse iteration.

VECIO prints eigenvectors and calculates the following checks:

$$(\underline{\underline{A}} - \lambda_i \underline{\underline{I}})\, \underline{u}^{(i)},\ \underline{\underline{U}}^T\underline{\underline{V}},\ \underline{\underline{V}}\,\underline{\underline{U}}^T.$$

SKIP spaces the response data tape past all previous data. It is controlled by data cards punched during prior response calculations.

SENTY calculates eigenvalue sensitivities using derivative matrices stored on unit 4.

RESPNS calculates the response of the state vector to a step change of the input vector and following initial conditions. A frequency response calculation is included but not debugged. If desired, the response data may be stored on unit 6 for subsequent plotting.

PLOT is a main program that controls plotting of the response data stored on unit 6. It provides for plotting in a variety of formats. The program uses subroutine GRAPH and actually only prepares a plot tape that is used subsequently for control of the incremental plotter by a system program. Both PLOT and GRAPH use a University of California, Berkeley computer center library subroutine (J5 BC XYP4) that does the mechanics of plot tape preparation.

GRAPH is a subroutine prepared by J. E. Crider[10] that specifies the frame and tick marks, places scales and labels on the axes, and draws the curves. Rectangular, semi-logarithmic, or logarithmic graphs may be specified.

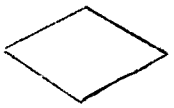
NOTE: The details (other than listings) for the various plotting programs are not included because they can only be used at the University of California, Berkeley Computer Center on the IBM 7094 computer in their present form.

G.8 Subroutine Flow Charts

On the following pages are flow charts for the more important programs that contain considerable logic. The numbers in circles or adjacent to boxes correspond to FORTRAN statement numbers. The symbols are as follows:

Terminals, or connectors for entry from, or exit to, another part of the flow chart.

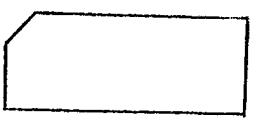
processing operations (may include input or output).



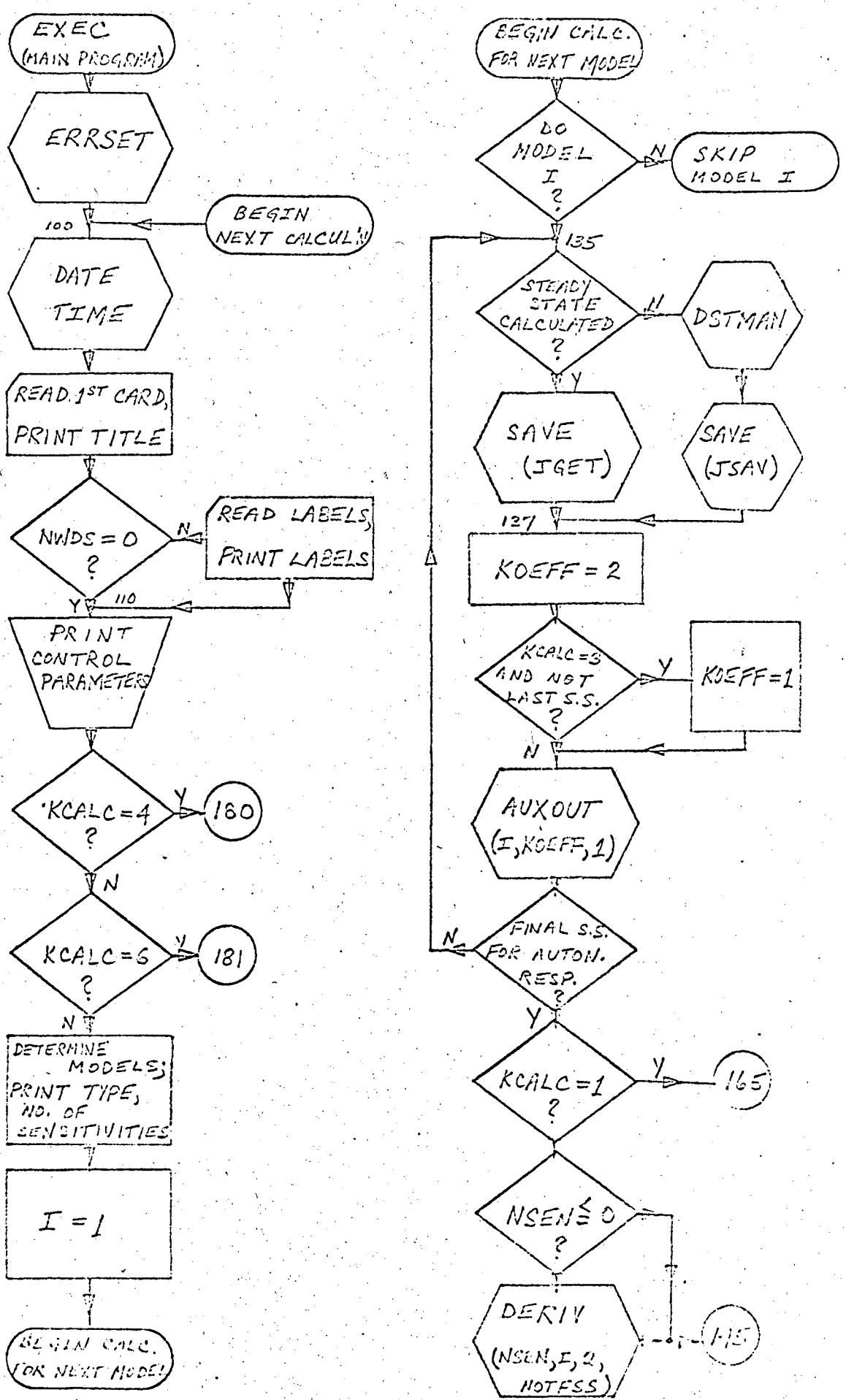
decisions or computed GO TO. Affirmative test is indicated by Y (yes) and negative by N (no).

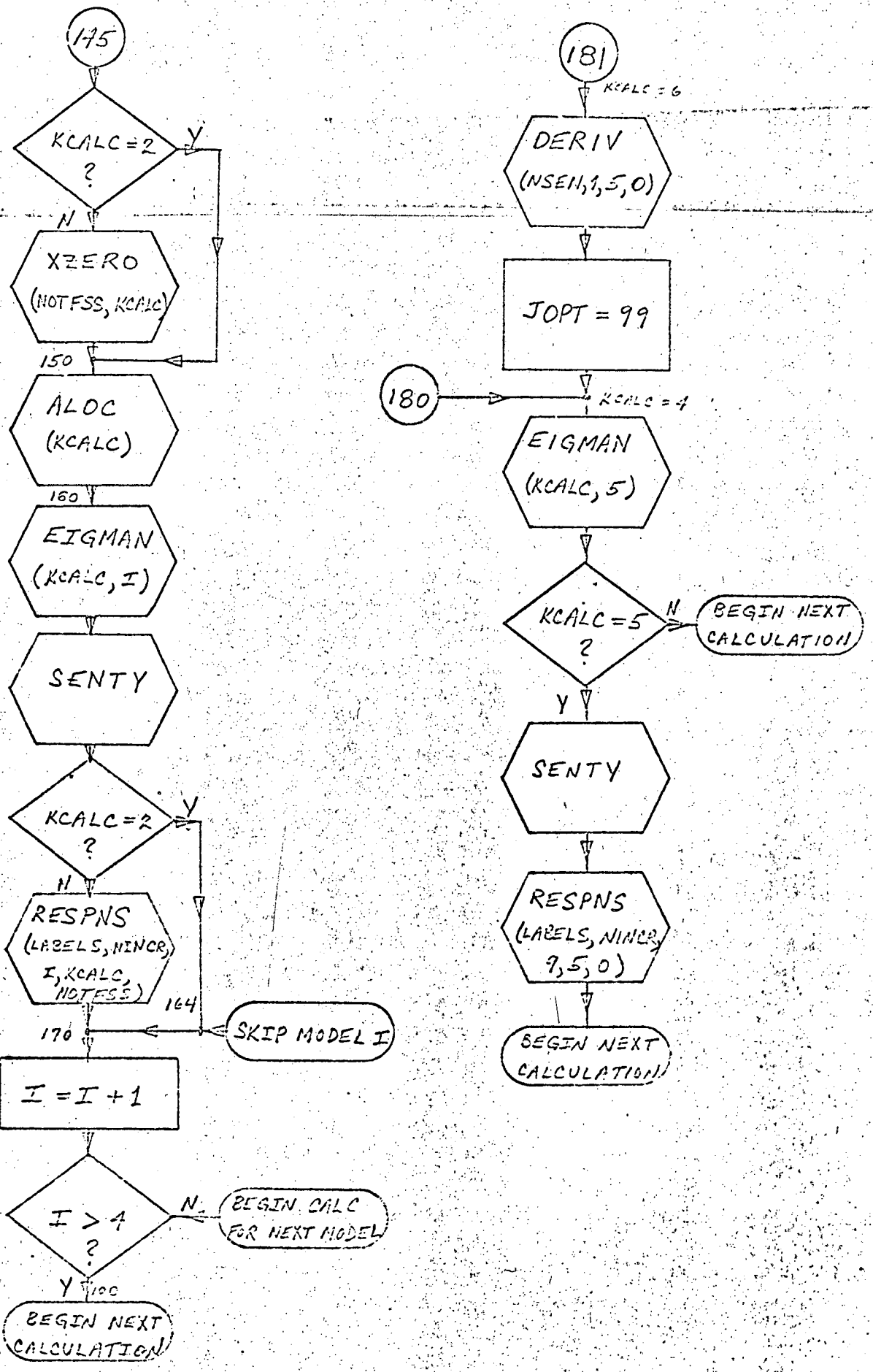
subroutine

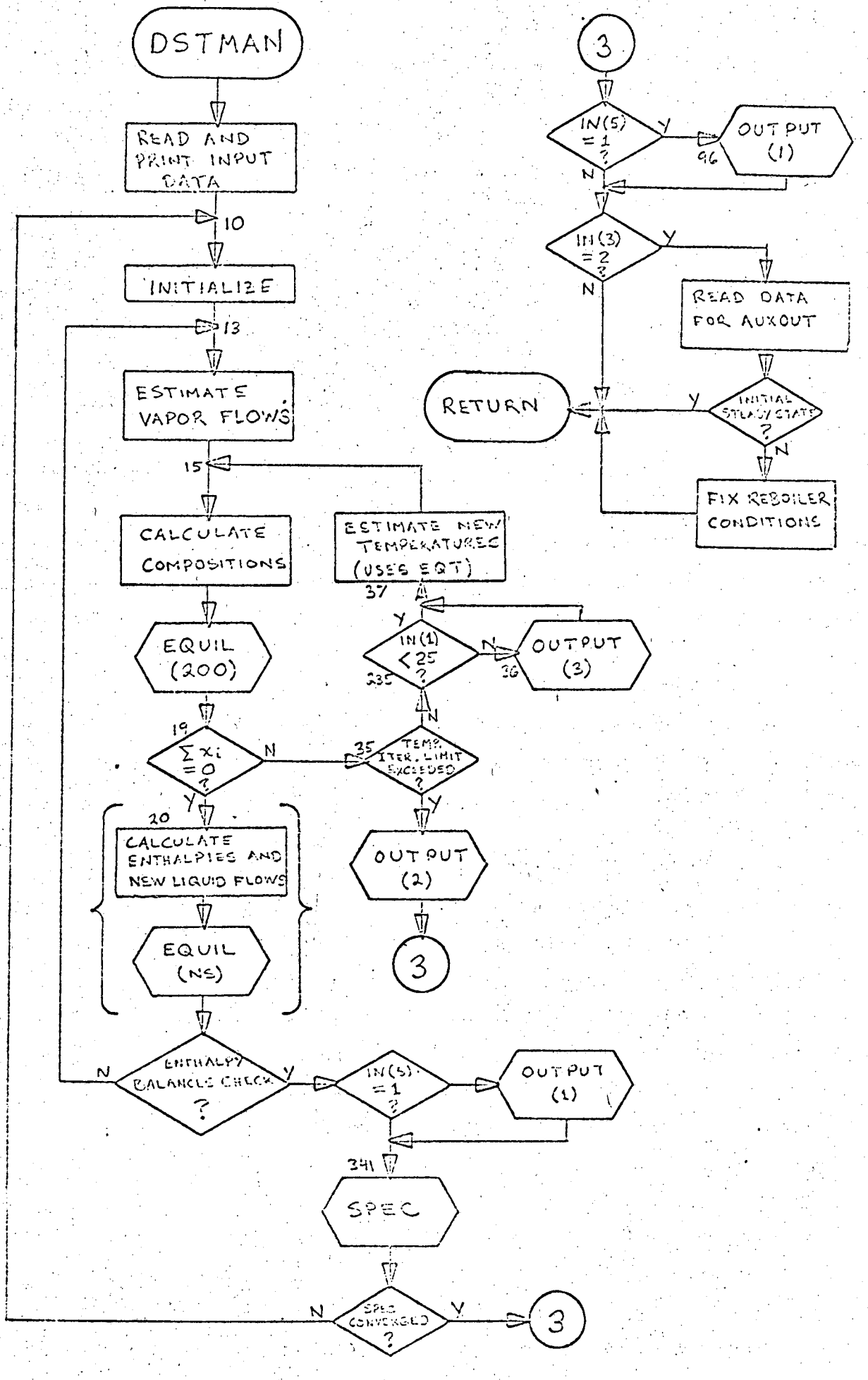
input/output (not always used).

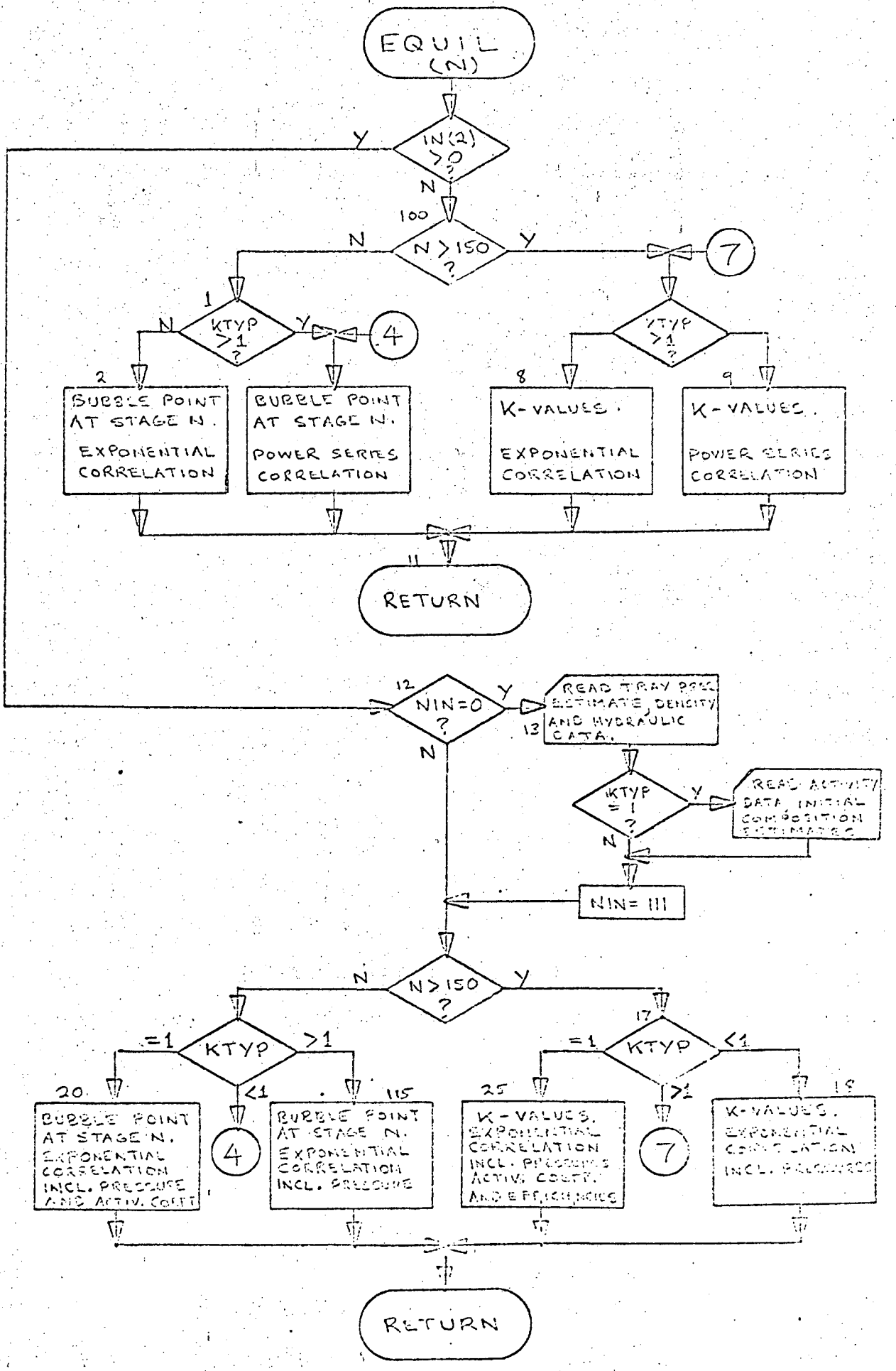


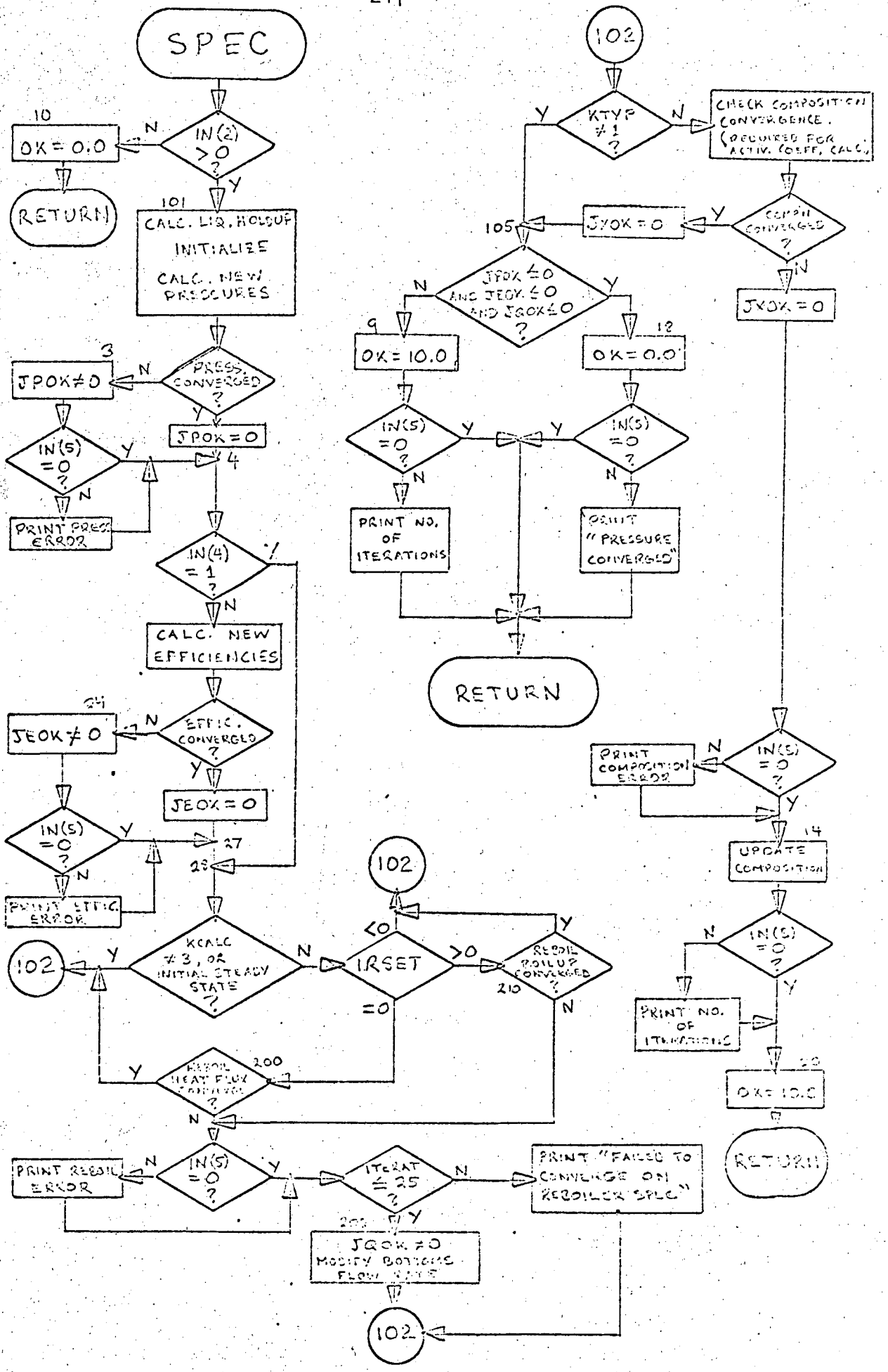
card input (not always used)

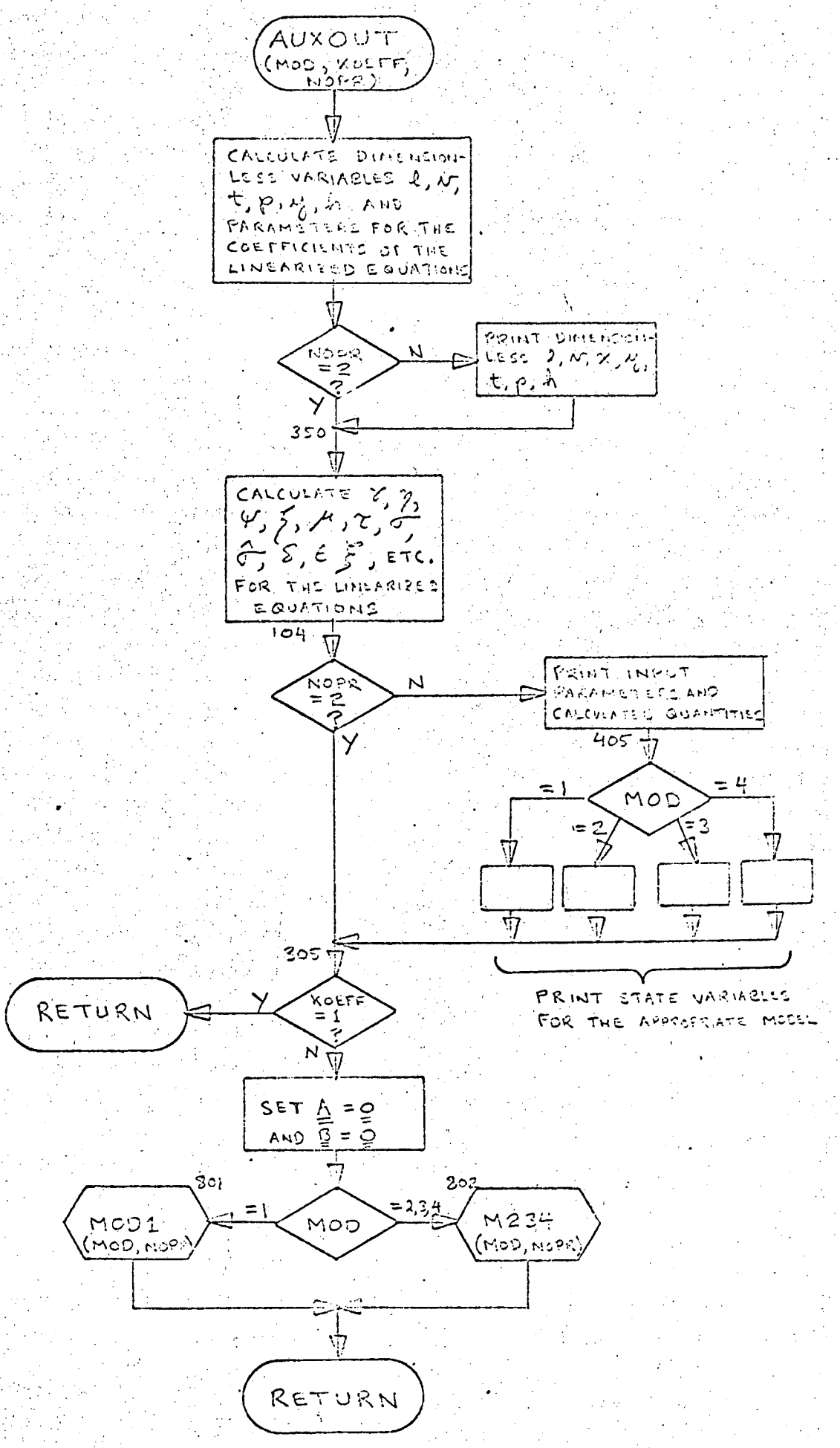

EXEC (MAIN PROGRAM)
ERRSET
100
BEGIN NEXT CALCUL'N
DATE TIME
READ 1ST CARD, PRINT TITLE
NWDS = 0 ?
N
READ LABELS, PRINT LABELS
Y
110
PRINT CONTROL PARAMETERS
KCALC=4 ?
Y
180
N
KCALC=6 ?
Y
181
N
DETERMINE MODELS; PRINT TYPE, NO. OF SENSITIVITIES
I = 1
BEGIN CALC. FOR NEXT MODEL
BEGIN CALC. FOR NEXT MODEL
DO MODEL I ?
N
SKIP MODEL I
135
STEADY STATE CALCULATED ?
N
DSTMAN
Y
SAVE (JGET)
SAVE (JSAV)
127
KOEFF = 2
KCALC=3 AND NOT LAST S.S. ?
Y
KOEFF=1
N
AUXOUT (I,KOEFF,1)
FINAL S.S. FOR AUTON. RESP. ?
N
Y
KCALC=1 ?
Y
165
NSEN ≥ 0 ?
DERIV (NSEN,I,2, NOTFSS)
145

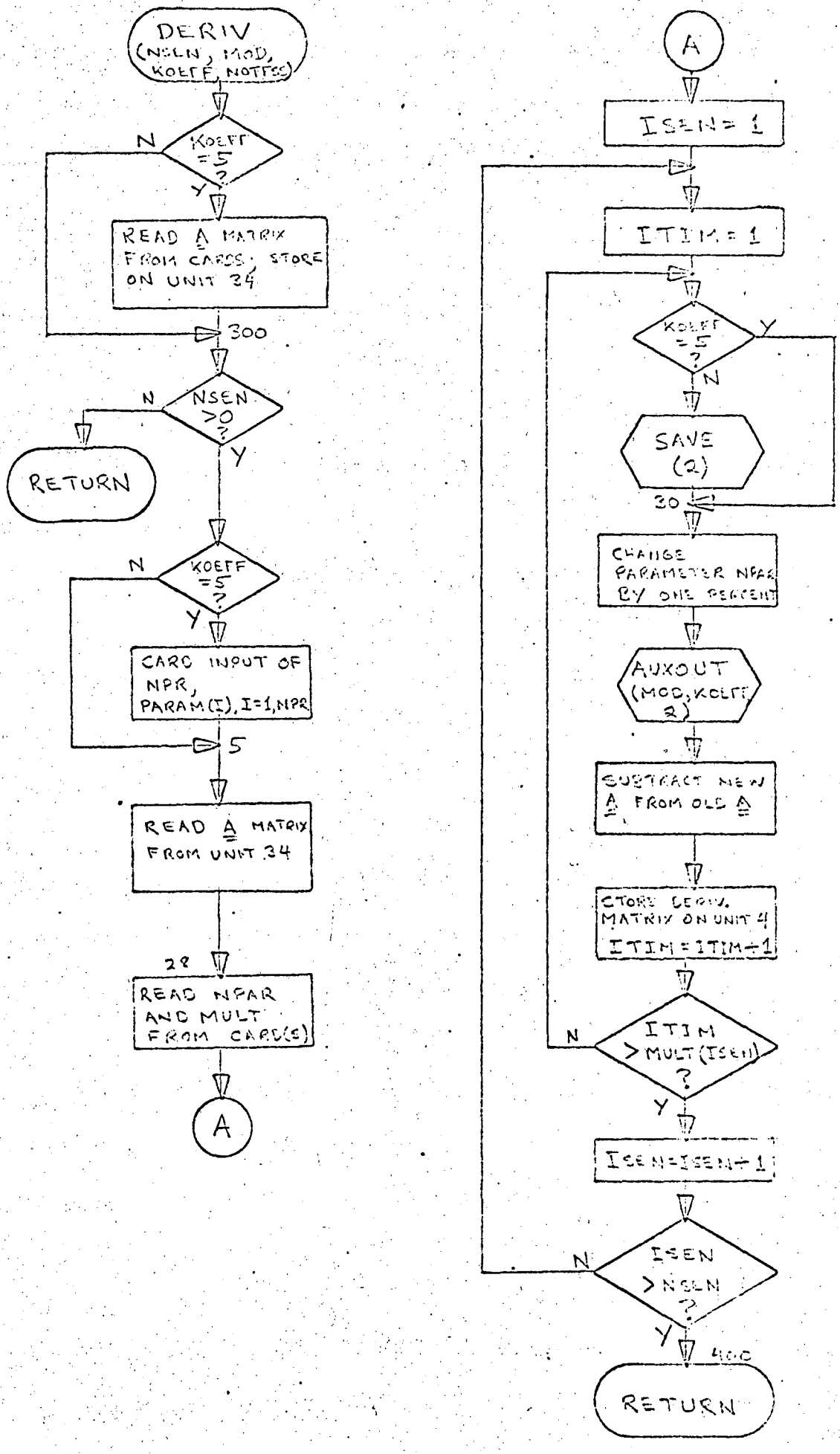

175
KCALC=2 ?
Y
N
XZERO (NOTFSS, KCALC)
150
ALOC (KCALC)
160
EIGMAN (KCALC, I)
SENTY
KCALC=2 ?
Y
N
RESPNS (LABELS, NINCR, I, KCALC, NOTFSS)
164
170
SKIP MODEL I
I = I + 1
I > 4 ?
N
BEGIN CALC FOR NEXT MODEL
Y
100
BEGIN NEXT CALCULATION
181
KCALC = 6
DERIV (NSEN, 1, 5, 0)
JOPT = 99
180
KCALC = 4
EIGMAN (KCALC, 5)
KCALC=5 ?
N
BEGIN NEXT CALCULATION
Y
SENTY
RESPNS (LABELS, NINCR, 9, 5, 0)
BEGIN NEXT CALCULATION

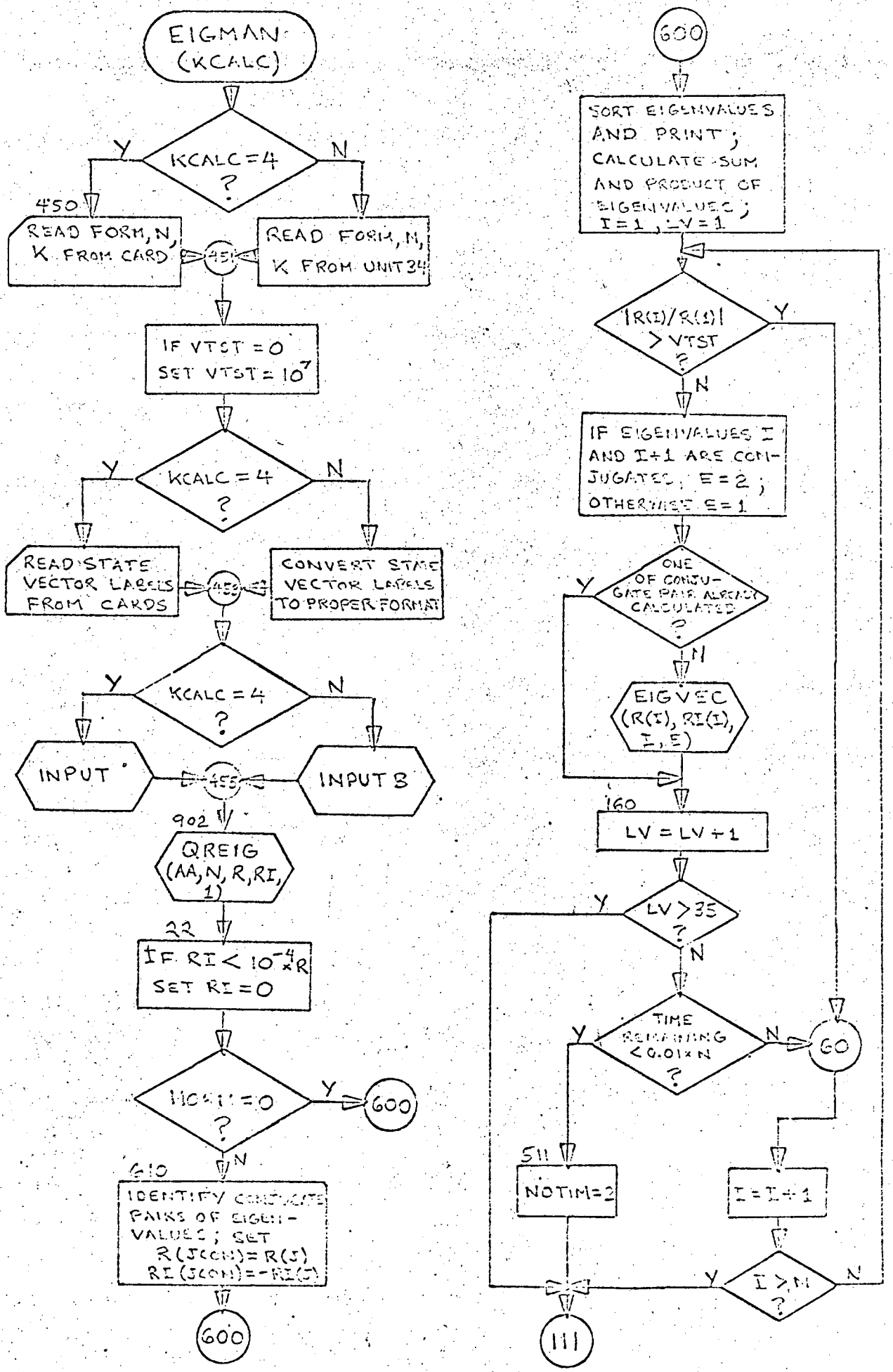

DSTMAN
READ AND PRINT INPUT DATA
10
INITIALIZE
13
ESTIMATE VAPOR FLOWS
15
CALCULATE COMPOSITIONS
ESTIMATE NEW TEMPERATURES (USES EQT)
37
EQUIL (200)
IN(1) < 25 ?
235
Y
N
OUTPUT (3)
36
19
Σ xi = 0 ?
N
35
TEMP. ITER. LIMIT EXCEEDED ?
Y
20
CALCULATE ENTHALPIES AND NEW LIQUID FLOWS
EQUIL (NS)
OUTPUT (2)
3
ENTHALPY BALANCE CHECK ?
N
Y
IN(5) = 1 ?
OUTPUT (1)
341
SPEC
SPEC CONVERGED ?
N
Y
3
3
IN(5) = 1 ?
Y
96
OUTPUT (1)
N
IN(3) = 2 ?
Y
READ DATA FOR AUXOUT
INITIAL STEADY STATE ?
Y
N
RETURN
FIX REBOILER CONDITIONS

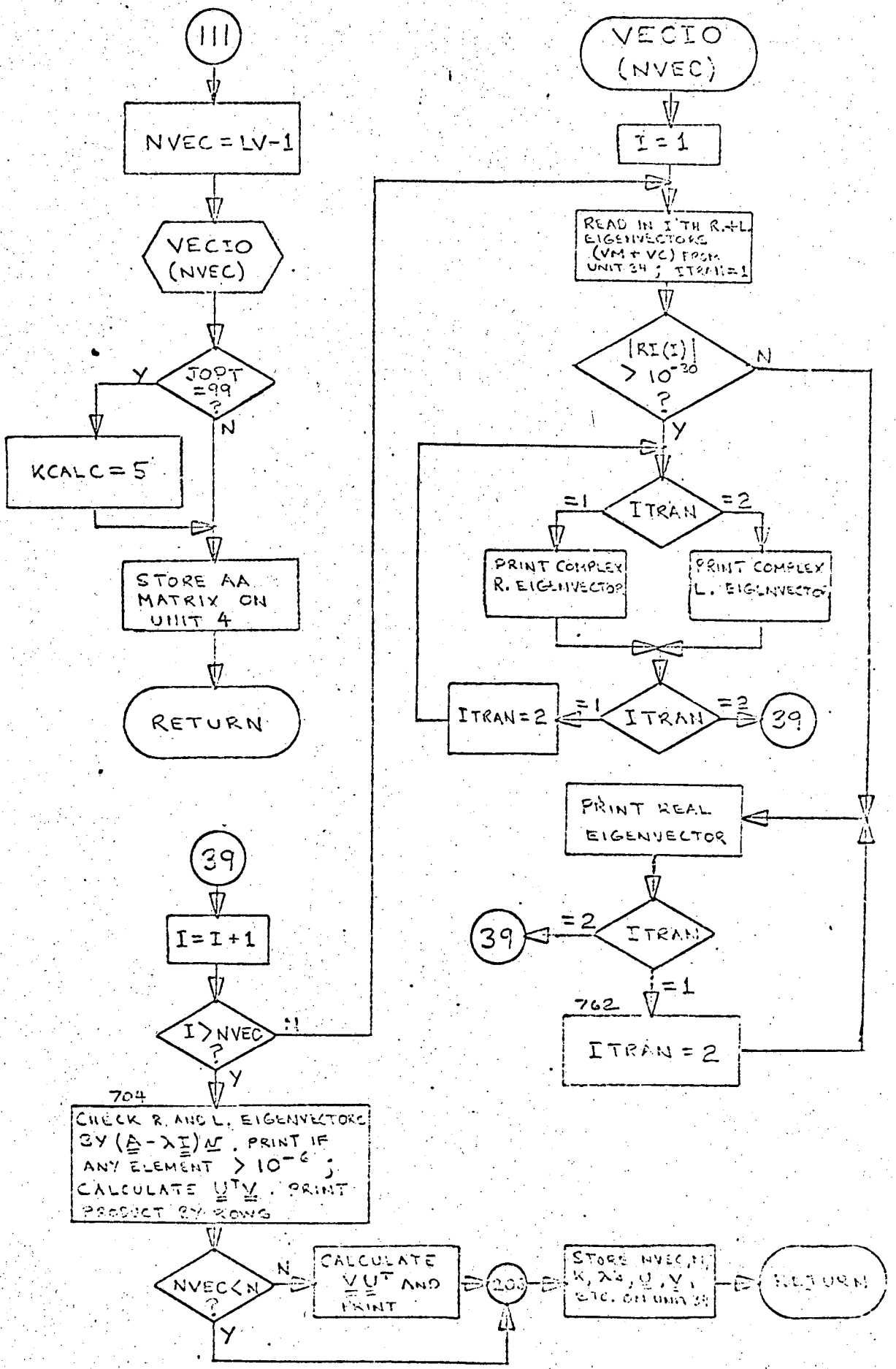

EQUIL (N)
IN(2) > 0 ?
Y
N
100
N > 150 ?
N
Y
7
1
KTYP > 1 ?
N
Y
4
2
BUBBLE POINT AT STAGE N. EXPONENTIAL CORRELATION
BUBBLE POINT AT STAGE N. POWER SERIES CORRELATION
KTYP > 1 ?
8
K-VALUES. EXPONENTIAL CORRELATION
9
K-VALUES. POWER SERIES CORRELATION
11
RETURN
12
NIN=0 ?
Y
N
13
READ TRAY PARA. ESTIMATE, DENSITY AND HYDRAULIC DATA.
KTYP = 1 ?
Y
N
READ ACTIVITY DATA, INITIAL COMPOSITION ESTIMATES
NIN= 111
N > 150 ?
N
Y
KTYP
=1
>1
<1
20
BUBBLE POINT AT STAGE N. EXPONENTIAL CORRELATION INCL. PRESSURE AND ACTIV. COEFF.
4
115
BUBBLE POINT AT STAGE N. EXPONENTIAL CORRELATION INCL. PRESSURE
17
KTYP
=1
<1
>1
25
K-VALUES. EXPONENTIAL CORRELATION INCL. PRESSURE ACTIV. COEFF. AND EFFICIENCIES
7
18
K-VALUES. EXPONENTIAL CORRELATION INCL. PRESSURE
RETURN

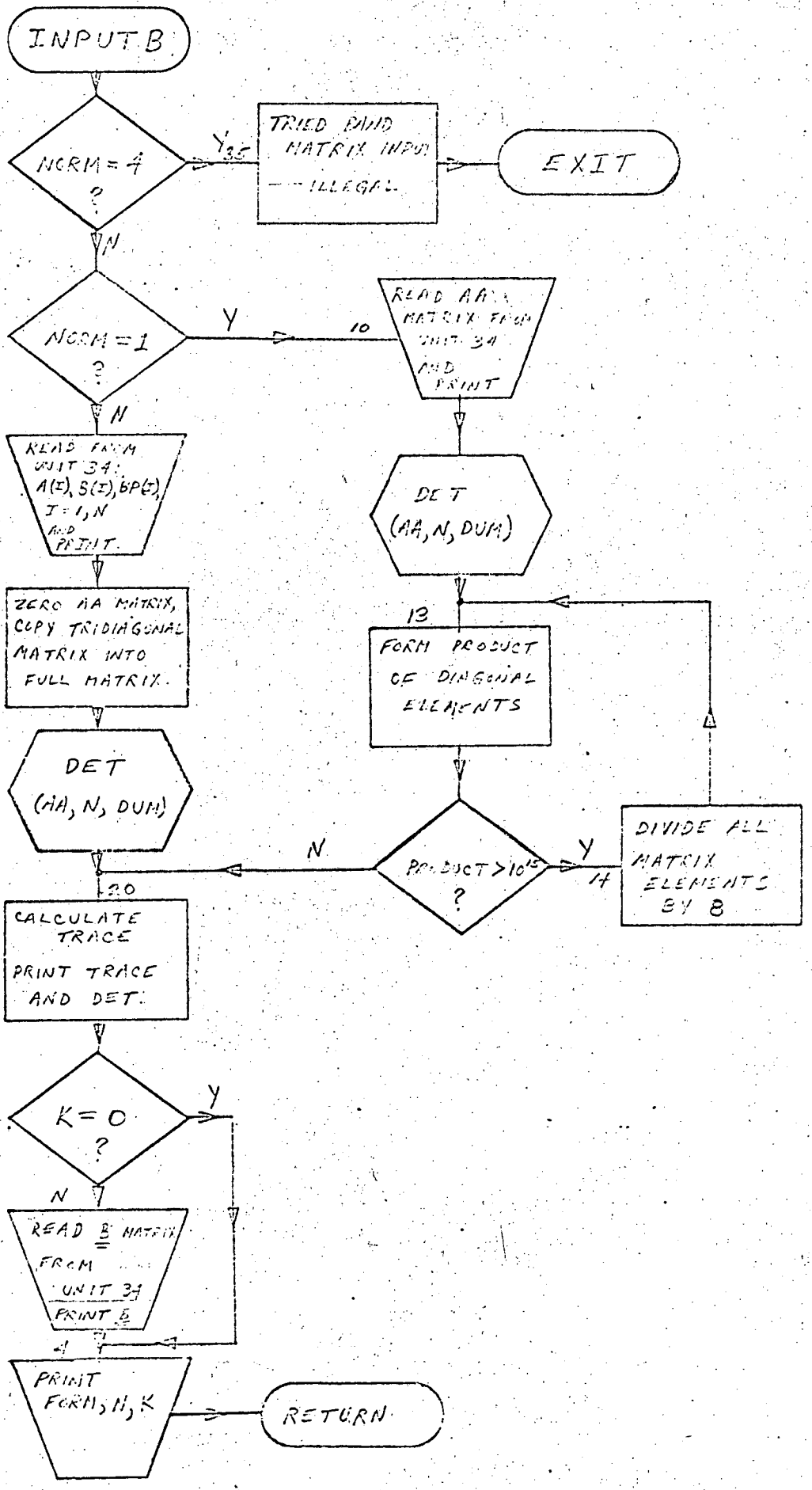

SPEC
10
IN(2) > 0 ?
N
OK = 0.0
RETURN
Y
101
CALC. LIQ. HOLDUP
INITIALIZE
CALC. NEW PRESSURES
3
PRESS. CONVERGED ?
JPOK ≠ 0
N
IN(5) = 0 ?
Y
N
PRINT PRESS ERROR
JPOK = 0
4
IN(4) = 1 ?
N
CALC. NEW EFFICIENCIES
24
EFFIC. CONVERGED ?
JEOK ≠ 0
N
IN(5) = 0 ?
Y
N
PRINT EFFIC. ERROR
JEOK = 0
27
28
KCALC ≠ 3, OR INITIAL STEADY STATE ?
Y
102
N
IRSET
<0
>0
=0
REBOIL ROLLUP CONVERGED ?
210
N
Y
REBOIL HEAT FLUX CONVERGED ?
200
N
IN(5) = 0 ?
Y
N
PRINT REBOIL ERROR
ITERAT ≤ 25 ?
Y
N
PRINT "FAILED TO CONVERGE ON REBOILER SPEC"
205
JQOK ≠ 0
MODIFY BOTTOMS FLOW RATE
102
102
KTYP ≠ 1 ?
Y
N
CHECK COMPOSITION CONVERGENCE. (REQUIRED FOR ACTIV. COEFF. CALC.)
COMPN CONVERGED ?
Y
N
JVOK = 0
105
JPOK ≤ 0 AND JEOK ≤ 0 AND JQOK ≤ 0 ?
N
Y
9
OK = 10.0
12
OK = 0.0
IN(5) = 0 ?
Y
N
PRINT NO. OF ITERATIONS
PRINT "PRESSURE CONVERGED"
RETURN
JVOK = 0
PRINT COMPOSITION ERROR
IN(5) = 0 ?
N
Y
14
UPDATE COMPOSITION
IN(5) = 0 ?
N
Y
PRINT NO. OF ITERATIONS
20
OK = 10.0
RETURN

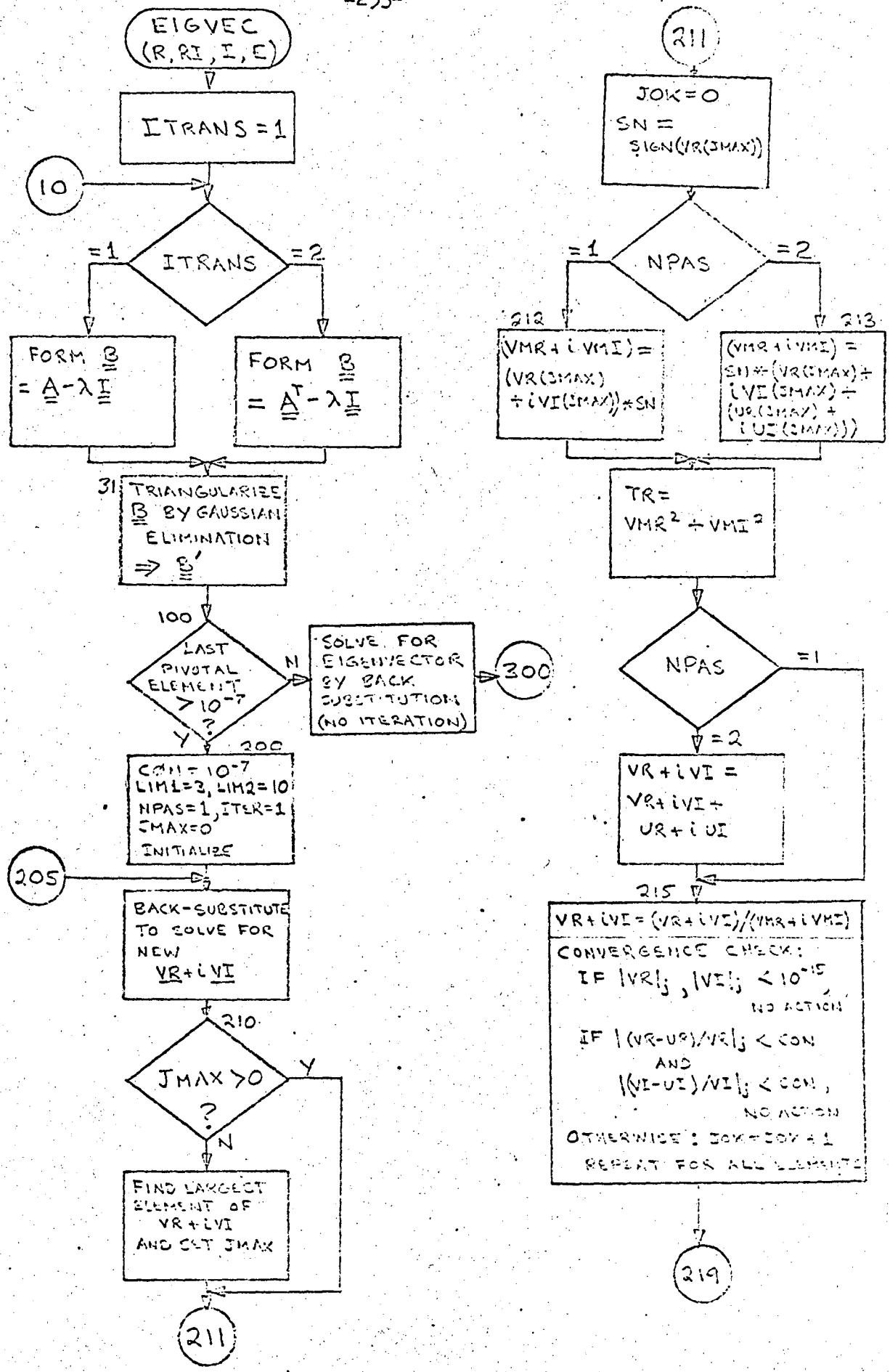

AUXOUT (MOD, KOEFF, NOPR)
CALCULATE DIMENSION-LESS VARIABLES ℓ, N, t, p, μ, h AND PARAMETERS FOR THE COEFFICIENTS OF THE LINEARIZED EQUATIONS
NOPR = 2 ?
N
PRINT DIMENSION-LESS ℓ, N, χ, μ, t, p, h
Y
350
CALCULATE γ, η, Ψ, ζ, μ, τ, σ, σ̂, δ, ε ξ, ETC. FOR THE LINEARIZED EQUATIONS
104
NOPR = 2 ?
N
PRINT INPUT PARAMETERS AND CALCULATED QUANTITIES
405
Y
MOD
=1
=2
=3
=4
PRINT STATE VARIABLES FOR THE APPROPRIATE MODEL
305
KOEFF = 1 ?
Y
RETURN
N
SET A = 0 AND B = 0
MOD
=1
=2,3,4
801
MOD1 (MOD, NOPR)
802
M234 (MOD, NOPR)
RETURN

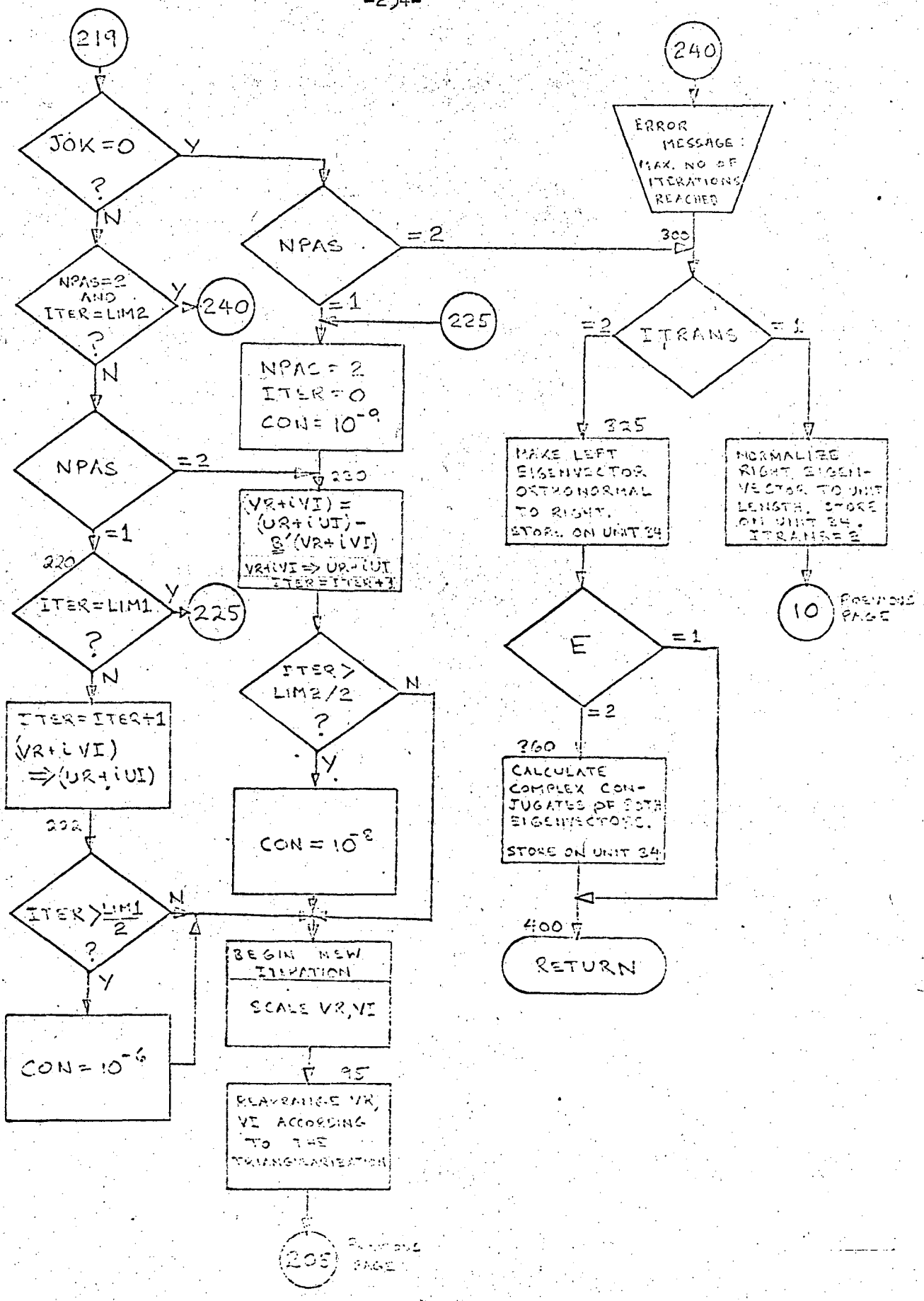

DERIV (NSLN, MOD, KOEFF, NOTFSS)
KOEFF =5 ?
N
Y
READ A MATRIX FROM CARDS, STORE ON UNIT 34
300
NSEN >0 ?
N
Y
RETURN
KOEFF =5 ?
N
Y
CARD INPUT OF NPR, PARAM(I), I=1,NPR
5
READ A MATRIX FROM UNIT 34
28
READ NPAR AND MULT FROM CARD(S)
A
A
ISEN = 1
ITIM = 1
KOEFF =5 ?
Y
N
SAVE (2)
30
CHANGE PARAMETER NPAR BY ONE PERCENT
AUXOUT (MOD, KOEFF 2)
SUBTRACT NEW A FROM OLD A
STORE DERIV. MATRIX ON UNIT 4
ITIM = ITIM-1
ITIM > MULT(ISEN) ?
N
Y
ISEN = ISEN-1
ISEN > NSLN ?
N
Y
400
RETURN

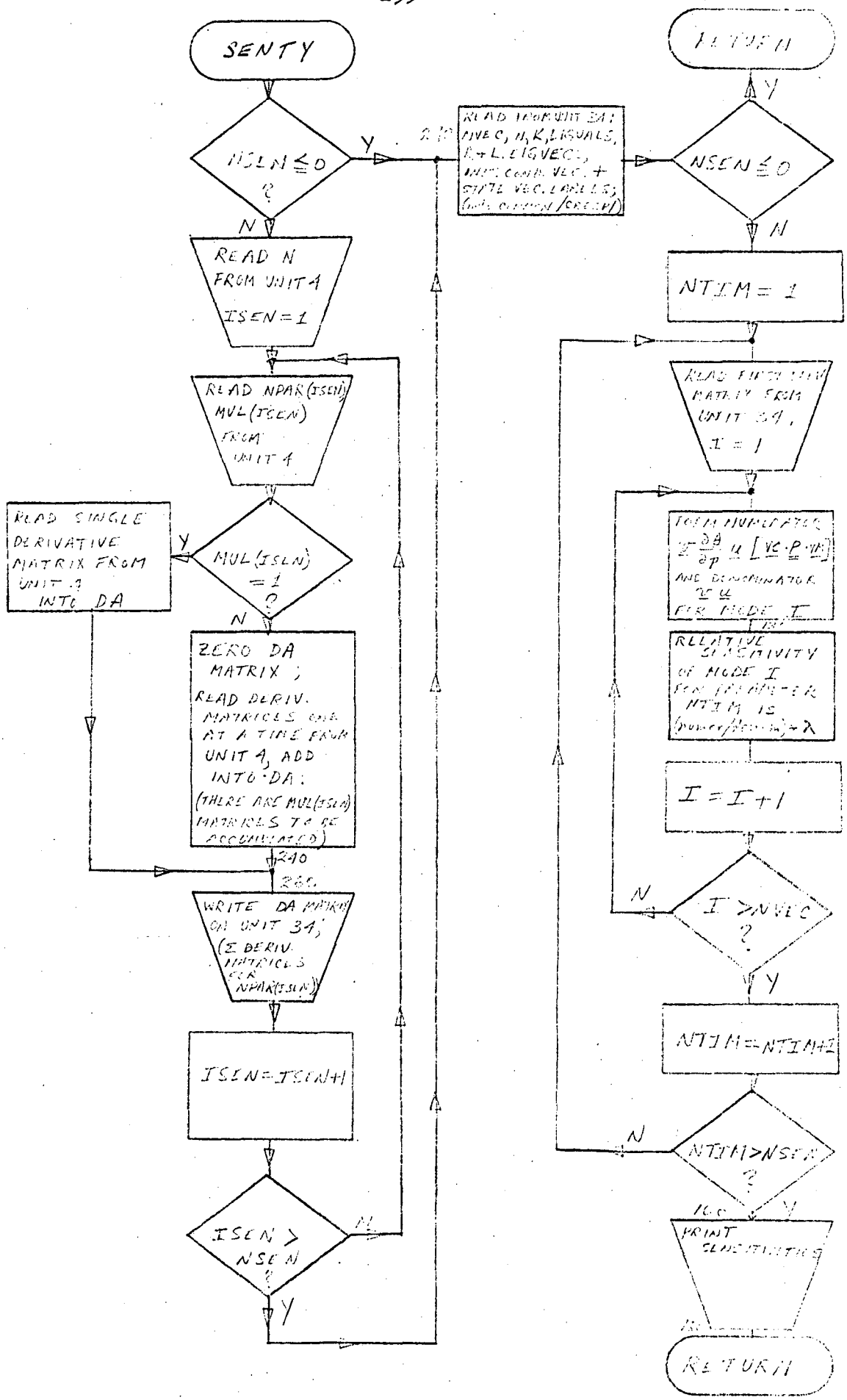

EIGMAN (KCALC)
KCALC=4 ?
Y
N
450
READ FORM, N, K FROM CARD
READ FORM, N, K FROM UNIT34
451
IF VTST=0 SET VTST=10^-7
KCALC=4 ?
READ STATE VECTOR LABELS FROM CARDS
CONVERT STATE VECTOR LABELS TO PROPER FORMAT
455
INPUT
INPUT B
902
QREIG (AA,N,R,RI, 1)
22
IF RI<10^-4×R SET RI=0
IOW1=0 ?
600
610
IDENTIFY CONJUGATE PAIRS OF EIGENVALUES; SET R(JCON)=R(J) RI(JCON)=-RI(J)
600
600
SORT EIGENVALUES AND PRINT; CALCULATE SUM AND PRODUCT OF EIGENVALUES; I=1, LV=1
|R(I)/R(1)| > VTST ?
IF EIGENVALUES I AND I+1 ARE CONJUGATES, E=2; OTHERWISE E=1
ONE OF CONJUGATE PAIR ALREADY CALCULATED ?
EIGVEC (R(I), RI(I), I, E)
160
LV=LV+1
LV>35 ?
TIME REMAINING <0.01×N ?
GO
511
NOTIM=2
I=I+1
I>N ?
111

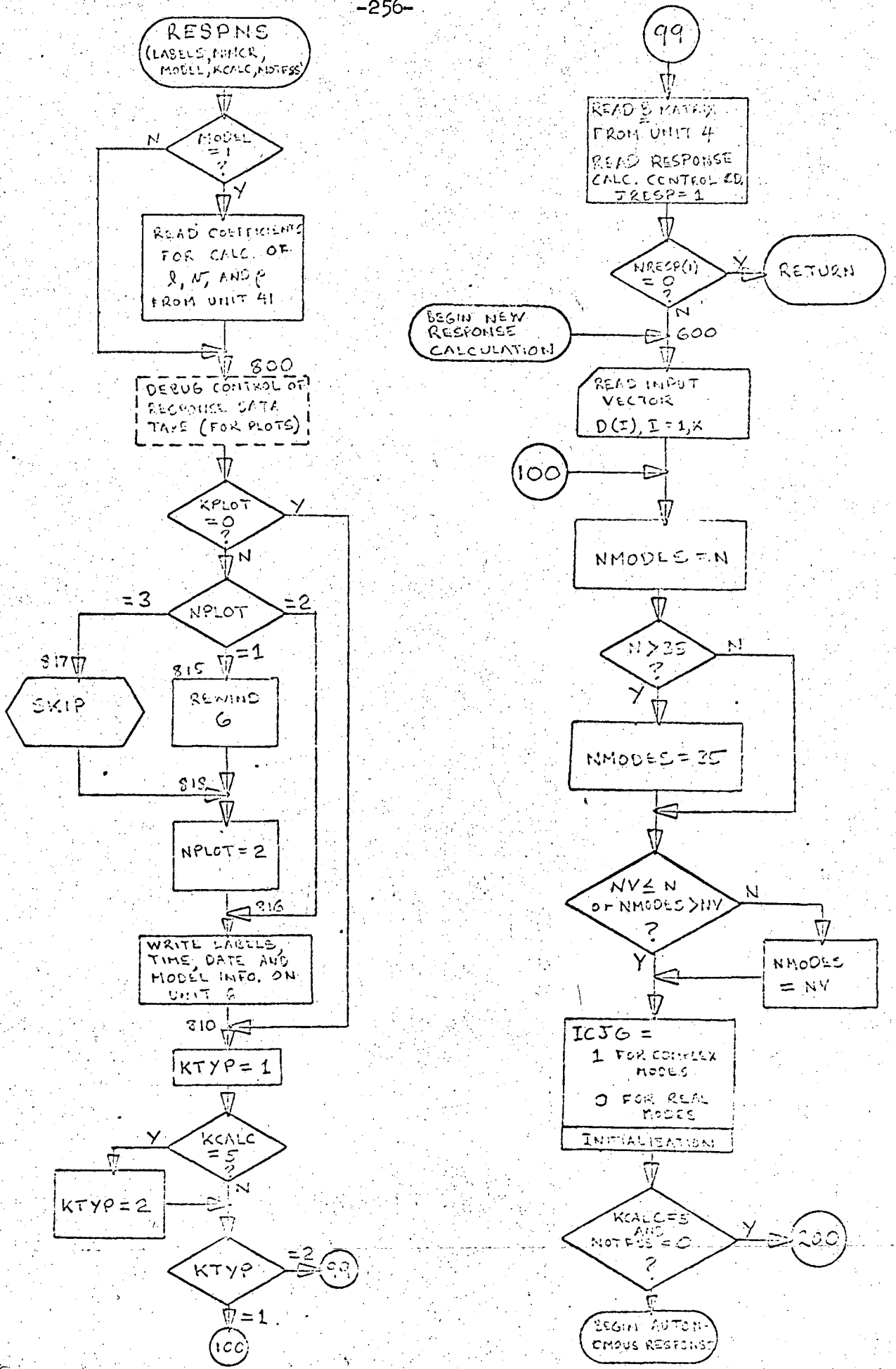

111
NVEC = LV-1
VECIO (NVEC)
JOPT =99 ?
Y
N
KCALC = 5
STORE AA MATRIX ON UNIT 4
RETURN
VECIO (NVEC)
I = 1
READ IN I'TH R.+L. EIGENVECTORS (VM + VC) FROM UNIT 34 ; ITRAN=1
|RI(I)| > 10^-30 ?
N
Y
ITRAN
=1
=2
PRINT COMPLEX R. EIGENVECTOR
PRINT COMPLEX L. EIGENVECTOR
ITRAN = 2
ITRAN
=1
=2
39
PRINT REAL EIGENVECTOR
39
ITRAN
=2
=1
762
ITRAN = 2
39
I = I + 1
I > NVEC ?
N
Y
704
CHECK R. AND L. EIGENVECTORS BY (A - λI)V . PRINT IF ANY ELEMENT > 10^-6 ; CALCULATE U^T V . PRINT PRODUCT BY ROWS
NVEC < N ?
N
Y
CALCULATE V U^T AND PRINT
203
STORE NVEC, N, K, λ's, U, V, ETC. ON UNIT 34
RETURN

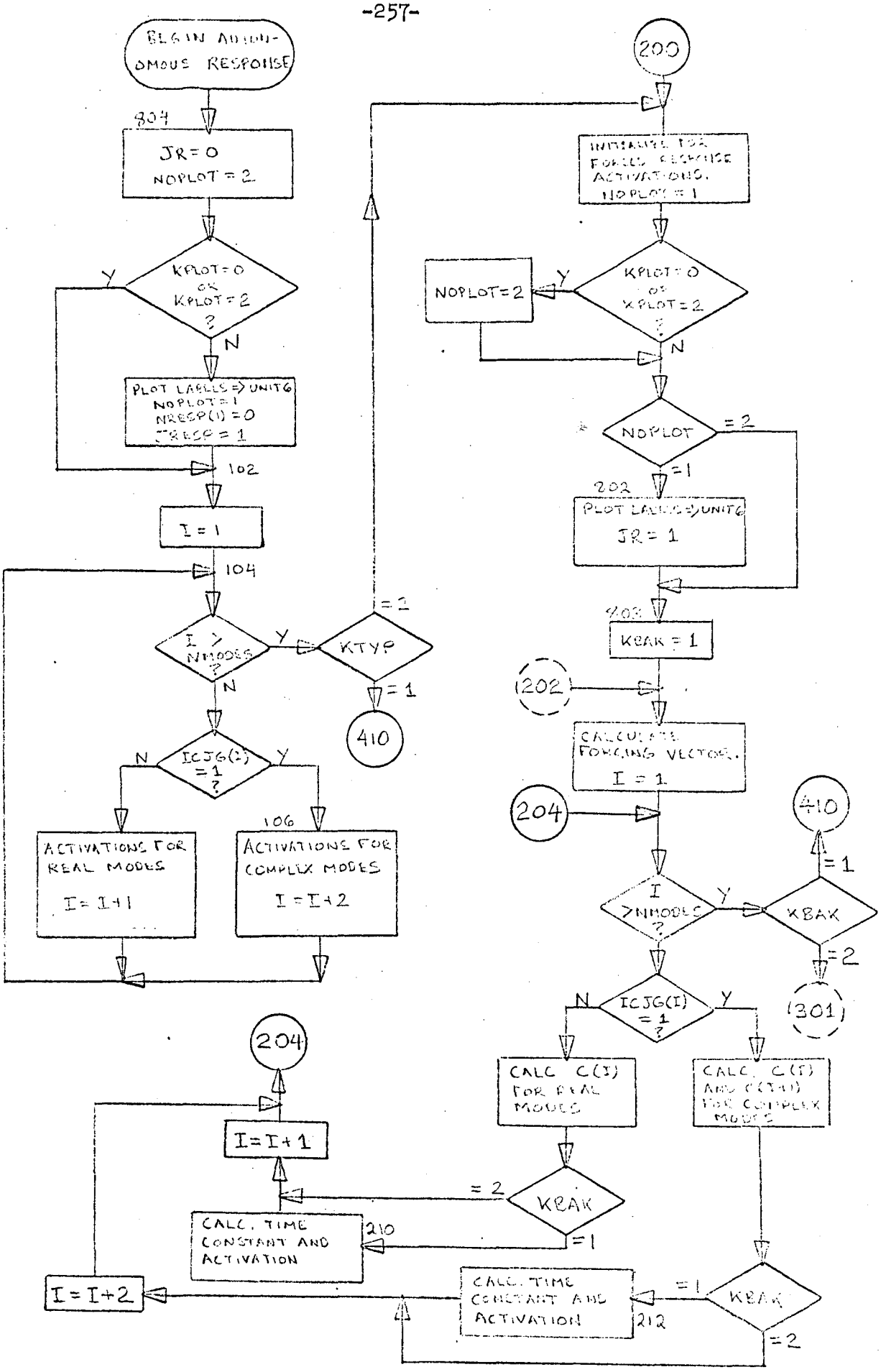

INPUT B
NORM = 4 ?
Y 35
TRIED BAND MATRIX INPUT — ILLEGAL.
EXIT
N
NORM = 1 ?
Y
10
READ AA MATRIX FROM UNIT 34 AND PRINT
N
READ FROM UNIT 34: A(I), S(I), BP(I), I = 1, N AND PRINT.
DET (AA, N, DUM)
ZERO AA MATRIX, COPY TRIDIAGONAL MATRIX INTO FULL MATRIX.
13
FORM PRODUCT OF DIAGONAL ELEMENTS
DET (AA, N, DUM)
PRODUCT > 10^15 ?
N
Y
14
DIVIDE ALL MATRIX ELEMENTS BY 8
20
CALCULATE TRACE
PRINT TRACE AND DET.
K = 0 ?
Y
N
READ B MATRIX FROM UNIT 34 PRINT B
4
PRINT FORM, N, K
RETURN

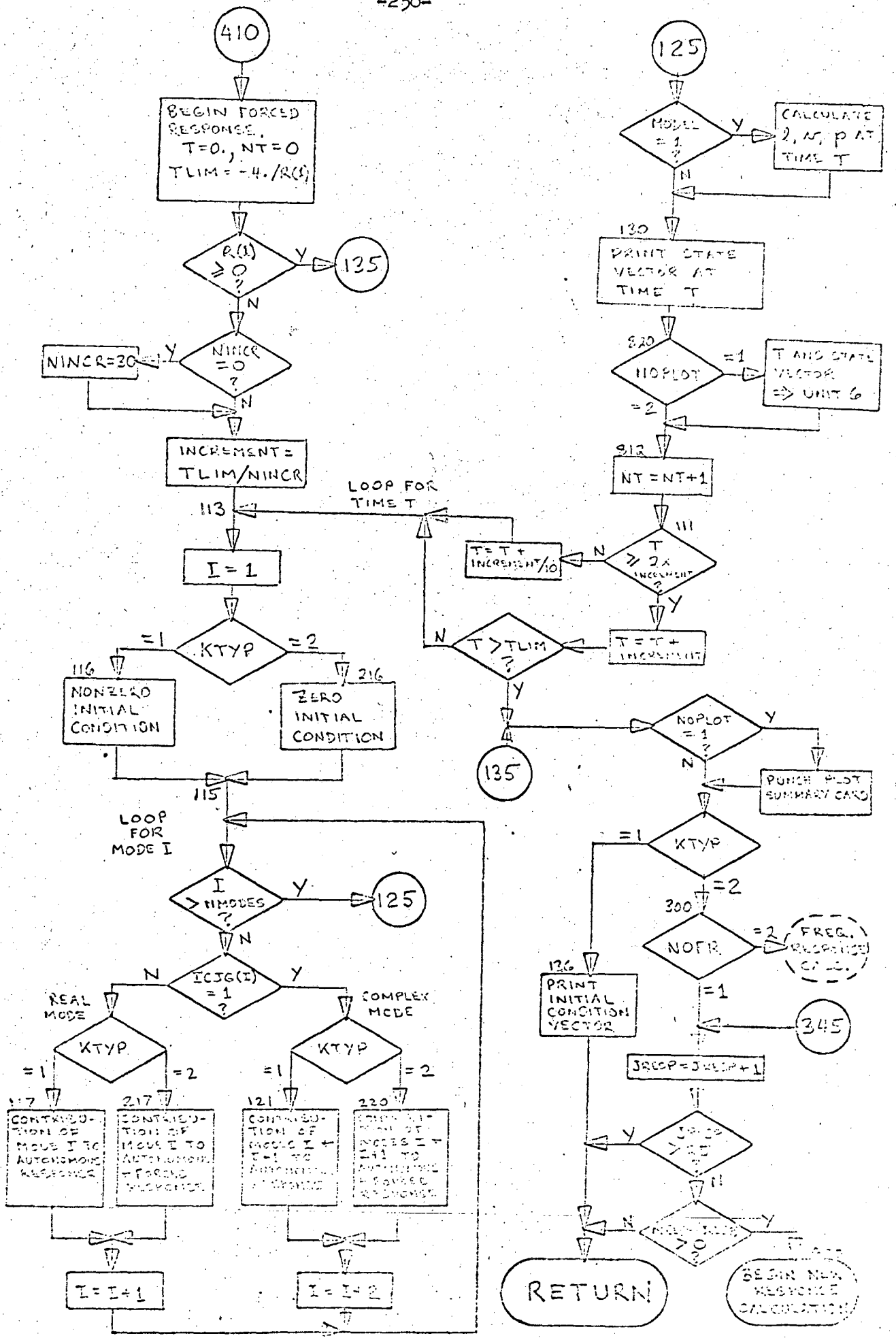

EIGVEC (R, RI, I, E)
ITRANS = 1
10
ITRANS
=1
=2
FORM B = A - λI
FORM B = A^T - λI
31
TRIANGULARIZE B BY GAUSSIAN ELIMINATION ⇒ B'
100
LAST PIVOTAL ELEMENT > 10^-7 ?
N
SOLVE FOR EIGENVECTOR BY BACK SUBSTITUTION (NO ITERATION)
300
Y
200
CON = 10^-7
LIM1=3, LIM2=10
NPAS=1, ITER=1
JMAX=0
INITIALIZE
205
BACK-SUBSTITUTE TO SOLVE FOR NEW VR+iVI
210
JMAX >0 ?
Y
N
FIND LARGEST ELEMENT OF VR+iVI AND SET JMAX
211
211
JOK=0
SN = SIGN(VR(JMAX))
NPAS
=1
=2
212
(VMR+iVMI) = (VR(JMAX) + iVI(JMAX)) * SN
213
(VMR+iVMI) = SN * (VR(JMAX) + iVI(JMAX) / (UR(JMAX) + iUI(JMAX)))
TR = VMR^2 + VMI^2
NPAS
=1
=2
VR+iVI = VR+iVI + UR+iUI
215
VR+iVI = (VR+iVI)/(VMR+iVMI)
CONVERGENCE CHECK:
IF |VR|_J , |VI|_J < 10^-15 NO ACTION
IF |(VR-UR)/VR|_J < CON AND |(VI-UI)/VI|_J < CON , NO ACTION
OTHERWISE : JOK = JOK + 1
REPEAT FOR ALL COMPONENTS
219


219
JOK = 0 ?
Y
N
NPAS = 2
NPAS = 2 AND ITER = LIM2 ?
Y
240
N
NPAS = 2
=1
225
NPAC = 2
ITER = 0
CON = 10^-9
NPAS
=2
230
(VR+iVI) = (UR+iUI) - S'(VR+iVI)
VR+iVI ⇒ UR+iUI
ITER = ITER+1
220
ITER = LIM1 ?
Y
225
N
ITER > LIM2/2 ?
N
Y
CON = 10^-8
ITER = ITER+1
(VR+iVI) ⇒ (UR+iUI)
222
ITER > LIM1/2 ?
N
Y
CON = 10^-6
BEGIN NEW ITERATION
SCALE VR, VI
95
REARRANGE VR, VI ACCORDING TO THE TRIANGULARIZATION
205
240
ERROR MESSAGE: MAX. NO OF ITERATIONS REACHED
300
ITRANS
=2
=1
325
MAKE LEFT EIGENVECTOR ORTHONORMAL TO RIGHT. STORE ON UNIT 34
NORMALIZE RIGHT EIGENVECTOR TO UNIT LENGTH. STORE ON UNIT 34. ITRANS = 2
10
E
=1
=2
360
CALCULATE COMPLEX CONJUGATES OF BOTH EIGENVECTORS.
STORE ON UNIT 34
400
RETURN


SENTY
NSEN ≤ 0 ?
Y
N
READ N FROM UNIT 4
ISEN = 1
READ NPAR(ISEN), MUL(ISEN) FROM UNIT 4
MUL(ISEN) = 1 ?
Y
READ SINGLE DERIVATIVE MATRIX FROM UNIT 4 INTO DA
N
ZERO DA MATRIX ;
READ DERIV. MATRICES ONE AT A TIME FROM UNIT 4, ADD INTO DA ;
(THERE ARE MUL(ISEN) MATRICES TO BE ACCUMULATED)
240
REC.
WRITE DA MATRIX ON UNIT 34, (Σ DERIV. MATRICES FOR NPAR(ISEN))
ISEN = ISEN+1
ISEN > NSEN ?
N
Y
READ FROM UNIT 34: NVEC, N, K, EIGVALS, K+L EIGVECS, INIT. COND. VEC. + STATE VEC. LABELS; (only option /REC=1)
NSEN ≤ 0
Y
N
NTIM = 1
READ FIRST DERIV. MATRIX FROM UNIT 34, I = 1
FORM NUMERATOR $\underline{v}^T \frac{\partial \theta}{\partial p} \underline{u} \left[\underline{v}^T \underline{P} \underline{u} \right]$ AND DENOMINATOR $\underline{v}^T \underline{u}$ FOR MODE I
RELATIVE SENSITIVITY OF MODE I FOR PARAMETER NTIM IS (numerator/denominator) = λ
I = I+1
I > NVEC ?
N
Y
NTIM = NTIM+1
NTIM > NSEN ?
N
Y
100
PRINT STATISTICS
RETURN


RESPNS
(LABELS, MINCR, MODEL, KCALC, NOTFSS)
MODEL = 1 ?
N
Y
READ COEFFICIENTS FOR CALC. OF ℓ, N, AND P FROM UNIT 41
800
DEBUG CONTROL OF RESPONSE DATA TAPE (FOR PLOTS)
KPLOT = 0 ?
Y
N
NPLOT
=3
=2
=1
817
SKIP
815
REWIND 6
818
NPLOT = 2
816
WRITE LABELS, TIME, DATE AND MODEL INFO. ON UNIT 6
810
KTYP = 1
KCALC = 5 ?
Y
N
KTYP = 2
KTYP
=2
=1
ICC
99
READ Φ MATRIX FROM UNIT 4
READ RESPONSE CALC. CONTROL CD, JRESP = 1
NRESP(I) = 0 ?
Y
RETURN
N
BEGIN NEW RESPONSE CALCULATION
600
READ INPUT VECTOR D(I), I = 1,K
100
NMODES = N
N > 35 ?
N
Y
NMODES = 35
NV ≤ N OR NMODES > NV ?
N
Y
NMODES = NV
ICJG =
1 FOR COMPLEX MODES
0 FOR REAL MODES
INITIALIZATION
KCALC=5 AND NOTFSS = 0 ?
Y
200
BEGIN AUTONOMOUS RESPONSE


BEGIN AUTONOMOUS RESPONSE
304
JR = 0
NOPLOT = 2
KPLOT = 0 OR KPLOT = 2 ?
Y
N
PLOT LABELS ⇒ UNITG
NOPLOT = 1
NRESP(I) = 0
JRESP = 1
102
I = 1
104
I > NMODES ?
Y
N
KTYP
= 1
410
ICJG(I) = 1 ?
N
Y
ACTIVATIONS FOR REAL MODES
I = I+1
106
ACTIVATIONS FOR COMPLEX MODES
I = I+2
200
INITIALIZE FOR FORCED RESPONSE ACTIVATIONS.
NOPLOT = 1
KPLOT = 0 OR KPLOT = 2 ?
Y
NOPLOT = 2
N
NOPLOT
= 2
= 1
202
PLOT LABELS ⇒ UNITG
JR = 1
208
KBAK = 1
202
CALCULATE FORCING VECTORS.
I = 1
204
I > NMODES ?
Y
KBAK
= 1
= 2
410
301
ICJG(I) = 1 ?
N
Y
CALC C(I) FOR REAL MODES
CALC. C(I) AND C(I+1) FOR COMPLEX MODES
204
I = I+1
KBAK
= 2
= 1
CALC. TIME CONSTANT AND ACTIVATION
210
I = I+2
CALC. TIME CONSTANT AND ACTIVATION
212
KBAK
= 1
= 2


410
BEGIN FORCED RESPONSE, T=0., NT=0 TLIM=-4./R(1)
R(1) ≥ 0 ?
Y
125
N
NINCR=30
NINCR =0 ?
Y
N
INCREMENT = TLIM/NINCR
LOOP FOR TIME T
113
I = 1
KTYP
=1
=2
116
NONZERO INITIAL CONDITION
216
ZERO INITIAL CONDITION
115
LOOP FOR MODE I
I > NMODES ?
Y
125
N
ICJG(I) =1 ?
N
Y
REAL MODE
COMPLEX MODE
KTYP
KTYP
=1
=2
=1
=2
217
CONTRIBUTION OF MODE I TO AUTONOMOUS RESPONSE
CONTRIBUTION OF MODE I TO AUTONOMOUS + FORCED RESPONSE
121
220
I = I+1
I = I+2
125
MODEL =1 ?
Y
CALCULATE Q, N, P AT TIME T
N
130
PRINT STATE VECTOR AT TIME T
820
NOPLOT
=1
T AND STATE VECTOR => UNIT 6
=2
912
NT = NT+1
111
T ≥ 2x INCREMENT ?
N
T = T + INCREMENT/10
Y
T = T + INCREMENT
T > TLIM ?
N
Y
135
NOPLOT =1 ?
Y
N
PUNCH PLOT SUMMARY CARD
KTYP
=1
=2
300
NOFR
=2
FREQ. RESPONSE CALC.
=1
345
126
PRINT INITIAL CONDITION VECTOR
JRCOP = JRCOP+1
JRCOP > NFR ?
Y
N
NEXT MODE > 0 ?
Y
N
RETURN
BEGIN NEW RESPONSE CALCULATION

G.9 Subroutine Listings

The following pages give the FORTRAN listings for all of the subroutines used in the mode calculation and in plot preparation. However, programs that are part of the Berkeley Campus IBM 7094 computer library are not included.

```
$IBFTC EXEC.   DECK,SDD
CEXEC
C
C      EXECUTIVE PROGRAM FOR RESPONSE MODE CALCULATIONS
C      CONTROLS TYPE OF CALCULATION TO BE PERFORMED
C      R. E. LEVY    8/18/65
C
       DIMENSION LABELS(48),BIT(4),MES(16)
       COMMON /CEIG/ VTST,NSEN,JOPT
       COMMON /CDIST/ KCALC,J    ,NTIM,IRSET
       INTEGER BIT
       DATA MES(1)/96H, HEAT AND MASS BALANCE) AND HEAT BALANCE)       AN
      2D MASS BALANCE)       BALANCE ONLY)          /
       CALL ERRSET
  100  REWIND 34
       CALL DATE(DAT)
       CALL TIME(TIM)
       READ(2,02) KCALC,MODEL,NWDS,NINCR,NOTFSS,VTST,NSEN,JOPT,IRSET
    02 FORMAT(5I4,E8.4,5I4)
       WRITE(3,01) DAT,TIM
    01 FORMAT(1H1,28X,30HRESPONSE MODE ANALYSIS PROGRAM,//20X,10HR. E. LE
      2VY,25X,A6,///20H BEGIN CALCULATION
      3   ,F7.2)
C
C      KCALC INDICATES TYPE OF CALCULATION DESIRED
C           = 1 FOR DIST ONLY (STEADY STATE AND DIMENSIONLESS STATE VAR)
C           = 2 FOR DIST + EIG
C           = 3 FOR AUTONOMOUS RESPONSE (USES 2 STEADY STATES)
C           = 4 FOR EIG ONLY (REQUIRES CARD INPUT OF COEFFS), NO SENS
C           = 5 FOR FORCED RESPONSE  (REQUIRES INPUT OF FORCING VECTOR)
C           = 6 FOR EIG ALONE + FORCED RESPONSE.  SENSITIVITIES REQUIRE
C      SPECIAL AUXOUT AND CARD INPUT OF PARAMETER VALUES (SEE DERIV)
C      MODEL INDICATES DIST MODELS TO BE USED
C           = 1 FOR COMP, HEAT, MASS ONLY
C           = 2 FOR COMP, HEAT ONLY
C           = 4 FOR COMP, MASS ONLY
C           = 8 FOR COMP ONLY
C           = APPROPRIATE SUM FOR ANY DESIRED COMBINATION OF MODELS
C      NINCR IS NUMBER OF TIME INCREMENTS  BETWEEN T = 0 AND T = 3/R(1)
C      IF NINCR  = 0, ASSUMED VALUE IS 20
C      NOTFSS = 1 INDICATES THAT FINAL SS PARAMETERS ARE NOT TO BE USED
C      IN RESPONSE CALCULATION.  CONDITIONS FOR SS SUPPLIED AS THIRD SET
C      OF DIST INPUT DATA.  OTHERWISE NOTFSS = 0
C      IF KCALC = 5 AND NOTFSS = 1  CALC RESPONSE WITH NONZERO INIT CONDX
C      NWDS IS NUMBER OF LABEL WORDS SUPPLIED (A6)    (MAX = 48, 4 CDS)
C      VTST IS THE RATIO OF THE LARGEST EIGENVALUE TO BE USED TO THE
C      SMALLEST (FIRST) EIGENVALUE.
C      NSEN = NO. OF SENSITIVITY CALCULATIONS
C      JOPT AVAILABLE FOR ANYTHING, EXCEPT WHEN KCALC = 6
C      IRSET = 0 FIXES REBOILER STEAM TEMP,  IRSET = 1 FIXES REBOILER
C      VAPOR RATE
C
       IF(NWDS.EQ.0) GO TO 110
       READ(2,03) (LABELS(I),I=1,NWDS)
    03 FORMAT(12A6)
       WRITE(3,11) (LABELS(I),I=1,48)
    11 FORMAT(//4(10X,12A6/))
   110 WRITE(3,21) KCALC,NINCR,NOTFSS,JOPT,IRSET,VTST
    21 FORMAT(///9H KCALC = ,I2,10H  NINCR = ,I3,11H  NOTFSS = ,I2,9H  JO
      2PT = ,I2,10H  IRSET = ,I2,9H  VTST = ,1PE11.4)
       IF(KCALC.EQ.4) GO TO 180
       IF(KCALC.EQ.6) GO TO 181
       BIT(4)=MODEL/8
       MODEL=MODEL-8*BIT(4)
       BIT(3)=MODEL/4
       MODEL=MODEL-4*BIT(3)
       BIT(2)=MODEL/2
       MODEL=MODEL-2*BIT(2)
       BIT(1)=MODEL
       IF(KCALC.EQ.1) WRITE(3,04)
       IF(KCALC.EQ.2) WRITE(3,05)
       IF(KCALC.EQ.3.OR.KCALC.EQ.5) WRITE(3,06)
    04 FORMAT( //30H DISTILLATION CALCULATION ONLY)
    05 FORMAT( //48H DISTILLATION, EIGENVALUES AND EIGENVECTORS ONLY)
    06 FORMAT( //30H COMPLETE RESPONSE CALCULATION)
       IF(NSEN.GT.0) WRITE(3,20) NSEN
    20 FORMAT(27HOEIGENVALUE SENSITIVITY TO ,I2,11H PARAMETERS)
       WRITE(3,07)
       NMODL=0
       DO 130 I=1,4
       JHI=4*I
       JLO=JHI-3
       IF(BIT(I).EQ.1) WRITE(3,08) I,(MES(J),J=JLO,JHI)
   130 NMODL=NMODL+BIT(I)
    07 FORMAT(//36H THE FOLLOWING MODEL(S) WILL BE USED)
    08 FORMAT(20X,5HMODEL,I2,12H  (COMPONENT,4A6)
C
C      SET UP OVERALL DO LOOP FOR MULTIPLE MODELS
C      KOEFF = 1 GIVES STATE VARIABLES ONLY.  KOEFF = 2 GIVES ENTIRE
C      MATRIX ARRAY
C
       REWIND 41
       NDIST=0
       DO 170 I=1,4
       IF(BIT(I).EQ.0) GO TO 170
       NTIM=1
       IF(KCALC.EQ.3) NTIM=2+NOTFSS
       J=1
C      BEGIN LOOP FOR INITIAL - FINAL SS
   135 JSAV=1
       IF(J.GT.1) JSAV=3
       JGET=JSAV+1
       IF(NDIST.EQ.1) GO TO 136
       CALL DSTMAN
C       DSTMAN DOES NOT CALL AUXOUT
       CALL SAVE(JSAV)
       GO TO 137
   136 CALL SAVE(JGET)
   137 KOEFF=1
       IF(KCALC.EQ.2.OR.J.EQ.2) KOEFF=2
```

```
      IF(NTIM.EQ.3.AND.J.LT.NTIM) KOEFF=1
      IF(KCALC.EQ.5) KOEFF=2
C     AUXOUT WRITES STATE VARIABLES AND INPUT FOR EIG ON TAPE
C     SEQUENCE  -  INITIAL SS, FINAL SS, (SS FOR MATRIX CALC)
      CALL TIME(TIM)
      WRITE(3,12) I,TIM
   12 FORMAT(//30X,20H********************,///13X,11HBEGIN MODEL,I2,
     25X,6H TIME ,F7.2)
      IF(J.EQ.1.AND.KCALC.EQ.3) WRITE(3,14)
      IF(J.EQ.2) WRITE(3,15)
   14 FORMAT(25X,20HINITIAL STEADY STATE)
   15 FORMAT(25X,18HFINAL STEADY STATE)
      CALL AUXOUT(I,KOEFF,1)
      J=J+1
      IF(J.LE.NTIM) GO TO 135
C     END LOOP FOR INITIAL - FINAL SS
  140 NDIST=1
      IF(KCALC.EQ.1) GO TO 165
      REWIND 4
      IF(NSEN.LE.0) GO TO 145
      CALL DERIV(NSEN,I,2,NOTFSS)
  145 REWIND 34
      IF(KCALC.EQ.2) GO TO 150
C     XZERO CALCULATES INITIAL STATE VECTOR (DEVIATION FROM FINAL SS)
      CALL XZERO(NOTFSS,KCALC)
C     SET UP FOR CALC OF EIGENVALUES AND EIGENVECTORS
C     ALOC POSITIONS TAPE WITH AA MATRIX READY TO BE READ
  150 CALL TIME(TIM)
      WRITE(3,09) I,TIM
   09 FORMAT(/////35X,5HMODEL,I2,10H CONTINUES//,6H TIME ,F7.2)
      CALL ALOC(KCALC)
  160 CALL EIGMAN(KCALC,1)
C     EIG WRITES N, INITIAL STATE VECTOR, EIGENVALUES AND EIGENVECTORS
C     ON TAPE (PICKS UP INITIAL VECTOR FROM TAPE INPUT)
C     DERIV MATRICES ON UN04
      CALL SENTY
  260 IF(KCALC.EQ.2) GO TO 164
      CALL TIMREM(TIM)
  261 IF(TIM.LT.0.1) GO TO 164
      CALL RESPNS(LABELS,NINCR,1,KCALC,NOTFSS)
  164 REWIND 34
  165 CALL TIME(TIM)
      WRITE(3,13) I,TIM
   13 FORMAT(///13X,9HEND MODEL,I2,5X,6H TIME ,F7.2)
  170 CONTINUE
      GO TO 190
C     FOR KCALC = 4 OR 6    USE EIG VERSION WHICH READS CARDS
  181 WRITE(3,16)
   16 FORMAT(///63H EIGENVALUES, EIGENVECTORS AND RESPONSE.  CARD INPUT
     2OF MATRIX.)
      CALL DERIV(NSEN,1,5,0)
      JOPT=99
  180 REWIND 41
      REWIND 34
      CALL EIGMAN(KCALC,5)
      IF(KCALC.NE.5) GO TO 190
      REWIND 34
      CALL SENTY
      CALL RESPNS(LABELS,NINCR,9,5,0)
  190 CALL TIME(TIM)
      WRITE(3,10) TIM
   10 FORMAT(////18H END CALCULATION  ,F7.2)
      GO TO 100
      END
```

```
$IBFTC ERSET.  DECK,SDD
      SUBROUTINE ERRSET
C     OVERRIDE THE FOLLOWING
C          1) MAX 10 ERROR MESSAGES (36)
C          2) FIELD WIDTH ERROR MESSAGE (46)
      CALL FXMSET(DUM,DUM,-3,36,46,-8)
C     SET MAX NO. OF OVFLOS AND DIV CHKS TO NMAX
      NMAX=100
      ASSIGN 10 TO M
      CALL FTMOPT(5,NMAX,M)
C     ALLOW PRINTING OF TRUNCATED NUMBERS
      CALL TRUNC(.TRUE.)
      RETURN
   10 CALL FXMSET(DUM,DUM,-9)
      WRITE(3,100) NMAX
  100 FORMAT(/////9H LIMIT OF,I4,37H TRAPS REACHED.  TRACE AND TERMINATE
     2.//)
      CALL EXIT
      RETURN
      END


$IBFTC SAVE.   DECK
CSAVE
      SUBROUTINE SAVE(I)
C     STORES AND RETRIEVES DIST COMMON
      COMMON /DCOM/DSTCOM(3450)
      GO TO (100,150,110,160), I
C     STORES COMMON
  100 REWIND 41
  110 WRITE (41) DSTCOM
      RETURN
C     RETRIEVES COMMON
  150 REWIND 41
  160 READ (41) DSTCOM
      RETURN
      END


$IBFTC RHOMW.  DECK,SDD
CRHOMW
C     SUBROUTINE TO CALCULATE AVG VAPOR MOLEC WT AND AVG LIQ MOLAR DENS
C     PHASE = 1 FOR LIQ DENSITY,    PHASE = 2 FOR VAPOR MOLEC WT
      SUBROUTINE RHOMW(PHASE,JSTAGE,VALUE)
      INTEGER PHASE
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10) ,BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),FILL(21)
      VALUE=0.0
      GO TO (1,3), PHASE
    1 DO 2 I=1,NC
    2 VALUE=VALUE+X(I,JSTAGE)*(DENS(I)+ADENS(I)*T(JSTAGE))/WT(I)
      RETURN
    3 DO 4 I=1,NC
    4 VALUE=VALUE+WT(I)*X(I,JSTAGE)
      RETURN
      END


$IBFTC VHCAL.  DECK
CVHCALC
C     FUNCTION TO CALCULATE HT OF VAP ON ANY TRAY
      FUNCTION VHCALC(A,B,C,D,X,T)
      VHCALC=X*(A-B*T)+(1.-X)*(C-D*T)
      RETURN
      END


$IBFTC CPCAL.  DECK
CCPCALC
C     FUNCTION TO CALCULATE CP ON ANY TRAY
      FUNCTION CPCALC(A,B,C,D,X,T)
      CPCALC=X*(A+B*T)+(1.-X)*(C+D*T)
      RETURN
      END
```

```
$IBFTC DISTM.  DECK,SDD
CDISTMAN
C  EXECUTIVE PROGRAM FOR FRACTIONATING COLUMN DESIGN
C  ORIGINAL PROGRAM BY J. S. NEWMAN
C  ADAPTED FOR MODE CALCULATION OF BINARY DISTILLATION COLUMN
      SUBROUTINE DSTMAN
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),I(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),W1(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),CMC,CMR,
     XWMC,WMR,AMC,AMR,UMCP,UCP,UMRP,URP,FILL(11)
      DIMENSION E(70)
      EQUIVALENCE(E,FX(631))
      COMMON /CDIST/ KCALC,JTIM,NTIM,IRSET
      DIMENSION A(70,70)
  101 FORMAT (74H1COMPONENTS STAGES   FEEDS   COTYP   KTYP    LIMIT   DR
     1AWS    1NSTRUCTIONS,26X,7HPROBLEM/(1318))
  102 FORMAT (118H0 I      AK(I)        BK(I)        CK(I)        DK(I)
     1 AHL(I)       BHL(I)       CHL(I)      AHV(I)      BHV(I)      CHV(I)/
     2(I3,7E12.4,3E11.4))
  103 FORMAT (60H0     STAGE             FEED          ENTHALPY        COMPO
     1NENTS/18,E22.7,6E15.7/(8E15.7))
  104 FORMAT (40H0     STAGE    LIQUID DRAW       VAPOR DRAW/(I8,2E15.7))
  105 FORMAT (69H0    SUMERR          HETERR          SUBCOL          DTLIM
     1          SPECS/(8E15.7))
    1 FORMAT (9E8.4)
    2 FORMAT (1314)
C  BASIC DATA INPUT
      READ(2,2) NC,NS,NF,JCOTYP,KTYP,NIT,NDRAW,(IN(I),I=1,5),NPROB
      READ(2,1) (AK(I),BK(I),CK(I),DK(I),AHL(I),BHL(I),CHL(I),AHV(I),
     1BHV(I),CHV(I),I=1,NC)
      READ(2,1) (AL(J),J=1,NS)
      READ(2,1) (T(J),J=1,NS)
      WRITE (3,101) NC,NS,NF,JCOTYP,KTYP,NIT,NDRAW,(IN(I),I=1,5),NPROB
      WRITE(3,102) (I,AK(I),BK(I),CK(I),DK(I),AHL(I),BHL(I),CHL(I),AHV(I
     1),BHV(I),CHV(I),I=1,NC)
      DO 4 J=1,NS
      E(J)=0.70
      SL(J)= 0.0
      SV(J)= 0.0
      F(J)= 0.0
      HF(J)= 0.0
      DO 4 I=1,NC
      X(I,J)=1.0
    4 FX(I,J)= 0.0
      E(1)=1.0
      E(NS)=1.0
C  FEED PLATE
      DO 6 JF=1,NF
      READ(2,2) J
      READ(2,1) HF(J),(FX(I,J),I=1,NC)
      DO 5 I=1,NC
    5 F(J)= F(J) + FX(I,J)
    6 WRITE(3,103) J,F(J),HF(J),(FX(I,J),I=1,NC)
      IF (NDRAW)  9,9,7
    7 DO 8 J=1,NDRAW
      READ(2,2) JD
      READ(2,1) SL(JD),SV(JD)
    8 WRITE(3,104) JD,SL(JD),SV(JD)
    9 READ(2,1) SUMERR,HETERR,SUBCOL,DTLIM,(SPECS(I),I=1,4),CHECK
C  END BASIC DATA INPUT
      WRITE(3,105) SUMERR,HETERR,SUBCOL,DTLIM,(SPECS(I),I=1,4)
      ITERAT= 0
      NIN=0
      IF (ABS (CHECK - 11.111) - 0.01)  10,10,3
C  BEGIN OUTER LOOP
   10 ITERAT= ITERAT + 1
      JC= -1
      ITHEAT= - 1
      ITTEMP= 0
   11 N= L
      DO 12 I=1,NC
   12 EQ(I,NS)= 1.0
C  BEGIN ENTHALPY BALANCE LOOP
   13 NM1= N - 1
      V(1)= AL(2) - AL(1) - SL(1) - SV(1) + F(1)
      DO 14 J=2,L
   14 V(J)= AL(J+1) + V(J-1) - AL(J) - SL(J) - SV(J) + F(J)
      V(NS)= V(L) - AL(NS) - SL(NS) - SV(NS) + F(NS)
C  BEGIN COMPONENT BALANCE LOOP
   15 CALL EQUIL(200)
      DO 17 I=1,NC
      ERR(1)= 1.0/(AL(1) + SL(1) + (V(1)+SV(1))*EQ(I,1))
      X(I,1)= FX(I,1)*ERR(1)
      DO 16 J=2,NS
      ERR(J)= 1.0/(AL(J) + SL(J) + (V(J)+SV(J))*EQ(I,J)
     1 - ERR(J-1)*V(J-1)*EQ(I,J-1)*AL(J))
   16 X(I,J)= (FX(I,J) + V(J-1)*EQ(I,J-1)*X(I,J-1))*ERR(J)
      DO 17 JD=1,L
      J= NS - JD
   17 X(I,J)= X(I,J) + ERR(J)*X(I,J+1)*AL(J+1)
      DO 18 J=1,NS
      ERR(J)= - 1.0
      DO 18 I=1,NC
   18 ERR(J)= ERR(J) + X(I,J)
      DO 19 J=1,NS
      IF (ABS (ERR(J)) - SUMERR)  19,19,35
   19 CONTINUE
C  TO TEMP CORRECTION IF SUM OF X(I,J) .NE. 1.0
      ITHEAT= ITHEAT + 1
      IF (JCOTYP - 1)  21,20,20
   20 CALL EQUIL(NS)
      T(NS)= T(NS) - SUBCOL
   21 DO 22 J=1,NS
      HL(J)= 0.0
```

```
      HV(J)= 0.0
      DO 22 I=1,NC
      HL(J)= HL(J) + X(I,J)*(AHL(I)+BHL(I)*T(J)+CHL(I)*T(J)**2)
   22 HV(J)= HV(J) + X(I,J)*EQ(I,J)*(AHV(I)+BHV(I)*T(J)+CHV(I)*T(J)**2)
      IF (JCOTYP - 1)  24,23,23
   23 HV(NS)= HL(NS)
   24 QNET= HV(L)*V(L) - HL(NS)*AL(NS)
      QC= QNET - SL(NS)*HL(NS) - (V(NS)+SV(NS))*HV(NS) + HF(NS)
      IF (JC)  226,224,225
  224 DAMP= DAMP*(SUM/FLOAT (L-1) + 1.0)
      EPSP= 0.0
      JC= 1
      GO TO 228
  225 DAMP= DAMP*EPS1/(EPS1 - EPSP)
      IF (ABS (DAMP - 0.5) - 0.5)  227,227,226
  226 DAMP= 1.0
  227 JC= 0
      SUM= 0.0
  228 EPS1= EPS
      EPS= 0.0
      DO 32 K=2,L
      J= L - K + 2
      QNET= QNET + HV(J)*SV(J) + HL(J)*SL(J) - HF(J)
      QER= QNET + HL(J)*AL(J) - HV(J-1)*V(J-1)
      IF (JC)  27,27,25
   25 EPSP= EPSP + QERR(J)*(QER/ABS (QERR(J)))
      IF (ABS (QERR(J) - QER) - ABS (QERR(J) + QER)/3.0)   27,26,26
   26 DL= QER*(OLDDL(J)/(QERR(J) - QER))
      GO TO 31
   27 DL= QER/(HV(J-1) - HL(J))*DAMP
      CHECK= AL(J)
      IF (V(J-1) - AL(J))  28,29,29
   28 CHECK= V(J-1)
   29 IF (ABS (DL) - 0.25*CHECK)  31,31,30
   30 SUM= SUM + 0.25*CHECK/ABS (DL) - 1.0
      DL=0.25*CHECK*DL/ABS (DL)
   31 OLDDL(J)= DL
      QERR(J)= QER
      AL(J)= AL(J) + DL
   32 EPS= EPS + ABS (QER)
   33 QR= QNET + (AL(1)+SL(1))*HL(1) + SV(1)*HV(1) - HF(1)
      DO 34 J=2,L
      IF (ABS (QERR(J)) - 0.5*HETERR*ABS (QC + QR))  34,34,13
   34 CONTINUE
C  END ENTHALPY BALANCE LOOP
      IF(IN(5)) 342,341,342
  342 CALL OUTPUT(1)
  341 OK = 0.0
      CALL SPEC
C  CHECK CONVERGENCE IN SPEC
      IF (OK - 1.0)  3,3,10
   35 IF(ITTEMP-NIT) 235,135,135
  135 CALL OUTPUT(2)
      GO TO 3
  235 IF(IN(1)-25) 37,36,36
   36 CALL OUTPUT(3)
C  BEGIN TEMP CORRECTION
   37 DO 38 J=1,N
      HV(J)= - (ERR(J) + 1.0)*ALOG(ERR(J) + 1.0)
      DO 38 K=1,N
   38 A(J,K)= 0.0
      DO 44 I=1,NC
      ERR(1)= 1.0/(AL(1) + SL(1) + (V(1)+SV(1))*EQ(I,1))
      DO 39 J=2,NS
   39 ERR(J)= 1.0/(AL(J) + SL(J) + (V(J)+SV(J))*EQ(I,J)
     1 - ERR(J-1)*V(J-1)*EQ(I,J-1)*AL(J))
      DO 44 K=1,N
      DO 40 J=1,NS
   40 HL(J)= 0.0
      CHECK= -X(I,K)*EQT(AK(I),BK(I),CK(I),DK(I),T(K),EQ(I,K),KTYP)
      HL(K)= CHECK*(V(K) + SV(K))*ERR(K)
      IF (K - NS)  41,43,43
   41 HL(K+1)= - CHECK*V(K)
      DO 42 J=K,L
   42 HL(J+1)= (HL(J+1) + V(J)*EQ(I,J)*HL(J))*ERR(J+1)
   43 A(NS,K)= A(NS,K) + HL(NS)
      DO 44 JF=2,NS
      J= NS - JF + 1
      HL(J)= HL(J) + ERR(J)*HL(J+1)*AL(J+1)
   44 A(J,K)= A(J,K) + HL(J)
      DO 46 I=1,NM1
      IP1= I + 1
      A(I,I)= 1.0/A(I,I)
      HV(I)= HV(I)*A(I,I)
      DO 45 K=IP1,N
   45 A(I,K)= A(I,K)*A(I,I)
      DO 46 J=IP1,N
      HV(J)= HV(J) - HV(I)*A(J,I)
      DO 46 K=IP1,N
   46 A(J,K)= A(J,K) - A(I,K)*A(J,I)
      HV(N)= HV(N)/A(N,N)
      DO 47 I=1,NM1
      J= NM1 + 1 - I
      JP1= J + 1
      DO 47 K=1,J
   47 HV(K)= HV(K) - A(K,JP1)*HV(JP1)
      DO 49 J=1,N
      IF (ABS (HV(J)) - DTLIM)  49,49,48
   48 HV(J)= DTLIM*HV(J)/ABS (HV(J))
   49 T(J)= T(J) + HV(J)
      ITTEMP= ITTEMP + 1
      GO TO 15
C  END TEMP CORRECTION
    3 CONTINUE
      IF(IN(5)) 97,96,97
   96 CALL OUTPUT(1)
   97 IF(IN(3)-2) 98,100,98
  100 CONTINUE
C  INPUT DATA FOR AUXOUT
      READ(2,99) APO,BPO,APOP,BPOP,ACP,BCP,CCP,DCP,AVH,
```

```
     1 BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CMC,CMR,WMC,WMR,AMC,
     2 AMR
       IF(KCALC.NE.3.OR.JTIM.GT.1) RETURN
C  FIX REBOILER CONDITIONS IF THIS IS AN INITIAL SS TO BE FOLLOWED
C  BY A FINAL SS CALC
       TS=T(1)+DELTR
       UA=QR/DELTR
       VR=V(1)
       QRERR=1.0E-4*QR
    99 FORMAT(9E8.4)
    98 RETURN
       END
```

```
$IBFTC EQUIL.  DECK,SDD
CEQUIL
C       SUBROUTINE FOR EQUILIBRIUM CONSTANTS AND BUBBLE POINT
        SUBROUTINE EQUIL(N)
        COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
       2X(10,70),NC,L,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
       3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
       4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
       5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
       6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
       7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
       8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
       9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),CMC,CMR,
       XWMC,WMR,AMC,AMR,UMCP,UCP,UMRP,URP,FILL(11)
        EQUIVALENCE (A,QC),(B,QR),(C,QNET), (D,CHECK),(SUMX,DL),(SUMD,OK)
        DIMENSION E(70)
        EQUIVALENCE(E,FX(631))
        IF(IN(2)) 100,100,12
  100 CONTINUE
        IF (N - 150)  1,1,7
    1 IF (KTYP - 1)  2,2,4
C  BUBBLE POINT ON STAGE N
C  EXPONENTIAL EQUIL CORRELATION
    2 SUMX= 0.0
      SUMD= 0.0
      DO 3 I=1,NC
      A= EXP (AK(I)/(T(N)+DK(I)) + BK(I) + CK(I)*(T(N)+DK(I)))
      SUMX= SUMX + X(I,N)*(A - 1.0)
    3 SUMD= SUMD + X(I,N)*A*(CK(I) - AK(I)/((T(N)+DK(I))**2))
      T(N)= T(N) - SUMX/SUMD
      IF (ABS (SUMX) - 0.00001)  11,11,2
C  BUBBLE PT ON STAGE N
C  POWER SERIES EQUIL CORRELATION
    4 A= 0.0
      B= 0.0
      C= 0.0
      D= 0.0
      DO 5 I=1,NC
      A= A + (AK(I) - 1.0)*X(I,N)
      B= B + BK(I)*X(I,N)
      C= C + CK(I)*X(I,N)
    5 D= D + DK(I)*X(I,N)
    6 SUMX= A + B*T(N) + C*T(N)**2 + D*T(N)**3
      SUMD= B + 2.0*C*T(N) + 3.0*D*T(N)**2
      T(N)= T(N) - SUMX/SUMD
      IF (ABS (SUMX) - 0.00001)  11,11,6
C  K VALUES
    7 DO 10 J=1,L
      DO 10 I=1,NC
      IF (KTYP - 1)  8,8,9
C  EXPONENTIAL EQUIL
    8 EQ(I,J)= EXP (AK(I)/(T(J)+DK(I)) + BK(I) + CK(I)*(T(J)+DK(I)))
      GO TO 10
C POWER SERIES EQUIL
    9 EQ(I,J)= AK(I) + BK(I)*T(J) + CK(I)*T(J)**2 + DK(I)*T(J)**3
```

```
   10 CONTINUE
   11 RETURN
   12 IF(NIN) 14,13,14
C READ DATA FOR INITIAL P EST, HYDRAULICS AND DENSITY
C  READ ONLY ON FIRST PASS.
   13 READ(2,1000) (P(J),J=1,NS)
      PTOP=P(NS)
      READ(2,1000) (WT(J),DENS(J),ADENS(J),J=1,NC)
      READ(2,1000) AT,RHLDUP,ALPHA,BETA,PERR,BETAN,CAP
      IF(KTYP.NE.1) GO TO 113
      READ(2,1000) (ACTCON(I),I=1,4),((XX(I,J),I=1,NC),J=1,NS)
 1000 FORMAT(9E8.4)
  113 NIN=111
C     THE FOLLOWING INCORPORATES EXPONENTIAL EQUIL EXPRESSION WITH
C     INVERSE PRESSURE DEPENDENCE
   14 IF(N-150) 15,15,17
   15 IF(KTYP-1) 115,20,4
C  BUBBLE PT
  115 SUMX=0.0
      SUMD=0.0
      DO 16 I=1,NC
      A=EXP(AK(I)/(T(N)+DK(I))+BK(I)+CK(I)*(T(N)+DK(I)))/P(N)
      SUMX=SUMX+X(I,N)*(A-1.0)
   16 SUMD=SUMD+X(I,N)*A*(CK(I)-AK(I)/((T(N)+DK(I))**2))
      T(N)=T(N)-SUMX/SUMD
      IF(ABS(SUMX)-0.00001)  11,11,115
   17 IF(KTYP-1) 18,25,7
C  K VALUES
   18 DO 19 J=1,L
      DO 19 I=1,NC
   19 EQ(I,J)=EXP(AK(I)/(T(J)+DK(I))+BK(I)+CK(I)*(T(J)+DK(I)))/P(J)
      RETURN
C     EQUILIBRIUM CALCULATION FOR NONIDEAL MIXTURES
C  WITH PRESSURE DEPENDENCE
C  ACTIVITY COEFFICIENTS BY VAN LAAR EQN
C  BUBBLE PT
   20 SUMX=0.0
      SUMD=0.0
      DO 21 I=1,NC
      ACTCOF=EXP(2.303*ACTCON(I)/(1.+(XX(I,N)*ACTCON(I)/((1.-XX(I,N))
     1*ACTCON(I+1))))**2.)
      A=(ACTCOF/P(N))*EXP(AK(I)/(T(N)+DK(I))+BK(I)+CK(I)*(T(N)+DK(I)))
      SUMX=SUMX+X(I,N)*(A-1.0)
   21 SUMD=SUMD+X(I,N)*A*(CK(I)-AK(I)/((T(N)+DK(I))**2))
      T(N)=T(N)-SUMX/SUMD
      IF(ABS(SUMX)-0.00001) 11,11,20
C  K VALUES
   25 DO 26 J=1,L
      DO 26 I=1,NC
      ACTCOF=EXP(2.303*ACTCON(I)/(1.+(XX(I,J)*ACTCON(I)/((1.-XX(I,J))
     1*ACTCON(I+1))))**2.)
   26 EQ(I,J)=(ACTCOF/P(J))*EXP(AK(I)/(T(J)+DK(I))+BK(I)+CK(I)*(T(J)
     1+DK(I)))
      DO 28 I=1,NC
      DO 28 J=1,L
   28 EQ(I,J)=(EQ(I,J)/E(J))*(1.0-XX(I,J+1)*(1.0-E(J))/XX(I,J))
      RETURN
      END
```

```
$IBFTC SPEC.   DECK,SDD
CSPEC
C     SUBROUTINE FOR CHECKING TRAY PRESSURES.   DETERMINES OK
      SUBROUTINE SPEC
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLODL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),CMC,CMR,
     XWMC,WMR,AMC,AMR,UMCP,UCP,UMRP,URP,FILL(11)
      DIMENSION E(70)
      EQUIVALENCE(E,FX(631))
      COMMON /CDIST/ KCALC,JTIM,NTIM,IRSET
      DATA ILIM/25/,EFERR/0.01/
    1 FORMAT(22H NEW PRESSURE ON TRAY ,I2,48H EXCEEDS PERR.  DIFFERENCE
     1FROM PREVIOUS VALUE =,E14.6)
      INTST=IN(2)
 1000 IF(INTST) 10,10,101
C  CALC HOLDUPS AND PRESSURES
  101 DO 2 I=2,N
      RHOV=P(1)/(0.730*T(1))
      CALL RHOMW(1,I,RHO)
    2 HLDUP(I)=RHLDUP+ALPHA*AT*37.4*AL(I)-CAP*V(I-1)*RHO/(12.*RHOV)
      JPOK=0
      JEOK=0
      JXOK=0
      JQOK=0
      JF=FJF
      P(NS)=PTOP
      DO 4 I=1,N
      J=NS-I
      CALL RHOMW(1,J,RHO)
      CALL RHOMW(2,J,VMW)
      PTEMP=P(J)
      IF(I.GT.1) GO TO 110
      P(J)=P(NS)/2.+SQRT((P(NS)/2.)**2+((V(J)/BETAN)**2)*VMW*1544.*
     2T(J)/(32.2*(14.7*144.)**2))
      GO TO 111
  110 CONTINUE
      P(J)=0.5*(P(J+1)+HLDUP(J+1)*VMW/(AT*144.*14.7))+(VMW/64.4)*SQRT
     1((32.2*P(J+1)/VMW+32.2*HLDUP(J+1)/(AT*144.*14.7))**2 +4.*((V(J)/
     2BETA)**2)*32.2*1544./(144.*14.7)**2*T(J)/VMW)
  111 PDIFF=P(J)-PTEMP
```

```
      IF(ABS(PDIFF)-PERR) 4,3,3
    3 JPOK=JPOK+1
      IF(IN(5).EQ.0) GO TO 4
      WRITE(3,1) J,PDIFF
    4 CONTINUE
C  END HOLDUP AND PRESSURE CALC
      L=NS-1
      IF (IN(4) .EQ. 1) GO TO 28
C  CALC MURPHREE EFFICIENCY
      DO 27 J=2,L
      ETEMP=E(J)
      CALL RHOMW(2,J,VMW)
      RHOV=P(J)/(0.730*T(J))*VMW
      CALL RHOMW(1,J,RHOLM)
      SLOPE=EQ(1,J)*(1.0+X(1,J)*(-AK(1))*(EQ(2,J)-EQ(1,J))**2
     2/((-AK(2))*EQ(2,J)*(1.0-EQ(1,J))-(-AK(1))*EQ(1,J)*(1.0-EQ(2,J))))
      EMV=1.095-EXP(-1.353+0.389*V(J)*VMW/(2.45*SQRT(RHOV))-6.537*AL(J)
     2 /RHOLM)
      E(J)=1.0/(1.0+(1.0/EMV-1.0)/(SLOPE*V(J)/AL(J)))
      EDIF=E(J)-ETEMP
      IF(ABS(EDIF)-EFERR) 27,24,24
   24 JEOK=JEOK+1
      IF(IN(5).EQ.0) GO TO 27
      WRITE(3,30) J,EDIF
   30 FORMAT(20H DELTA EFF. ON TRAY ,I2,23H EXCEEDS 0.01.  DELTA =1PE12.
     24)
   27 CONTINUE
   28 CONTINUE
C  END EFF CALC
      IF(KCALC.NE.3.OR.JTIM.EQ.1) GO TO 102
C  HOLD REBOILER CONDITION CONSTANT FOR FINAL STEADY STATE
      IF(IRSET) 102,200,210
C  FIX REBOILER HEAT FLUX
  200 QRP=UA*(TS-T(1))
      QDIFF=QR-QRP
      IF(ABS(QDIFF).LE.QRERR) GO TO 102
      IF(IN(5).EQ.0) GO TO 206
      WRITE(3,201) QDIFF
  201 FORMAT(21H QR - UA*(TS-T(1)) = ,E11.4)
      GO TO 206
C  FIX BOILUP RATE
  210 IF(ITERAT.EQ.1) QRERR=0.005*VR
      QDIFF=V(1)-VR
      IF(ABS(QDIFF).LE.QRERR) GO TO 102
      IF(IN(5).EQ.0) GO TO 206
      WRITE(3,211) QDIFF
  211 FORMAT(13H V(1) - VR = ,E11.4)
  206 IF(ITERAT.LE.ILIM) GO TO 202
      WRITE(3,205)
  205 FORMAT(///49H *** FAILED TO CONVERGE ON REBOILER SPECIFICATION)
      GO TO 102
  202 JQOK=1
      IF(ITERAT.GT.1) GO TO 203
      ALDELT=0.1*QDIFF*F(JF)/QR
      GO TO 204
  203 ALDELT=(AL(1)-OLDL)*QDIFF/OLDQD
  204 OLDL=AL(1)
      OLDQD=QDIFF
      IF(AL(1)+ALDELT.GE.F(JF)) ALDELT=(F(JF)-AL(1))/2.
      IF(AL(1)+ALDELT.LE.0.) ALDELT=-AL(1)/2.
      AL(1)=AL(1)+ALDELT
C  ADJUST COMPOSITION FOR NEW ACTIV. COEFF CALC, CHECK CONVERGENCE
  102 IF(KTYP.NE.1) GO TO 105
      DO 13 I=1,NS
      XDIFF=X(1,I)-XX(1,I)
      IF(ABS(XDIFF)-0.01) 13,11,11
   11 JXOK=JXOK+1
      IF(IN(5).EQ.0) GO TO 13
      WRITE(3,16) I,XDIFF
   13 CONTINUE
      IF(JXOK) 105,105,14
   14 DO 15 I=1,NS
      XX(1,I)=X(1,I)
   15 XX(2,I)=1.-XX(1,I)
      IF(IN(5).EQ.0) GO TO 20
      WRITE(3,17) ITERAT
   20 OK=10.0
      RETURN
   16 FORMAT(14H COMP ON TRAY ,I2,36H DIFFERS FROM PREVIOUS ESTIMATE BY
     1  ,E11.4)
   17 FORMAT(//23H END OVERALL ITERATION ,I2,17H , BEGIN NEXT ONE///)
C  CHECK CONVERGENCE ON P, E, AND REBOILER CONDITION
  105 IF(JPOK) 6,6,9
    6 IF(JEOK) 306,306,9
  306 IF(JQOK) 18,18,9
C  CONVERGED
   18 OK=0.0
      IF(IN(5).NE.0) WRITE(3,5)
    5 FORMAT(19H PRESSURE CONVERGED)
    8 RETURN
C  NOT CONVERGED
    9 OK=10.0
      IF(IN(5).NE.0) WRITE(3,17) ITERAT
      RETURN
C  NO CALCS IN SPEC
   10 OK=0.0
      RETURN
      END
```

```
$IBFTC OUTPU.  DECK,SDD
COUTPUT
C       SUBROUTINE FOR OUTPUT
        SUBROUTINE OUTPUT(JOUT)
        COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
       2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
       3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
```

```
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),CMC,CMR,
     XWMC,WMR,AMC,AMR,UMCP,UCP,UMRP,URP,FILL(11)
      DIMENSION SUMX(70)
      DIMENSION E(70)
      EQUIVALENCE (SUMX,ERR),(E,FX(631))
  106 FORMAT(11H0ITERATIONS,3I8)
  107 FORMAT(11H0SUMX - 1.0/(8E15.7))
  108 FORMAT(13H0TEMPERATURES/(8E15.7))
  109 FORMAT(13H0LIQUID FLOWS/(8E15.7))
  110 FORMAT (11H1ITERATIONS,4I8)
  111 FORMAT (118H0 J       T(J)            AL(J)        SUMX - 1.0
     1X(1,J)          X(2,J)          X(3,J)          X(4,J)          X(5,J) /
     2(I3,5E15.6,3E14.6))
  112 FORMAT (119H0 J       X(6,J)          X(7,J)          X(8,J)
     1X(9,J)          X(10,J)         X(11,J)         X(12,J)         X(13,J) /
     2 (I3,5E15.6,3E14.6))
  113 FORMAT (105H0 J       X(14,J)         X(15,J)         X(16,J)
     1X(17,J)         X(18,J)         X(19,J)         X(20,J) /(I3,5E15.6,
     22E14.6))
  114 FORMAT (34H0TOP PRODUCT AMOUNTS BY COMPONENTS/E63.6,E15.6,3E14.6/
     1(E18.6,4E15.6,3E14.6))
  115 FORMAT (41H0HEAT BALANCE SATISFIED, CONDENSER LOAD =,E14.6,19H ,
     1REBOILER LOAD =,E14.6/////)
  134 FORMAT (15H0BOTTOM PRODUCT/E63.6,E15.6,3E14.6/(E18.6,4E15.6,3E14.6
     1))
  135 FORMAT  (20H0VAPOR DRAW ON STAGE,I4/E63.6,E15.6,3E14.6/(E18.6,4E
     115.6,3E14.6))
  136 FORMAT (21H0LIQUID DRAW ON STAGE,I4/E63.6,E15.6,3E14.6/(E18.6,4E
     115.6,3E14.6))
      GO TO (117,117,216),JOUT
C  X, T, AND L ONLY
  216 WRITE(3,106) ITERAT,ITHEAT,ITTEMP
      WRITE(3,107) (SUMX(J),J=1,NS)
      WRITE(3,108) (T(J),J=1,NS)
      WRITE(3,109) (AL(J),J=1,NS)
      RETURN
C  COMPLETE PRINTOUT
  117 WRITE(3,110) ITERAT,ITHEAT,ITTEMP
      IF (NC-10) 118,120,120
  118 DO 119 I=NC,9
      DO 119 J=1,NS
  119 X(I+1,J)= 0.0
  137 IF(IN(2)) 120,120,138
C  GENERAL OUTPUT
  120 WRITE(3,111) (J,T(J),AL(J),SUMX(J),(X(I,J),I=1,5),J=1,NS)
      IF (NC-5)  123,123,121
  121 WRITE(3,112) (J,(X(I,J),I=6,13),J=1,NS)
      IF (NC-13)  123,123,122
  122 WRITE(3,113) (J,(X(I,J),I=14,20),J=1,NS)
  123 DO 124 I=1,NC
  124 SUMX(I)= X(I,1)*AL(1)
      WRITE(3,134) (SUMX(I),I=1,NC)
      DO 125 I=1,NC
  125 SUMX(I)= X(I,NS)*EQ(I,NS)*V(NS)
      WRITE(3,114) (SUMX(I),I=1,NC)
      DO 131 J=1,NS
      IF (SL(J))  128,128,126
  126 DO 127 I=1,NC
  127 SUMX(I)= X(I,J)*SL(J)
      WRITE(3,135) J,(SUMX(I),I=1,NC)
  128 IF (SV(J))  131,131,129
  129 DO 130 I=1,NC
  130 SUMX(I)= X(I,J)*EQ(I,J)*SV(J)
      WRITE(3,136) J,(SUMX(I),I=1,NC)
  131 CONTINUE
      GO TO (132,133),JOUT
C  CONVERGED
  132 WRITE(3,115) QC,QR
  133 RETURN
  116 FORMAT(106H0 J       T(J)            P(J)            AL(J)        SUM
     1X - 1.0         E(J)            X(1,J)          X(2,J)/(I3,7E15.6))
C  FOR BINARY SYSTEM ONLY, INCLUDES P AND E
  138 WRITE(3,116) (J,T(J),P(J),AL(J),SUMX(J),E(J),X(1,J),X(2,J),J=1,NS)
      IF(NC-5) 123,123,120
      END
```

```
$IBFTC EQT.    DECK
CEQT
C      FUNCTION FOR DERIVATIVES OF EQUILIBRIUM CONSTANTS
       FUNCTION EQT(A,B,C,D,T,EQ,K)
       IF (K - 1)  1,1,2
     1 EQT= EQ*(C - A/(T+D)**2)
       GO TO 3
     2 EQT= B + 2.0*C*T + 3.0*D*T**2
     3 RETURN
       END
```

```
$IBFTC AUXOU.  DECK,SDD
CAUXOUT
C      SUBROUTINE TO CALCULATE COEFFICIENTS FOR LINEARIZED DYNAMIC
C      EQUATIONS
C  APPLIES FOR ALL MODELS
       SUBROUTINE AUXOUT(MOD,KOEFF,NOPR)
       DIMENSION GAM(70),DELT(70),EPS(70),XI(70),TAU(70),SIG(70),
      1ZETA(70),ETA(70),EMPTY(70),BETAP(70),PNU(70),CP(70),
      2VAPHT(70),COEFF(210),PSI(70),XMU(70),E(70),CAPA(70),XEQ(70),
      3SIGHT(70)
       COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
      2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
      3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
      4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
      5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
      6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
      7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
      8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
      9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),SC1,SC2,
      XSC3,SC4,TAUL3,AMR,USCP,UCP,UMRP,URP,FILL(11)
       COMMON /AUX/ L,CPF,CPO,VAPHTO,AA(70,70),TAU,SIG,ZETA,ETA,EMPTY,
      2BETAP,PNU,CP,VAPHT,PSI,XMU,Y(70),DEE,AJAY,CKP
       EQUIVALENCE (GAM(1),SL(1)),(DELT(1),SV(1)),(EPS(1),QERR(1)),
      1(XI(1),OLDDL(1)),(COEFF(1),ERR(1)),(E,FX(631)), (CAPA,XX),
      2(XEQ,XX(71)),(SIGHT,FX(561))
       VPO(TT,AA,BB)=AA*EXP(-BB/TT)
       ACT(A1,A2,X)=EXP(2.303*A1/(1.0+(X*A1/((1.0-X)*A2)))**2)
       HLDUP(1)=HLDUPB
       HLDUP(NS)=HLDUPA
       L=NS-1
       CPO=CPCALC(ACP,BCP,CCP,DCP,1.,T(L))
       VAPHTO=VHCALC(AVH,BVH,CVH,DVH,1.,T(L))
       JF=IFIX(FJF)
       VPTOP=VPO(T(L),APO,BPO)
       DO2 J=1,NS
       XEQ(J)=X(1,J)/E(J)+X(1,J+1)*(1.0-1.0/E(J))
       CP(J)=CPCALC(ACP,BCP,CCP,DCP,X(1,J),T(J))/CPO
     2 VAPHT(J)=VHCALC(AVH,BVH,CVH,DVH,X(1,J),T(J))/VAPHTO
       XEQ(NS)=X(1,NS)
       XF=FX(1,JF)/F(JF)
       CPF=CPCALC(ACP,BCP,CCP,DCP,XF,TF)/CPO
       ACT1=ACT(ACTCON(1),ACTCON(2),Y(L))
       ACT2=ACT(ACTCON(2),ACTCON(1),Y(L))
       TC=T(NS)+SUBCOL
       TCW=T(NS)-DELTC
C      GAMC IS 1.0/ALPHP
       GAMC=1.0/(ALPHA*37.4*AT*AL(NS)/RHLDUP)
       DO 3 J=2,NS
       RHOV=P(J)/(0.730*T(J))
       CALL RHOMW(1,J,RHO)
       CALL RHOMW(2,J,VMW)
       BETAP(J)=BETA*VPTOP*SQRT(32.2*CPO/(1544.  *VAPHTO*VMW))/AL(NS)
       BETAP(J)=BETAP(J)*144.*14.7
       CAPA(J)=CAP*AL(NS)*RHO/(12.*RHLDUP*RHOV)
     3 PNU(J)=VMW*RHLDUP/(VPTOP*AT*14.7*144.)
       CALL RHOMW(2,1,VMW)
       BETAP(1)=BETA*VPTOP*SQRT(32.2*CPO/(1544. *VAPHTO*VMW))/AL(NS)
       BETAP(1)=BETAP(1)*144.*14.7
       BETAP(L)=BETAN*BETAP(L)/BETA
       PNU(1)=VMW*RHLDUP/(VPTOP*AT*14.7*144.)
       PNU(L)=0.
       QC=QC+(V(L)-AL(NS))*(VAPHT(L)*VAPHTO+CP(NS)*CPO*SUBCOL)
       UMR=QR/DELTR
       USC=V(L)*CP(L)*CPO*(TC-T(NS))/(0.5*(TC+T(NS))-TCW)
       UC=V(L)*VAPHT(L)*VAPHTO/(TC-TCW)
C
C      CALCULATE DIMENSIONLESS TRAY VARIABLES
C
C  UMRP SAME AS URP IN DERIVATION
       UMRP=UMR/(CPO*AL(NS))
       USCP=USC/(CPO*AL(NS))
       UCP = UC/(CPO*AL(NS))
       HLDUP(NS)=HLDUP(NS)/RHLDUP
       DO 100 I=1,L
       AL(I)=AL(I)/AL(NS)
       V(I)=V(I)/AL(NS)
       T(I)=T(I)*CPO/VAPHTO
       P(I)=P(I)/VPTOP
       HLDUP(I)=HLDUP(I)/RHLDUP
   100 Y(I)=X(1,I)*EQ(1,I)
       IF(NOPR.EQ.2) GO TO 400
C  THE FOLLOWING ARE STILL DIMENSIONAL
       WRITE(3,102) AL(NS),V(NS),P(NS),F(JF),QC
   400 X(1,NS)=Y(L)
       P(NS)=P(NS)/VPTOP
       T(NS)=T(NS)*CPO/VAPHTO
       IF(NOPR.EQ.2) GO TO 350
C  TEMPORARILY MAKE L(N+1) DIMENSIONLESS (=1.0)
       TEMP1=AL(NS)
       AL(NS)=1.0
       WRITE(3,101) (I,AL(I),V(I),X(1,I),Y(I),T(I),P(I),HLDUP(I),I=1,NS)
   101 FORMAT(1HC,48X,24HDIMENSIONLESS QUANTITIES//20X,5HRATES,23X,
      112HCOMPOSITIONS/113H  TRAY      LIQUID          VAPOR           LI
      3QUID          VAPOR              TEMP            PRESS            HOLDU
      4P//(2X,I2,1P2E16.6,0P2E16.6,1P3E16.6))
       AL(NS)=TEMP1
   102 FORMAT(1H1///,14H REFLUX RATE =,1PE11.3,20H  TOP PRODUCT RATE =,
      2E11.3,24H  ACCUMULATOR PRESSURE =,E11.3,13H  FEED RATE =,E11.3//,
      314H   QC(TOTAL) =,E11.3,33X,17H(ALL DIMENSIONAL)////)
   350 TCW=TCW*CPO/VAPHTO
       TC=TC*CPO/VAPHTO
       LL=L-1
C
C  CALCULATE COEFFICIENTS OF LINEARIZED EQUATIONS
C
       DO 4 J=1,NS
       TTEM=T(J)*VAPHTO/CPO
       IF(J.EQ.NS) TTEM=TTEM+SUBCOL
       ACT1=ACT(ACTCON(1),ACTCON(2),X(1,J))
       IF(MOD.LT.3) GO TO 103
```

```
      ZETA(J)=EXP(AK(1)/TTEM+BK(1))*ACT1/(P(J)*VPTOP)
      GO TO 4
  103 ACT2=ACT(ACTCON(2),ACTCON(1),X(2,J))
      TEMP2=ACT1*EXP(AK(1)/TTEM+BK(1))
      TEMP3=ACT2*EXP(AK(2)/TTEM+BK(2))
      PSI(J)=(AK(1)*XEQ(J)*TEMP2+AK(2)*(1.-XEQ(J))*TEMP3)*(-1.*CPO/
     2VAPHTO)/(VPTOP*T(J)**2)
      XMU(J)=TEMP2*XEQ(J)*(-AK(1)*CPO/(VAPHTO*P(J)*T(J)**2)-PSI(J)/
     2(P(J)**2))/VPTOP
      ETA(J)=(TEMP2-TEMP3)/VPTOP
      ZETA(J)=TEMP2*(1.-ETA(J)*XEQ(J)/P(J))/(P(J)*VPTOP)
    4 CONTINUE
      IF(MOD.EQ.4) GO TO 104
      ZETA(NS)=0.0
      XMU(NS)=0.0
      DO 5 J=1,L
      TEMP1=2.*P(J)-P(J+1)-PNU(J)*HLDUP(J+1)
      TAU(J)=0.5*ETA(J)*TEMP1*BETAP(J)**2/(V(J)*T(J)*E(J))
      XI(J)=-0.5*P(J)*PNU(J)*BETAP(J)**2/(V(J)*T(J))
      IF(J.EQ.L) GO TO 106
      SIG(J)=XI(J)*ETA(J+1)/(PNU(J)*E(J+1))-TAU(J)*(1.-E(J))
      SIGHT(J)=-XI(J)*ETA(J+1)*(1.-E(J+1))/(PNU(J)*E(J+1))
      EPS(J)=XI(J)*PSI(J+1)/PNU(J)
  106 CONTINUE
      DELT(J)=PSI(J)*TAU(J)*E(J)/ETA(J)-0.5*V(J)/T(J)
    5 GAM(J)=GAMC
      EPS(L)=0.0
      SIGHT(L)=0.0
      TEMP1=0.5*(BETAP(L)**2)/(T(L)*V(L))
      TEMP2=1.+TEMP1*P(L)*PSI(NS)*VAPHT(L)/UCP
      TAU(L)=TEMP1*(ETA(L)*(2.*P(L)-P(NS))-P(L)*ETA(NS)*ZETA(L))/
     2(E(L)*TEMP2)
      TAU3=TAU(L)*TEMP2
      SIG(L)=-TAU(L)*(1.-E(L))
      DELT(L)=(TEMP1*(PSI(L)*(2.*P(L)-P(NS))-P(L)*ETA(NS)*XMU(L))-0.5*
     2V(L)/T(L))/TEMP2
      DEE=P(L)*TEMP1/TEMP2
      TEMP1=(VAPHT(L)*(V(L)*CP(L)-USCP/2.)/UCP+CP(L)*(TC-T(NS)))/
     2(V(L)*CP(L)+USCP/2.)
      SC1=TAU(L)*TEMP1
      SC2=-SC1*(1.-E(L))
      SC3=SC1*DELT(L)/TAU(L)
      SC4=(USCP+(V(L)*CP(L)-USCP/2.)*(1.-VAPHT(L)*PSI(NS)*DEE/UCP)
     2 -PSI(NS)*DEE*CP(L)*(TC-T(NS)))/(V(L)*CP(L)+USC/2.)
      GAM(NS)=0.
      SIG(NS)=0.0
      CAPA(1)=0.0
      TAU(NS)=0.0
      QC=QC/(AL(NS)*VAPHTO)
  104 CONTINUE
C
C  PRINT COEFFICIENTS IF DESIRED
C
      GO TO (401,402),NOPR
  401 CONTINUE
      WRITE(3,200) WT(1),DENS(1),ADENS(1),WT(2),DENS(2),ADENS(2),
     2(J,ACTCON(J),J=1,4),APO,BPO,APOP,BPOP,ACP,BCP,CCP,DCP,AVH,BVH,CVH,
     3DVH
      WRITE(3,202)                    HLDUP(NS),HLDUP(1),TF,PERR,BETAN,
     2BETA,ALPHA,CAP,RHLDUP,AT,TAUL3,TC,TCW,DELTC,DELTR,UC,USC,UMR,DEE,
     3SC1,SC2,SC3,SC4
  200 FORMAT(1H1,30X,10HPARAMETERS///,
     213H      MW(1) =1PE11.3,13H    DENS(1) =E11.3,13H   ADENS(1) =E11.
     33//,13H      MW(2) =E11.3,13H    DENS(2) = E11.3,13H   ADENS(2) =
     4E11.3//,4(9H  ACTCON(,I1,3H) =E11.3)//,13H         APO =,E11.3,13H
     5       BPO =E11.3,13H        APOP =E11.3,13H        BPOP =E11.3//,
     613H         ACP =E11.3,13H         BCP =E11.3,13H         CCP =E11.3,
     713H         DCP =E11.3//,
     8       13H         AVH =E11.3,13H         BVH =E11.3,13H         CVH
     9=E11.3,13H         DVH =E11.3//)
  202 FORMAT(                         13H  HLDUP(NS) =1PE11.3,13H   HLDUP(1
     3) =E11.3,13H          TF =E11.3,13H        PERR =E11.3//,13H       BE
     4TAN =E11.3,13H        BETA =E11.3,13H      ALPHA =E11.3,13H
     5CAP =E11.3//,13H      RHLDUP =E11.3,13H          AT =E11.3,13H    (T
     6AUL3) =E11.3//,13H          TC =E11.3,13H         TCW =E11.3,13H
     7  DELTC =E11.3,13H      DELTR =E11.3//,13H          UC =E11.3,
     813H         USC =E11.3,13H         UMR =E11.3,13H         DEE =E11.3/
     9/,13H         SC1 =E11.3,13H         SC2 =E11.3,
     X13H         SC3 =E11.3,13H         SC4 =E11.3/)
  402 CONTINUE
  105 CONTINUE
C  MORE ITEMS FOR NONDIMENSIONALIZING
      F(JF)=F(JF)/AL(NS)
      FX(1,JF)=FX(1,JF)/AL(NS)
      FX(2,JF)=FX(2,JF)/AL(NS)
C  FINALLY MAKE L(N+1) DIMENSIONLESS
      AL(NS)=1.0
      GO TO (403,404),NOPR
  403 CONTINUE
      WRITE(3,201) (J,GAM(J),ETA(J),PSI(J),ZETA(J),XMU(J),TAU(J),SIG(J),
     1DELT(J),EPS(J),XI(J),J=1,NS)
  201 FORMAT(/////,45X,31HCOEFFICIENTS RELATING VARIABLES//3H  J,4X,
     13HGAM,8X,3HETA,8X,3HPSI,8X,4HZETA,8X,2HMU,8X,3HTAU,8X,3HSIG,8X,4HD
     2ELT,7X,3HEPS,9X,2HXI,//(I3,1P10E11.3))
      WRITE(3,203) (J,XEQ(J),CAPA(J),SIGHT(J),J=1,NS)
  203 FORMAT(//3H  J,3X,5HX(EQ),7X,4HCAPA,6X,5HSIGHT,7X//(I3,1P3E11.3))
C     WRITE STATE VARIABLES (STEADY STATE VALUES)
  404 N=3*NS-2
      IF(MOD.EQ.2) N=2*NS
      IF(MOD.EQ.3) N=2*NS-2
      IF(MOD.EQ.4) N=NS
      GO TO (405,305),NOPR
  405 WRITE(3,310) N
      WRITE(34) N
      GO TO (301,302,303,304),MOD
  301 WRITE(34) (HLDUP(I),I=2,L),(X(1,I),I=1,NS),    (T(I),I=1,NS)
      WRITE(3,311) (HLDUP(I),I=2,L),(X(1,I),I=1,NS),    (T(I),I=1,NS)
      GO TO 305
  302 WRITE(34)    (X(1,I),I=1,NS),    (T(I),I=1,NS)
      WRITE(3,312) (X(1,I),I=1,NS),    (T(I),I=1,NS)
```

```
      GO TO 305
  303 WRITE(34)     (HLDUP(I),I=2,L),(X(1,I),I=1,NS)
      WRITE(3,313) (HLDUP(I),I=2,L),(X(1,I),I=1,NS)
      GO TO 305
  304 WRITE(34)     (X(1,I),I=1,NS)
      WRITE(3,314) (X(1,I),I=1,NS)
  305 IF(KOEFF.EQ.1) RETURN
  310 FORMAT(1H1,22HSTEADY STATE VALUES OF,I3,23H STATE VARIABLES FOLLOW
     2///)
  311 FORMAT(17H MASS, COMP, HEAT/,(10(2X,1PE10.3)))
  312 FORMAT(11H COMP, HEAT/,(10(2X,1PE10.3)))
  313 FORMAT(11H MASS, COMP/,(10(2X,1PE10.3)))
  314 FORMAT(5H COMP/,(10(2X,1PE10.3)))
C     GO TO CALC OF COEFFICIENTS.  FIRST WRITE MODEL USED
      DO 800 I=1,70
      DO 800 J=1,70
  800 AA(I,J)=0.0
      GO TO (801,802,802,802),MOD
C  MODEL 1 CALC
  801 CALL MOD1(MOD,NOPR)
      RETURN
C  MODEL 3 OR 4 CALC
  802 CALL M234(MOD,NOPR)
      RETURN
      END
```

```
$IBFTC DERIV.  DECK,SDD
C  CALCULATES THE DERIVATIVE OF MATRIX A WITH RESPECT TO ANY PARAMETER
      SUBROUTINE DERIV(NSEN,MOD,KOEFF,NOTFSS)
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),CMC,CMR,
     XSC3,SC4,AMC,AMR,USCP,UCP,UMRP,URP,FILL(11)
      DIMENSION GAM(70),DELT(70),EPS(70),XI(70),TAU(70),SIG(70),
     1ZETA(70),ETA(70),ALPHP(70),BETAP(70),PNU(70),CP(70),
     2VAPHT(70),COEFF(210),PSI(70),XMU(70),E(70),CAPA(70),XEQ(70),
     3SIGHT(70),A(70),B(70),BP(70)
      COMMON /AUX/ L,CPF,CPO,VAPHTO,AA(70,70),TAU,SIG,ZETA,ETA,ALPHP,
     2BETAP,PNU,CP,VAPHT,PSI,XMU,Y(70),DEE,AJAY,CKP
      COMMON /CDIST/ KCALC,NIL,NIX,NOL
      EQUIVALENCE (GAM,A,SL),(DELT,B,SV),(EPS,BP,QERR),
     1(XI(1),OLDDL(1)),(COEFF(1),ERR(1)),(E,FX(631)), (CAPA,XX),
     2(XEQ,XX(71)),(SIGHT,FX(561))
      DIMENSION TA(70),TB(70),TBP(70)
      DIMENSION Q(70,70),PARAM(3450),NPAR(35),MULT(35)
      DIMENSION VECT(140)
      EQUIVALENCE (PARAM,AK),(TA,Q),(TB,Q(71)),(TBP,Q(141))
      EQUIVALENCE (VECT,Q(211))
      IF(KOEFF.NE.5) GO TO 300
C  FOLLOWING READS STATE MATRIX AND AFFILIATED INFORMATION FROM
C  CARDS IF THIS OPTION HAS BEEN SELECTED
      REWIND 34
      READ(2,201) ZILCH,N,K
      IP=2*(N+K)
      READ(2,202) (VECT(I),I=1,IP)
  201 FORMAT(F10.2,2I10,F10.2,2I10)
  202 FORMAT(30A2)
      DO 210 I=1,N
  210 READ(2,203) (AA(I,J),J=1,N)
  203 FORMAT(6E12.5)
      IF(K.EQ.0) GO TO 230
      DO 220 I=1,K
      NI=N+I
  220 READ(2,203) (AA(J,NI),J=1,N)
  230 WRITE(34) N
      WRITE(34) (ZILCH,I=1,N)
      WRITE(34) ZILCH,N,K
      WRITE(34) (VECT(I),I=1,IP)
      WRITE(34) ((AA(I,J),J=1,N),I=1,N)
      IF(K.EQ.0) GO TO 250
      DO 240 I=1,K
      NI=N+I
  240 WRITE(34) (AA(J,NI),J=1,N)
  250 KCALC=5
  300 IF(NSEN.LE.0) RETURN
```

```
C  BEGIN DERIV CALC
      REWIND 34
      IF(KOEFF.NE.5) GO TO 5
      READ (2,2) NPR
C  SPECIFIES PARAM IF ALL DATA ARE ON CARDS
      READ(2,3) (PARAM(I),I=1,NPR)
    2 FORMAT(I4)
    3 FORMAT(9E8.4)
C  BEGIN USUAL DERIV CALC
    5 J=0
      NFSS=NOTFSS
    6 J=J+1
C  SPACE 34
      READ(34) N
      READ(34) (ZILCH,I=1,N)
      IF(KCALC.EQ.3.AND.J.EQ.1) GO TO 6
      IF(NFSS.EQ.0) GO TO 7
      NFSS=0
      GO TO 6
    7 READ(34) ZILCH,N,K
      J=(N+K)*2
      READ(34) (ZILCH,I=1,J)
      L=N-1
      IF(MOD.EQ.4) GO TO 10
C  READ A MATRIX
      READ(34) ((Q(I,J),J=1,N),I=1,N)
      GO TO 20
C  FOR MODEL 4
   10 READ(34) (TA(I),I=1,N),(TB(I),I=1,L),(TBP(I),I=1,L)
   20 REWIND 4
      WRITE(4) N
      IF(K.EQ.0) GO TO 28
      DO 25 I=1,K
   25 READ(34) (ZILCH,J=1,N)
C  SPECIFY PARAMETER(S) IN DCOM
   28 READ(2,1) (NPAR(ISEN),MULT(ISEN),ISEN=1,NSEN)
    1 FORMAT(12(I4,I2))
      DO 200 ISEN=1,NSEN
      WRITE(4) NPAR(ISEN),MULT(ISEN)
      NTIM=MULT(ISEN)
      DO 100 ITIM=1,NTIM
      IF(KOEFF.EQ.5) GO TO 30
      CALL SAVE(2)
      NOPR=2
   30 J=NPAR(ISEN)+ITIM-1
C  CHANGE PARAMETER BY ONE PER CENT
      PARAM(J)=1.01*PARAM(J)
C   PROVIDE SPECIAL AUXOUT WHEN KCALC = 6
C  CALC NEW A MATRIX
      CALL AUXOUT(MOD,KOEFF,NOPR)
   35 IF(MOD.EQ.4) GO TO 50
      DO 40 II=1,N
      DO 40 JJ=1,N
C  CALC DERIV MATRIX
   40 AA(II,JJ)=(AA(II,JJ)-Q(II,JJ))*100.
      GO TO 90
   50 DO 60 II=1,N
      DO 60 JJ=1,N
   60 AA(II,JJ)=0.0
C  FOR MODEL 4
      DO 70 I=1,L
      AA(I,I)=(A(I)-TA(I))*100.
      AA(I,I+1)=(B(I)-TB(I))*100.
   70 AA(I+1,I)=(BP(I)-TBP(I))*100.
      AA(N,N)=(A(N)-TA(N))*100.
   90 WRITE(4) ((AA(I,J),I=1,N),J=1,N)
  100 CONTINUE
  200 CONTINUE
  400 RETURN
      END
```

```
$IBFTC MOD1.   DECK,SDD
C  CALCULATES A AND B MATRICES FOR MODEL 1
      SUBROUTINE MOD1(MOD,NOPR)
      DIMENSION GAM(70),DELT(70),EPS(70),XI(70),TAU(70),SIG(70),
     1ZETA(70),ETA(70),ALPHP(70),BETAP(70),PNU(70),CP(70),
     2VAPHT(70),COEFF(210),PSI(70),XMU(70),E(70),CAPA(70),XEQ(70),
     3SIGHT(70),A(70),B(70),BP(70)
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,DK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),SC1,SC2,
     XSC3,SC4,TAUL3,AMR,USCP,UCP,UMRP,URP,FILL(10),NDCOM
      COMMON /AUX/ L,CPF,CPU,VAPHTO,AA(70,70),TAU,SIG,ZETA,ETA,ALPHP,
     2BETAP,PNU,CP,VAPHT,PSI,XMU,Y(70),DEE,AJAY,CKP
      EQUIVALENCE (GAM,A,SL),(DELT,B,SV),(EPS,BP,QERR),
     1(XI(1),OLDDL(1)),(COEFF(1),ERR(1)),(E,FX(631)), (CAPA,XX),
     2(XEQ,XX(71)),(SIGHT,FX(561))
      DATA AAA,BBB,CCC/2H H,2H X,2H T/
      DATA DDD/2HIN/
C     MODEL 1
      DO 9001 IDUM=1,1
C  SET KCON VIA DEBUG FOR CONTROL OPTIONS
C  CNTRL CALLED AFTER UNCONTROLLED CASE IS CALCULATED
      KCON=1
 9000 CONTINUE
C     SET UP COEFFICIENTS IN MATRIX FOR STATE SPACE FORMULATION
C     COLUMNS ARE ARRANGED WITH ELEMENTS IN THE FOLLOWING SEQUENCE
C     HOLDUPS (2 THROUGH L), COMPOSITIONS (1 THROUGH NS),
C     TEMPERATURES (1 THROUGH NS)      .  ROW ELEMENTS FOLLOW SAME SEQ.
C     LAST SIX ROWS ARE   F, TF, XF, R, TS, TCW
  112 FORMAT(////40X,34H MODEL 1 - COMP, MASS AND HEAT BAL///)
      NDCOM=3450
      N=3*NS-2
      NLIM=N
      KKK=6
      FORM=1.0
      WRITE(34) FORM,N,KKK
      WRITE(34) (AAA,I,I=2,L),(BBB,I,I=1,NS),      (CCC,I,I=1,NS)
     1,(DDD,I,I=1,6)
   23 FORMAT (15(A2,I2))
   24 FORMAT (35HOMATRIX ELEMENTS ORDERED AS FOLLOWS//(1X,29(A2,I2)))
   25 FORMAT (F10.2,I10,I10)
    7 FORMAT(1H1,40X,34HCOEFFICIENTS OF STATE SPACE MATRIX//////,50X,
     116HHOLDUP EQUATIONS///)
C  HOLDUP EQUATIONS
C     NO HOLDUP EQUATION FOR REBOILER
      DO 9 J=2,L
      TEMP1=1.0-GAM(J)*CAPA(J)
      TEMP2=1.0-GAM(J+1)*CAPA(J+1)
      J1=NS+J-3
      J2=NS+J-2
      J3=NS+J-1
      J34=NS+J
      J4=2*NS+J-3
      J5=2*NS+J-2
      J6=2*NS+J-1
      AA(J-1,J-1)=-GAM(J)+XI(J-1)*TEMP1
      AA(J-1,J  )=GAM(J+1)-XI(J)*TEMP2
      AA(J-1,J1)=TAU(J-1)*TEMP1
      AA(J-1,J2)=SIG(J-1)*TEMP1-TAU(J)*TEMP2
      AA(J-1,J3)=-SIG(J)*TEMP2+SIGHT(J-1)*TEMP1
      AA(J-1,J34)=-SIGHT(J)*TEMP2
      AA(J-1,J4)=DELT(J-1)*TEMP1
      AA(J-1,J5)=EPS(J-1)*TEMP1-DELT(J)*TEMP2
    9 AA(J-1 ,J6)=-EPS(J)*TEMP2
    8 FORMAT (1P6E12.5)
   10 FORMAT(/4H ROW,I3,//,(1X,1P8E14.4))
      L1=NS+L-3
      L2=NS+L-2
      L3=NS+L-1
      L4=2*NS+L-3
      L5=2*NS+L-2
      L6=2*NS+L-1
C  COMPOSITION EQNS
      TEMP1=GAM(2)*CAPA(2)*(X(1,2)-X(1,1))/HLDUP(1)*(-1.0)
      AA(L ,1)=(GAM(2)*(X(1,2)-X(1,1))+XI(1)*(X(1,1)-Y(1)))/HLDUP(1)
     1-XI(1)*TEMP1
      AA(L,L)=(TAU(1)*(X(1,1)-Y(1))-AL(1)-V(1)*ZETA(1)/E(1))/HLDUP(1)
     1-TAU(1)*TEMP1
      AA(L ,NS  )=(SIG(1)*(X(1,1)-Y(1))+AL(2))/HLDUP(1)
     1-SIG(1)*TEMP1+V(1)*ZETA(1)*(1.-E(1))/(E(1)*HLDUP(1))
      AA(L,NS+1)=SIGHT(1)*(-TEMP1+(X(1,1)-Y(1))/HLDUP(1))
      AA(L ,2*NS-1)=DELT(1)*(X(1,1)-Y(1))/HLDUP(1)-V(1)*XMU(1)/HLDUP(1)
     1-DELT(1)*TEMP1
      AA(L ,2*NS  )=EPS(1)*(X(1,1)-Y(1))/HLDUP(1)
     1-EPS(1)*TEMP1
   14 FORMAT (////48X,21HCOMPOSITION EQUATIONS////,18H  ROW 1    REBOILER
     2//,(1X,1P8E14.4))
C  PLATES 1 - N
      DO 17 J=2,L
      TEMP1=-GAM(J+1)*CAPA(J+1)*(X(1,J+1)-X(1,J))/HLDUP(J)
      J1=NS+J-3
      J2=NS+J-2
      J3=NS+J-1
      J34=NS+J
      J4=2*NS+J-3
      J5=2*NS+J-2
      J6=2*NS+J-1
      AA(J2,J-1)=XI(J-1)*(Y(J-1)-X(1,J))/HLDUP(J)
      AA(J2,J  )=(GAM(J+1)*(X(1,J+1)-X(1,J))+XI(J)*(X(1,J)-Y(J)))/HLDUP(
     1J)-XI(J)*TEMP1
      AA(J2,J1)=(V(J-1)*ZETA(J-1)/E(J-1)+TAU(J-1)*(Y(J-1)-X(1,J)))/
     2HLDUP(J)
      AA(J2,J2)=(TAU(J)*(X(1,J)-Y(J))+SIG(J-1)*(Y(J-1)-X(1,J))-AL(J)
     1-V(J)*ZETA(J)/E(J)-V(J-1)*ZETA(J-1)*(1.-E(J-1))/E(J-1))/HLDUP(J)
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```
     2-TAU(J)*TEMP1
      AA(J2,J3)=(SIG(J)*(X(1,J)-Y(J))+AL(J+1))/HLDUP(J)
     1-SIG(J)*TEMP1+(SIGHT(J-1)*(Y(J-1)-X(1,J))+ZETA(J)*V(J)*(1.-E(J))/
     2E(J))/HLDUP(J)
      AA(J2,J34)=SIGHT(J)*(-TEMP1+(X(1,J)-Y(J))/HLDUP(J))
      AA(J2,J4)=(DELT(J-1)*(Y(J-1)-X(1,J))+V(J-1)*XMU(J-1))/HLDUP(J)
      AA(J2,J5)=(DELT(J)*(X(1,J)-Y(J))+EPS(J-1)*(Y(J-1)-X(1,J))
     1-V(J)*XMU(J))/HLDUP(J)-DELT(J)*TEMP1
   17 AA(J2,J6)=EPS(J)*(X(1,J)-Y(J))/HLDUP(J)
     1-EPS(J)*TEMP1
C  ACCUMULATOR
      AA(L3,L2)=V(L)*ZETA(L)/(E(L)*HLDUP(NS))
      AA(L3,L3)=-V(L)*(1.+ZETA(L)*(1.-E(L))/E(L))/HLDUP(NS)
      AA(L3    ,L5)=V(L)*XMU(L)/HLDUP(NS)
   20 FORMAT(/4H ROW,I3,12H   CONDENSER//,(1X,1P8E14.4))
C  TEMP EQNS
      TEMP1=-GAM(2)*(CP(2)*T(2)-CP(1)*T(1))*CAPA(2)/(CP(1)*HLDUP(1))
      AA(L3+1,1)=(GAM(2)*(CP(2)*T(2)-CP(1)*T(1))-VAPHT(1)*XI(1))/(CP(1)*
     1HLDUP(1))-TEMP1*XI(1)
      AA(L3+1,NS-1)=-VAPHT(1)*TAU(1)/(CP(1)*HLDUP(1))
     1-TEMP1*TAU(1)
      AA(L3+1,NS)=AA(L3+1,NS-1)*SIG(1)/TAU(1)
      AA(L3+1,NS+1)=AA(L3+1,NS)*SIGHT(1)/SIG(1)
      AA(L3+1,L3+1)=-(AL(1)+V(1))/HLDUP(1)-(VAPHT(1)*DELT(1)+UMRP)/
     1(CP(1)*HLDUP(1))
     2-DELT(1)*TEMP1
      AA(L3+1,2*NS   )=(CP(2)*AL(2)-VAPHT(1)*EPS(1))/(CP(1)*HLDUP(1))
     1-EPS(1)*TEMP1
   21 FORMAT(////48X,21HTEMPERATURE EQUATIONS////,18H  ROW 1   REBOILER/
     2/,(1X,1P8E14.4))
C  PLATES 1 - N
      DO 22 J=2,L
      TEMP2=-GAM(J+1)*CAPA(J+1)*(CP(J+1)*T(J+1)-CP(J)*T(J))/(CP(J)*
     2HLDUP(J))
      J1=NS+J-3
      J2=NS+J-2
      J3=NS+J-1
      J34=NS+J
      J4=2*NS+J-3
      J5=2*NS+J-2
      J6=2*NS+J-1
      TEMP1=(CP(J-1)*T(J-1)-CP(J)*T(J)+VAPHT(J-1))/(CP(J)*HLDUP(J))
      AA(J5,J-1)=TEMP1*XI(J-1)
      AA(J5,J   )=(GAM(J+1)*(CP(J+1)*T(J+1)-CP(J)*T(J))-XI(J)*VAPHT(J))
     1/(CP(J)*HLDUP(J))-XI(J)*TEMP2
      AA(J5,J1)=TEMP1*TAU(J-1)
      AA(J5,J2)=TEMP1*SIG(J-1)-VAPHT(J)*TAU(J)/(CP(J)*HLDUP(J))
     1-TAU(J)*TEMP2
      AA(J5,J3)=-VAPHT(J)*SIG(J)/(CP(J)*HLDUP(J))-SIG(J)*TEMP2+SIGHT(J-1
     2)*TEMP1
      AA(J5,J34)=SIGHT(J)*(-TEMP2-VAPHT(J)/(CP(J)*HLDUP(J)))
      AA(J5,J4)=TEMP1*DELT(J-1)+V(J-1)/HLDUP(J)
      AA(J5,J5)=TEMP1*EPS(J-1)-(CP(J)*(AL(J)+V(J))+VAPHT(J)*DELT(J))
     1/(CP(J)*HLDUP(J))-DELT(J)*TEMP2
      AA(J5,J6)=(CP(J+1)*AL(J+1)-VAPHT(J)*EPS(J))/(CP(J)*HLDUP(J))
     1-EPS(J)*TEMP2
   22 CONTINUE
C  ACCUMULATOR
      AA(L6,L2)=SC1*V(L)/HLDUP(NS)
      AA(L6,L3)=SC2*V(L)/HLDUP(NS)
      AA(L6,L5)=SC3*V(L)/HLDUP(NS)
      AA(L6,L6)=-V(L)/HLDUP(NS)
  200 CONTINUE
C  MODIFY A MATRIX FOR CONTROL IF DESIRED
      CALL CNTRL(KCON,MOD,1,N)
      WRITE(34) ((AA(I,J),J=1,N),I=1,N)
C     PREPARE VECTORS OF B MATRIX IN SEQUENCE -
C     F, TF, XF, AL(NS), TS, TCW
      JF1=L+JF-1
      JF2=NS+L+JF-1
      AA(JF-1,N+1)=1.0
      AA(JF1,N+1)=FX(1,JF)/(F(JF)*HLDUP(JF))
      AA(JF2,N+1)=TF*CPO/(HLDUP(JF)*VAPHTO)*CPF/CP(JF)
   26 FORMAT(///28H COLUMN VECTOR FOR FEED RATE/,
     2(1X,1P8E14.4))
      AA(JF2,N+2)=F(JF)/(HLDUP(JF)*AL(NS))*CPF/CP(JF)
   27 FORMAT(///28H COLUMN VECTOR FOR FEED TEMP/,(1X,1P8E14.4))
      AA(JF1,N+3)=F(JF)/(HLDUP(JF)*AL(NS))
   28 FORMAT(///28H COLUMN VECTOR FOR FEED COMP/,(1X,1P8E14.4))
      AA(L-1,N+4)=1.0
      AA( L2,N+4)=(X(1,NS)-X(1,L))/HLDUP(L)
      AA( L5,N+4)=(CP(NS)*T(NS)-CP(L)*T(L))/(CP(L)*HLDUP(L))
   29 FORMAT(///30H COLUMN VECTOR FOR REFLUX RATE/,(1X,1PE14.4))
      AA(L3+1,N+5)=UMRP/(CP(1)*HLDUP(1))
   30 FORMAT(///32H COLUMN VECTOR FOR REBOILER DUTY/(1X,
     21P8E14.4))
      AA(L-1,N+6)=+PSI(NS)*DEE
      AA(L2,N+6)=+PSI(NS)*DEE*(Y(L)-X(1,L))/HLDUP(L)
      AA(L5,N+6)=+PSI(NS)*DEE*VAPHT(L)/(CP(L)*HLDUP(L))
      AA(L6,N+6)=SC4*V(L)/HLDUP(NS)
   31 FORMAT(///39H COLUMN VECTOR FOR CONDENSER WATER TEMP/
     2,(1X,1P8E14.4))
  201 CONTINUE
C  MODIFY B MATRIX FOR CONTROL IF DESIRED
      CALL CNTRL(KCON,MOD,2,N)
      DO 801 I=1,KKK
      NI=N+I
  801 WRITE(34) (AA(J,NI),J=1,N)
      IF(NOPR.EQ.2) RETURN
C  PRINT MATRICES
      WRITE(3,112)
      IF(KCON.EQ.2) WRITE(3,1100)
      IF (KCON.EQ.3) WRITE(3,1101)
 1100 FORMAT(2X,46HCONDENSER PRESSURE CONTROLLED BY ADJUSTING TCW///)
 1101 FORMAT(2X,48HOVERHEAD FLOW DISTURBANCES TRANSMITTED TO REFLUX///)
      WRITE(3,24) (AAA,I,I=2,L),(BBB,I,I=1,NS),      (CCC,I,I=1,NS)
      WRITE(3,7)
      DO 1009 J=2,L
 1009 WRITE(3,10) J,(AA(J-1,I),I=1,NLIM)
      WRITE(3,14) (AA(L ,1),I=1,NLIM)
```

```
      DO 1017 J=2,L
      J1=NS+J-2
 1017 WRITE(3,10) J,(AA(J1,I),I=1,NLIM)
      WRITE(3,20) NS,(AA(L3     ,I),I=1,NLIM)
      WRITE(3,21) (AA(L3+1,I),I=1,NLIM)
      DO 1022 J=2,L
      J4=2*NS+J-2
 1022 WRITE(3,10) J,(AA(J4,I),I=1,NLIM)
      WRITE(3,20) NS,(AA(L6     ,I),I=1,NLIM)
      WRITE(3,26) (AA(I,N+1),I=1,NLIM)
      WRITE(3,27) (AA(I,N+2),I=1,NLIM)
      WRITE(3,28) (AA(I,N+3),I=1,NLIM)
      WRITE(3,29) (AA(I,N+4),I=1,NLIM)
      WRITE(3,30) (AA(I,N+5),I=1,NLIM)
      WRITE(3,31) (AA(I,N+6),I=1,NLIM)
C  THE FOLLOWING IS READ BY RESPNS FOR CALC OF L, V AND P
      REWIND 41
      NWDS=11*NS
      N2=L-1
      READ (41) (ZILCH,J=1,NDCOM)
      WRITE (41) NWDS,NS,L,N2,DEE,VAPHT(L),UCP,XMU(L)
      WRITE (41) (CAPA(J),TAU(J),GAM(J),PSI(J),EPS(J),DELT(J),SIGHT(J),
     2 SIG(J),XI(J),ETA(J), E(J),ZETA(J),J=1,NS)
      REWIND 41
 9001 CONTINUE
      RETURN
      END



$IBFTC CNTRL.  DECK,SDD
      SUBROUTINE CNTRL(KCON,MOD,JAB,N)
C  SUBROUTINE FOR VARIOUS CONTROL OPTIONS
C      KCON = 1 FOR NO OPTIONS
C           = 2 FOR CONDENSER PRESSURE CONTROL
C           = 3 FOR ALTERNATE REFLUX CONFIGURATION
C           = 4 FOR MODAL CONTROL - MANIP AL(NS),TS AND TCW,
C                                 - MEASURE T(1), T(NS), AND X(NS)
C           = 5 FOR OPTIONS 2 AND 4 COMBINED
C
C  SET KCON VIA DEBUG FROM MOD1, 9000
C      JAB = 1 FOR A MATRIX CALC, = 2 FOR B MATRIX CALC
      DIMENSION GAM(70),DELT(70),EPS(70),XI(70),TAU(70),SIG(70),
     1ZETA(70),ETA(70),ALPHP(70),BETAP(70),PNU(70),CP(70),
     2VAPHT(70),COEFF(210),PSI(70),XMU(70),E(70),CAPA(70),XEQ(70),
     3SIGHT(70),A(70),B(70),BP(70)
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),SC1,SC2,
     XSC3,SC4,TAUL3,AMR,USCP,UCP,UMRP,URP,FILL(10),NDCOM
      COMMON /AUX/ L,CPF,CPO,VAPHTO,AA(70,70),TAU,SIG,ZETA,ETA,ALPHP,
     2BETAP,PNU,CP,VAPHT,PSI,XMU,Y(70),DEE,AJAY,CKP
      EQUIVALENCE (GAM,A,SL),(DELT,B,SV),(EPS,BP,QERR),
     1(XI(1),OLDDL(1)),(COEFF(1),ERR(1)),(F,FX(631)), (CAPA,XX),
     2(XEQ,XX(71)),(SIGHT,FX(561))
C
C  SET AA1, ETC  VIA DEBUG AT CNTRL. 400
C
      DATA AA1,AA2,AA3,AA4,AA5,BB1,BB2,BB3,BB4,BB5,CC1,CC2,CC3,CC4,CC5
     2/2.464,6.268,0.,0.,0.2672,0.2908,0.740,0.,0.,0.0315,-0.3504,
     3 -0.888,0.,0.,-0.0379/
      L1=NS+L-3
      L2=NS+L-2
      L3=NS+L-1
      L4=2*NS+L-3
      L5=2*NS+L-2
      L6=2*NS+L-1
      JF1=L+JF-1
      JF2=NS+L+JF-1
      GO TO (100,200,300,400,200),KCON
  100 RETURN
  200 PCK=2.0
  201 GO TO (202,203), JAB
  202 CONTINUE
      PC1=1.0/(1.0+PCK*PSI(NS)/(1.0+0.5*PSI(NS)*VAPHT(L)*(BETAP(L)**2)
     2*P(L)/(UCP*T(L)*V(L))))
      PC2=PCK*(ETA(NS)*ZETA(L)/E(L)+PSI(NS)*TAU(L)*VAPHT(L)/UCP)/PC1
      PC3=PCK*(-ETA(NS)*ZETA(L)*(1.-E(L))/E(L)+PSI(NS)*SIG(L)*
     2VAPHT(L)/UCP)/PC1
      PC4=PCK*(ETA(NS)*XMU(L)+PSI(NS)*DELT(L)*VAPHT(L)/UCP)/PC1
      TMP1=PSI(NS)*DEE
      AA(L-1,L2)=AA(L-1,L2)-PC2*TMP1
      AA(L-1,L3)=AA(L-1,L3)-PC3*TMP1
      AA(L-1,L5)=AA(L-1,L5)-PC4*TMP1
      TMP=TMP1*(Y(L)-X(1,L))/HLDUP(L)
      AA(L2,L2)=AA(L2,L2)-PC2*TMP
      AA(L2,L3)=AA(L2,L3)-PC3*TMP
      AA(L2,L5)=AA(L2,L5)-PC4*TMP
      TMP=TMP1*VAPHT(L)/(CP(L)*HLDUP(L))
      AA(L5,L2)=AA(L5,L2)-PC2*TMP
      AA(L5,L3)=AA(L5,L3)-PC3*TMP
      AA(L5,L5)=AA(L5,L5)-PC4*TMP
      TMP=V(L)*SC4/HLDUP(NS)
      AA(L6,L2)=AA(L6,L2)-PC2*TMP
      AA(L6,L3)=AA(L6,L3)-PC3*TMP
      AA(L6,L5)=AA(L6,L5)-PC4*TMP
      IF(KCON.EQ.5) GO TO 400
      RETURN
  203 CONTINUE
      AA(L-1,N+6)=AA(L-1,N+6)*PC1
      AA(L2,N+6)=AA(L2,N+6)*PC1
      AA(L5,N+6)=AA(L5,N+6)*PC1
```

```
      AA(L6,N+6)=AA(L6,N+6)*PC1
      IF(KCON.EQ.5) GO TO 400
      RETURN
  300 GO TO (301,302), JAB
  301 AA(L-1,L2)=AA(L-1,L2)+TAU(L)
      AA(L-1,L3)=AA(L-1,L3)+SIG(L)
      AA(L-1,L5)=AA(L-1,L5)+DELT(L)
      DUM1=(X(1,NS)-X(1,L))/HLDUP(L)
      AA(L2,L2)=AA(L2,L2)+DUM1*TAU(L)
      AA(L2,L3)=AA(L2,L3)+DUM1*SIG(L)
      AA(L2,L5)=AA(L2,L5)+DUM1*DELT(L)
      DUM2=(CP(NS)*T(NS)-CP(L)*T(L))/(CP(L)*HLDUP(L))
      AA(L5,L2)=AA(L5,L2)+DUM2*TAU(L)
      AA(L5,L3)=AA(L5,L3)+DUM2*SIG(L)
      AA(L5,L5)=AA(L5,L5)+DUM2*DELT(L)
      RETURN
  302 AA(L-1,N+6)=AA(L-1,N+6)-PSI(NS)*DEE
      AA(L2,N+6)=AA(L2,N+6)-PSI(NS)*DEE*DUM1
      AA(L5,N+6)=AA(L5,N+6)-PSI(NS)*DEE*DUM2
      RETURN
C  MODAL CONTROL
  400 GO TO (401,402),JAB
  401 TMP = PSI(NS)*DEE
      JX=L-1+NS+JF
      AA(L-1,L3+1)=AA(L-1,L3+1)+AA1 + CC1*TMP
      AA(L-1,N)=AA(L-1,N)+AA2 + CC2*TMP
      AA(L-1,L3)=AA(L-1,L3)+AA3 + CC3*TMP
      AA(L-1,L) = AA(L-1,L) + AA4 + CC4*TMP
      AA(L-1,JX) = AA(L-1,JX) + AA5 + CC5*TMP
      TMP = TMP*(Y(L)-X(1,L))/HLDUP(L)
      DUM=(X(1,NS)-X(1,L))/HLDUP(L)
      AA(L2,L3+1)=AA(L2,L3+1)+AA1*DUM + CC1*TMP
      AA(L2,N)=AA(L2,N)+AA2*DUM + CC2*TMP
      AA(L2,L3)=AA(L2,L3)+AA3*DUM + CC3*TMP
      AA(L2,L) = AA(L2,L) + AA4*DUM + CC4*TMP
      AA(L2,JX) = AA(L2,JX) + AA5*DUM + CC5*TMP
      TMP = PSI(NS)*DEE*VAPHT(L)/(CP(L)*HLDUP(L))
      DUM=(CP(NS)*T(NS)-CP(L)*T(L))/(CP(L)*HLDUP(L))
      AA(L5,L3+1)=AA(L5,L3+1)+AA1*DUM + CC1*TMP
      AA(L5,N)=AA(L5,N)+AA2*DUM + CC2*TMP
      AA(L5,L3)=AA(L5,L3)+AA3*DUM + CC3*TMP
      AA(L5,L) = AA(L5,L) + AA4*DUM + CC4*TMP
      AA(L5,JX) = AA(L5,JX) + AA5*DUM + CC5*TMP
      AA(L3+1,L3+1)=AA(L3+1,L3+1)+BB1*UMRP/(CP(1)*HLDUP(1))
      AA(L3+1,N)=AA(L3+1,N)+BB2*UMRP/(CP(1)*HLDUP(1))
      AA(L3+1,L3)=AA(L3+1,L3)+BB3*UMRP/(CP(1)*HLDUP(1))
      AA(L3+1,L) = AA(L3+1,L) + BB4*UMRP/(CP(1)*HLDUP(1))
      AA(L3+1,JX) = AA(L3+1,JX) + BB5*UMRP/(CP(1)*HLDUP(1))
      TMP = V(L)*SC4/HLDUP(NS)
      AA(N,L3+1) = AA(N,L3+1) + CC1*TMP
      AA(N,N) = AA(N,N) + CC2*TMP
      AA(N,L3) = AA(N,L3) + CC3*TMP
      AA(N,L) = AA(N,L) + CC4*TMP
      AA(N,JX) = AA(N,JX) + CC5*TMP
  402 RETURN
      END
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$IBFTC M234.   DECK,SDD
C  CALCULATES A AND B MATRICES FOR MODELS 3 AND 4
      SUBROUTINE M234(MOD,NOPR)
      DIMENSION GAM(70),DELT(70),EPS(70),XI(70),TAU(70),SIG(70),
     1ZETA(70),ETA(70),ALPHP(70),BETAP(70),PNU(70),CP(70),
     2VAPHT(70),COEFF(210),PSI(70),XMU(70),E(70),CAPA(70),XEQ(70),
     3SIGHT(70),A(70),B(70),BP(70)
      COMMON /DCOM/ AK(10),BK(10),CK(10),DK(10),KTYP,EQ(10,70),T(70),
     2X(10,70),NC,N,QC,QR,QNET,CHECK,DL,OK,ITERAT,ITHEAT,ITTEMP,NIT,
     3AL(70),ERR(70),V(70),SL(70),SV(70),NS,NF,NDRAW,JCOTYP,IN(5),
     4SPECS(4),F(70),HF(70),FX(10,70),DTLIM,SUMERR,HETERR,SUBCOL,NPROB,
     5HL(70),HV(70),OLDDL(70),QERR(70),JF,P(70),HLDUP(70),WT(10),
     6DENS(10),ADENS(10),ACTCON(10),PERR,SW,AT,ALPHA,BETA,RHLDUP,PTOP,
     7XX(2,70),NIN,APO,BPO,APOP,BPOP,A1,B1,A2,B2,ACP,BCP,CCP,DCP,AVH,
     8BVH,CVH,DVH,HLDUPA,HLDUPB,TF,FJF,DELTR,DELTC,CAP,TS,UA,VR,QRERR,
     9BETAN,WC,AHL(10),BHL(10),CHL(10),AHV(10),BHV(10),CHV(10),SC1,SC2,
     XSC3,SC4,TAUL3,AMR,USCP,UCP,UMRP,URP,FILL(11)
      COMMON /AUX/ L,CPF,CPO,VAPHTO,AA(70,70),TAU,SIG,ZETA,ETA,ALPHP,
     2BETAP,PNU,CP,VAPHT,PSI,XMU,Y(70),DEE,AJAY,CKP
      EQUIVALENCE (GAM,A,SL),(DELT,B,SV),(EPS,BP,QERR),
     1(XI(1),OLDDL(1)),(COEFF(1),ERR(1)),(E,FX(631)), (CAPA,XX),
     2(XEQ,XX(71)),(SIGHT,FX(561))
      DATA AAA,BBB,CCC/2H H,2H X,2H T/
      DATA DDD/2HIN/
      TF=TF*CPO/VAPHTO
      GO TO (999,222,333,444),MOD
C
C     MODEL 2    **** NOT DEBUGGED ***
C
  222 CONTINUE
      DO 9002 IDUM=1,1
C     SET UP COEFFICIENTS IN MATRIX FOR STATE SPACE FORMULATION
C     COLUMNS ARE ARRANGED WITH ELEMENTS IN THE FOLLOWING SEQUENCE
C     COMPOSITIONS (1 THROUGH NS),
C     TEMPERATURES (1 THROUGH NS).   ROW ELEMENTS FOLLOW SAME SEQUENCE
C     LAST FOUR ROWS ARE TF, XF, TS, TCW
  223 FORMAT(////40X,28H MODEL 2 - COMP AND HEAT BAL///)
      NLIM=2*NS
      N=NLIM
      KKK=4
      FORM=1.0
      WRITE(34) FORM,N, KKK
      WRITE(34) (BBB,I,I=1,NS),(CCC,I,I=1,NS),
     1(DDD,I,I=1,4)
  507 FORMAT(1H1,40X,34HCOEFFICIENTS OF STATE SPACE MATRIX//////)
      L1=L-1
      L2=L
      L3=NS
      L4=NS+L-1
      L5=NS+L
      L6=2*NS
      DP=SC1/TAU(L)
      AA(1,1)=-(AL(1)+V(1)*ZETA(1))/HLDUP(1)
      AA(1,2)=AL(2)/HLDUP(1)
      AA(1,NS+1)=-V(1)*XMU(1)/HLDUP(1)
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      DO 517 J=2,L
      AA(J,J-1)=V(J-1)*ZETA(J-1)/(HLDUP(J)*E(J-1))
      AA(J,J)=-(AL(J)+V(J)*ZETA(J  )/E(J)+V(J-1)*ZETA(J-1)*(1.-E(J-1))
     2/E(J-1))/HLDUP(J)
      AA(J,J+1)=(AL(J+1)+V(J)*ZETA(J)*(1.-E(J))/E(J))/HLDUP(J)
      J1=NS+J
      AA(J,J1-1)=V(J-1)*XMU(J-1)/HLDUP(J)
      AA(J,J1)=-V(J)*XMU(J)/HLDUP(J)
  517 CONTINUE
      AA(NS,L)=V(L)*ZETA(L)/(E(L)*HLDUP(NS))
      AA(NS,NS)=V(L)/HLDUP(NS)*(-1.)
     2-V(L)*ZETA(L)*(1.-E(L))/(E(L)*HLDUP(NS))
      AA(NS,L5)=V(L)*XMU(L)/HLDUP(NS)
      AA(NS+1,NS+1)=-(AL(1)+V(1))/HLDUP(1)-UMRP/(CP(1)*HLDUP(1))
      AA(NS+1,NS+2)=CP(2)*AL(2)/(CP(1)*HLDUP(1))
      DO 522 J=2,L
      J1=NS+J
      AA(J1,J1-1)=CP(J-1)*V(J-1)/(CP(J)*HLDUP(J))
      AA(J1,J1)=-(AL(J)+V(J))/HLDUP(J)
      AA(J1,J1+1)=CP(J+1)*AL(J+1)/(CP(J)*HLDUP(J))
  522 CONTINUE
      AA(L6  ,L6)=-V(L)/HLDUP(NS)
      WRITE(34) ((AA(I,J),J=1,N),I=1,N)
C     PREPARE VECTORS CORRESPONDING TO SINGULAR ROWS  IN SEQUENCE
C     TF, XF, TS, TCW
      JF1=NS+JF
C  TF
      AA(JF1,N+1)=F(JF)*(CPF)/(CP(JF)*HLDUP(JF))
C  XF
      AA(JF,N+2)=F(JF)/HLDUP(JF)
C  TS
      AA(NS+1,N+3)=UMRP/(CP(1)*HLDUP(1))
C  TCW
      AA(L6,N+4)=V(L)/HLDUP(NS)
      DO 802 I=1,KKK
      NI=N+I
  802 WRITE(34) (AA(J,NI),J=1,N)
      IF(NOPR.EQ.2) RETURN
      WRITE(3,223)
      WRITE(3,24) (BBB,I,I=1,NS),(CCC,I,I=1,NS)
      WRITE(3,507)
      WRITE(3,14) (AA(1,I),I=1,NLIM)
      DO 1517 J=2,L
 1517 WRITE(3,10) J,(AA(J,I),I=1,NLIM)
      WRITE(3,20) NS,(AA(NS,I),I=1,NLIM)
      WRITE(3,21) (AA(NS+1,I),I=1,NLIM)
      DO 1522 J=2,L
      J1=NS+J
 1522 WRITE(3,10) J,(AA(J1,I),I=1,NLIM)
      WRITE(3,20) NS,(AA(L6  ,I),I=1,NLIM)
      WRITE(3,27) (AA(I,N+1),I=1,NLIM)
      WRITE(3,28) (AA(I,N+2),I=1,NLIM)
      WRITE(3,30) (AA(I,N+3),I=1,NLIM)
      WRITE(3,31) (AA(I,N+4),I=1,NLIM)
 9002 CONTINUE
      RETURN
C
C     MODEL 3   SIMILAR TO MODEL OF LAMB ET. AL.
C
  333 CONTINUE
      DO 9003 IDUM=1,1
C     SET UP COEFFICIENTS IN MATRIX FOR STATE SPACE FORMULATION
C     COLUMNS ARE ARRANGED WITH ELEMENTS IN THE FOLLOWING SEQUENCE
C     HOLDUPS (2 THROUGH L),  COMPOSITIONS (1 THROUGH NS),
C     INPUTS ARE F, TF, XF, R, V(0)
  334 FORMAT(////40X,28H MODEL 3 - COMP AND MASS BAL///)
      N=2*NS-2
      NLIM=N
      KKK=5
      FORM=1.0
      WRITE(34) FORM,N,KKK
      WRITE(34) (AAA,I,I=2,L ),(BBB,I,I=1,NS),
     1 (DDD,I,I=1,5)
  607 FORMAT(1H1,40X,34HCOEFFICIENTS OF STATE SPACE MATRIX//////,50X,
     116HHOLDUP EQUATIONS///)
C  HOLDUP EQNS
C     NO HOLDUP EQUATION FOR REBOILER
      DO 609 J=2,L
      J1=NS+J-3
      J2=NS+J-2
      J3=NS+J-1
      J34=NS+J
      AA(J-1,J-1)=-GAM(J)
      AA(J-1,J) = GAM(J+1)
  609 CONTINUE
C  COMPOSITION EQNS
      L1=NS+L-3
      L2=NS+L-2
      L3=NS+L-1
      AA(L,1)=(GAM(2)*(X(1,2)-X(1,1))                              )/HLDUP(1)
      AA(L  ,L  )=(                        -AL(1)-V(1)*ZETA(1))/HLDUP(1)
      AA(L  ,NS  )=(                         +AL(2))/HLDUP(1)
      DO 617 J=2,L
      J1=NS+J-3
      J2=NS+J-2
      J3=NS+J-1
      J34=NS+J
      AA(J2,J     )=(GAM(J+1)*(X(1,J+1)-X(1,J))                     )/
     2HLDUP(J)
      AA(J2,J1)=(V(J-1)*ZETA(J-1)/E(J-1)                           )/HLDUP
     2(J)
      AA(J2  ,J2)=(                                               -AL(J)
     1 -V(J)*ZETA(J)/E(J)-V(J-1)*ZETA(J-1)*(1.-E(J-1))/E(J-1))
     2 /HLDUP(J)
      AA(J2  ,J3)=(                        +AL(J+1))/HLDUP(J)
     1+                                          (+V(J)*ZETA(J)*(1.-E(J))
     2 /E(J))/HLDUP(J)
  617 CONTINUE
      AA(L3,L2)=V(L)*ZETA(L)/(E(L)*HLDUP(NS))
      AA(L3,L3)=-V(L)*(1.+ZETA(L)*(1.-E(L))/E(L))/HLDUP(NS)
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      WRITE(34) ((AA(I,J),J=1,N),I=1,N)
C     PREPARE VECTORS OF B MATRIX  IN SEQUENCE
C     F, XF, AL(NS), TS
      JF1=L+JF-1
      TEMP1=CP(L)*(T(L)-T(NS))/VAPHT(L)
      AA(JF1,N+3) = F(JF)/HLDUP(JF)
      AA(L-1,N+4)=1.+TEMP1
      AA(L2,N+4)=(X(1,NS)-X(1,L)*(1.+TEMP1)+Y(L)*TEMP1)/HLDUP(L)
      DO 620 J=2,L
      J1=L-1+J
      AA(J-1,N+5)=GAM(J+1)*CAPA(J+1)-GAM(J)*CAPA(J)
  620 AA(J1,N+5) = (GAM(J+1)*CAPA(J+1)*(X(1,J+1)-X(1,J))+Y(J-1)-Y(J))
     2/HLDUP(J)
      AA(L,N+5)=(GAM(2)*CAPA(2)*(X(1,2)-X(1,1))+X(1,1)-Y(1))/HLDUP(1)
      TEMP1=CP(JF)*(T(JF)-TF*CPO/VAPHTO)/VAPHT(JF)
      AA(JF-1,N+1)=TEMP1*(1.-GAM(JF+1)*CAPA(JF+1))
      TEMP2=F(JF)*CP(JF)/VAPHT(JF)
      AA(JF-1,N+2)=-TEMP2*(1.-GAM(JF+1)*CAPA(JF+1))
      TMP=-Y(JF)+GAM(JF+1)*CAPA(JF+1)*(X(1,JF+1)-X(1,JF))
      AA(JF1,N+1)=(-TMP*TEMP1+XF+TEMP1*(Y(JF-1)-X(1,JF)))/HLDUP(JF)
      AA(JF1,N+2)=TEMP2*(TMP+X(1,JF)-Y(JF-1))/HLDUP(JF)
      JLO=JF+1
      DO 621 J=JLO,L
      TMP=GAM(J+1)*CAPA(J+1)-GAM(J)*CAPA(J)
      AA(J-1,N+1)=TMP*(-TEMP1)
      AA(J-1,N+2)=TMP*TEMP2
      J1=L-1+J
      TMP=(Y(J-1)-Y(J)+CAPA(J+1)*GAM(J+1)*(X(1,J+1)-X(1,J)))/HLDUP(J)
      AA(J1,N+1)=-TMP*TEMP1
  621 AA(J1,N+2)=TMP*TEMP2
      DO 803 I=1,KKK
      NI=N+I
  803 WRITE(34) (AA(J,NI),J=1,N)
      IF(NOPR.EQ.2) RETURN
      WRITE(3,334)
      WRITE(3,24) (AAA,I,I=2,L ),(BBB,I,I=1,NS)
      WRITE(3,607)
      DO 1609 J=2,L
 1609 WRITE(3,10) J,(AA(J-1,I),I=1,NLIM)
      WRITE(3,14) (AA(L ,I),I=1,NLIM)
      DO 1617 J=2,L
      J2=NS+J-2
 1617 WRITE(3,10) J,(AA(J2,I),I=1,NLIM)
      WRITE(3,20) NS,(AA(L3,I),I=1,NLIM)
      WRITE(3,26) (AA(I,N+1),I=1,NLIM)
      WRITE(3,27) (AA(I,N+2),I=1,NLIM)
      WRITE(3,28) (AA(I,N+3),I=1,NLIM)
      WRITE(3,29) (AA(I,N+4),I=1,NLIM)
      WRITE(3,30) (AA(I,N+5),I=1,NLIM)
 9003 CONTINUE
      RETURN
C
C     MODEL 4
C
  444 CONTINUE
      DO 9004 IDUM=1,1
C     SET UP COEFFICIENTS IN MATRIX FOR STATE SPACE FORMULATION
  445 FORMAT(////40X,24H MODEL 4 - COMP BAL ONLY///)
      KKK=1
      FORM=0.
      WRITE(34) FORM,NS,KKK
      WRITE(34) (BBB,I,I=1,NS),(DDD,I,I=1,1)
  707 FORMAT(1H1,40X,34HCOEFFICIENTS OF STATE SPACE MATRIX//////)
C     MAIN DIAG
      A(1)=-(V(1)*ZETA(1)/E(1)+AL(1))/HLDUP(1)
      DO 709 J=2,L
  709 A(J)=-(V(J)*ZETA(J)/E(J)+AL(J)+V(J-1)*ZETA(J-1)*(1.-E(J-1))
     2 /E(J-1))/HLDUP(J)
      A(NS)=-V(L)*(1.+ZETA(L)*(1.-E(L))/E(L))/HLDUP(NS)
  710 FORMAT(/10H MAIN DIAG//,(1X,1P8E14.4))
C     UPPER DIAG
      DO 11 J=1,L
   11 B(J)=(AL(J+1)+V(J)*ZETA(J)*(1.-E(J))/E(J))/HLDUP(J)
   12 FORMAT(/11H UPPER DIAG//,(1X,1P8E14.4))
C     LOWER DIAG
      DO 13 J=2,NS
   13 BP(J-1)=V(J-1)*ZETA(J-1)/(E(J-1)*HLDUP(J))
  714 FORMAT(/11H LOWER DIAG//,(1X,1P8E14.4))
      WRITE(34) (A(I),I=1,N),(B(I),I=1,L),(BP(I),I=1,L)
C  INPUT VECTOR
      AA(JF,N+1)=F(JF)/(HLDUP(JF)*AL(NS))
      WRITE(34) (AA(I,N+1),I=1,N)
   15 FORMAT(///29H COLUMN VECTOR FOR FEED COMP/,(1X,1P8E14.4))
      IF(NOPR.EQ.2) RETURN
      WRITE(3,445)
      WRITE(3,24) (BBB,I,I=1,NS)
      WRITE(3,707)
      WRITE(3,710) (A(I),I=1,NS)
      WRITE(3,12) (B(J),J=1,L)
      WRITE(3,714) (BP(I),I=1,L)
      WRITE(3,15) (AA(I,N+1),I=1,N)
 9004 CONTINUE
  999 RETURN
   24 FORMAT (35HOMATRIX ELEMENTS ORDERED AS FOLLOWS//(1X,29(A2,I2)))
   10 FORMAT(/4H ROW,I3,//,(1X,1P8E14.4))
   14 FORMAT (////48X,21HCOMPOSITION EQUATIONS////,18H  ROW 1   REBOILER
     2//,(1X,1P8E14.4))
   20 FORMAT(/4H ROW,I3,12H   CONDENSER//,(1X,1P8E14.4))
   21 FORMAT(////48X,21HTEMPERATURE EQUATIONS////,18H  ROW 1   REBOILER/
     2/,(1X,1P8E14.4))
   26 FORMAT(///29H COLUMN VECTOR FOR FEED RATE/,
     2(1X,1P8E14.4))
   27 FORMAT(///29H COLUMN VECTOR FOR FEED TEMP/,(1X,1P8E14.4))
   28 FORMAT(///29H COLUMN VECTOR FOR FEED COMP/,(1X,1P8E14.4))
   29 FORMAT(///30H COLUMN VECTOR FOR REFLUX RATE/,(1X,1P8E14.4))
   30 FORMAT(///32H COLUMN VECTOR FOR REBOILER DUTY/(1X,
     21P8E14.4))
   31 FORMAT(///39H COLUMN VECTOR FOR CONDENSER WATER TEMP/
     2,(1X,1P8E14.4))
      END
```

```
$IBFTC EIGMA.  DECK,SDD
C  PROGRAM FOR CONTROL OF CALCULATION OF EIGENVALUES AND EIGENVECTORS
      SUBROUTINE EIGMAN(KCALC,IMOD)
      COMMON /EIGCOM/ AA(70,70),R(70),RI(70),N,K,MATFAC,VECT(140)
      COMMON /CCHAR/ A(70),B(70),BP(70),GP(71),FORM
      COMMON /CXZERO/ XZERO(70)
      COMMON /CEIG/ VTST,IOPT,JOPT
      DIMENSION COEFF(71),ROOT(70),U(70),D(6),NRESP(25)
      DIMENSION BB(16,16)
      EQUIVALENCE (BB,A)
      DOUBLE PRECISION SUMD
      COMPLEX COEFF,ROOT,Z
      INTEGER TCHK,U,RLCK,E
      EQUIVALENCE (DTNT,R(1))
      DATA ZERO,IBY,NOTIM/1.0E-30,1,1/
      DATA EPS/0146400000000/
      NDIM = 70
      CALL TIME(TIM)
      WRITE(3,850) TIM
  850 FORMAT(///18H BEGIN EIG   TIME ,F7.2)
    1 TEST = 0.
C     NATURE OF MATRIX INDICATED BY VALUE OF FORM
      IF(KCALC.EQ.4) GO TO 450
      READ (34) FORM,N,K
      GO TO 451
C  CARD INPUT OF MATRIX IF NOT ALREADY READ BY DERIV
  450 READ(2,300) FORM,N,K
  451 NORM=FORM
      IF(VTST.EQ.0.) VTST=1.0E07
      IP=N+K
      IBP=N
      IF(KCALC.EQ.4) GO TO 452
      IP2=2*IP
      READ (34) (VECT(I),I=1,IP2)
      REWIND 5
C  CONVERT STATE VECTOR LABELS TO PROPER FORMAT
      IF(JOPT.NE.99) GO TO 456
      WRITE(5,457) (VECT(I),I=1,IP2)
  457 FORMAT(A2,A2)
      GO TO 458
  456 WRITE(5,461) (VECT(I),I=1,IP2)
  461 FORMAT(A2,I2)
  458 REWIND 5
      READ(5,462) (VECT(I),I=1,IP)
  462 FORMAT(A4)
      GO TO 453
  452 READ(2,312) (VECT(I),I=1,IP)
  453 NN=N+1
      M=N-1
      IF(KCALC.EQ.4) GO TO 454
C  FOR MATRIX ALREADY ON TAPE
      CALL INPUTB
      GO TO 455
C  FOR CARD INPUT
  454 CALL INPUT
  455 CONTINUE
  103 CALL TIME(TIM)
      WRITE(3,851) TIM
  851 FORMAT(///21H BEGIN EIGVAL   TIME ,F7.2)
      IF (IMOD.NE.3) GO TO 902
C  SPECIAL EIGENVALUE CALC FOR MODEL 3, PARTITIONED MATRIX
C  SEE APPENDIX A.3
  800 NH=(N-2)/2
      NC=NH+2
      IF (NC.GT.16) GO TO 902
      DO 801 J=1,NC
      JC = J + NH
      DO 801 JJ=1,NC
      JJC=JJ+NH
  801 BB(J,JJ) = AA(JC,JJC)
      CALL QREIG(BB,NC,R,RI,1,16)
      CALL QREIG(AA,NH,A,B,1,NDIM)
      RIEN = +0.
      TST = 0.
      DO 802 J=1,NH
      JH= J+NC
      R(JH) = A(J) + RIEN
      RI(JH) = B(J)
      TST = TST + 1.0
  802 RIEN = RIEN - SIGN(3.*EPS*TST , RIEN)
      GO TO 22
C  EIGENVALUES BY QR ALGORITHM
  902 CALL QREIG(AA,N,R,RI,1,NDIM)
   22 DO 23 I=1,N
      IF(ABS(R(I)).LT.1.0E-20) GO TO 23
      IF(ABS(RI(I)/R(I)).LE.1.0E-4) RI(I)=0.
   23 CONTINUE
C  PAIR UP CONJUGATES
      IPROD=1
      NVEC=N
      CRIT=0.1
  610 JCON=0
      DO 120 J=1,NVEC
  120 U(J)=1
      IF(NORM.EQ.0) GO TO 600
      DO 505 I=1,NVEC
      IF(U(I).EQ.0.OR.ABS(RI(I)).LT.ZERO) GO TO 505
      DO 502 J=1,N
      IF(ABS((RI(I)+RI(J))/RI(I)).LE.CRIT) GO TO 503
      GO TO 502
  503 IF(U(J).EQ.0) GO TO 502
      JCON=J
      IF(ABS((R(I)-R(JCON))/R(I)).GT.CRIT) GO TO 504
      GO TO 506
  504 JCON=0
  502 CONTINUE
      GO TO 505
C     CONJUGATE IDENTIFIED
  506 U(JCON)=0
      U(I)=0
```

```
  620 RI(JCON)=-RI(I)
      R(JCON)=R(I)
  505 CONTINUE
  600 CONTINUE
C   SORT EIGENVALUES ACCORDING TO MAGNITUDES OF REAL PART
   25 DO 27 I=1,M
      TST=R(I)
      TEM1=RI(I)
      ITMP=U(I)
      DO 26 J=I,N
      IF(ABS(TST).LE.ABS(R(J))) GO TO 26
      TEMP=TST
      TST=R(J)
      R(J)=TEMP
      TEMP=TEM1
      TEM1=RI(J)
      RI(J)=TEMP
      JTMP=ITMP
      ITMP=U(J)
      U(J)=JTMP
   26 CONTINUE
      U(I)=ITMP
      RI(I)=TEM1
   27 R(I)=TST
C   EIGENVALUES ARRANGED IN R(I) AND RI(I)
   50 WRITE(3,712) VTST
  712 FORMAT(//8H VTST = ,E11.4)
      IF(MATFAC.NE.0) WRITE(3,592) MATFAC
  592 FORMAT(//40H ALL MATRIX ELEMENTS DIVIDED BY 8 TO THE ,I3,6H POWER)
      WRITE(3,310)
      WRITE (3,306)
      LIM=N
      IF(MATFAC.EQ.0) GO TO 670
C   RECONSTITUTE THE MATRIX AND EIGENVALUES (FORMERLY SCALED)
      TEMP=8.**MATFAC
      DO 101 I=1,N
      DO 100 J=1,N
  100 AA(I,J)=AA(I,J)*TEMP
      A(I)=A(I)*TEMP
      B(I)=B(I)*TEMP
      BP(I)=BP(I)*TEMP
      R(I)=R(I)*TEMP
  101 RI(I)=RI(I)*TEMP
  670 IKX=0
      TRACE=0.0
      SUMD=1.0
      SOFLO = 1.0
C   CALC SUM AND PROD OF EIGENVALUES , AND PRINT
      DO 32 I=1,N
      TRACE=TRACE+R(I)
      IF(ABS(RI(I)).LT.ZERO) GO TO 30
      IKX=IKX+1
      SUMD=SUMD*CABS(CMPLX(R(I),RI(I)))
      WRITE (3,307)              I,R(I),RI(I)
      GO TO 31
   30 WRITE (3,308)              I,R(I)
      SUMD=SUMD*R(I)
   31 IF(DABS(SUMD).LE.1.0D25) GO TO 32
C   PRODUCT OF ROOTS IS SCALED TO PREVENT OVERFLOW
      SUMD = SUMD/1.0D5
      SOFLO = SOFLO*1.0E5
   32 CONTINUE
      PROD=SNGL(SUMD)
      WRITE (3,328) TRACE,PROD,SOFLO
      CALL TIME(TIM)
      WRITE(3,852) TIM
  852 FORMAT(///21H BEGIN EIGVEC   TIME ,F7.2)
C     CALCULATE EIGENVECTORS
   40 WRITE (3,313)
   42 WRITE(3,314)
      LV=1
      REWIND 34
      R1=R(1)
      IF (ABS(R1) .LT. 1.0E-5) R1 = R(LIM)/VTST
      DO 60 I=1,LIM
      I=I
      E=1
      IF (ABS(R(I)/R1) .GT. VTST) GO TO 60
      IF (U(I) .NE. 0) GO TO 760
      IF(I.EQ.1) GO TO 740
      IF(ABS(R(I)-R(I-1)).LE.ZERO) GO TO 160
  740 E=2
  760 CALL EIGVEC(R(I),RI(I),I,E)
  160 LV=LV+1
      IF(LV.GT.35) GO TO 111
      CALL TIMREM(TIM)
C   THROW OFF IF INSUFFICIENT TIME LEFT
      IF(TIM.LT.0.01*FLOAT(N)) GO TO 511
   60 CONTINUE
      GO TO 111
  511 NOTIM=2
  111 NVEC=LV-1
      E=NVEC
      LV=NVEC
      CALL TIME(TIM)
  853 FORMAT(///19H END EIGVEC   TIME ,F7.2)
      REWIND 34
C   PRINT EIGENVECTORS AND CHECK
      CALL VECIO(NVEC)
      WRITE(3,853) TIM
   99 CONTINUE
      IF(JOPT.EQ.99) KCALC=5
C   STORE A MATRIX
      WRITE(4) ((AA(I,J),J=NN,IP),I=1,N)
      REWIND 4
  715 CALL TIME(TIM)
      WRITE(3,854) TIM
  854 FORMAT(///16H END EIG   TIME ,F7.2)
      RETURN
  300 FORMAT(F10.2,2I10,F10.2,2I10)
```

```
306 FORMAT (//9H ROOT NO.,10X,4HREAL,14X,9HIMAGINARY//)
307 FORMAT (3X,I3,8X,1PE12.5,8X,E12.5)
308 FORMAT (3X,I3,8X,1PE12.5)
310 FORMAT (1H1,11HEIGENVALUES)
312 FORMAT (15A4)
313 FORMAT (1H1,43HEIGENVALUES WITH CORRESPONDING EIGENVECTORS/////)
314 FORMAT(7X,10HEIGENVALUE,18X,22HEIGENVECTOR COMPONENTS)
328 FORMAT(///16H SUM OF ROOTS  =,1PE15.7,/16H PROD OF ROOTS =,E15.7,
   2 5H  X  ,E7.0)
    END
```

```
$IBFTC ALOC.   DECK
CALOC
C  FINDS BEGINNING OF INPUT FOR EIGMA. ON UN34
      SUBROUTINE ALOC(KCALC)
      IF(KCALC.EQ.2) GO TO 100
      RETURN
  100 REWIND 34
      READ (34) N
      READ (34) (DUM,I=1,N)
      RETURN
      END
```

```
$IBFTC XZERO.  DECK
CXZERO
C  CALCULATES INITIAL STATE VECTOR BY DIFFERENCE BETWEEN
C  TWO STEADY STATES     CALLED BY EXEC
      SUBROUTINE XZERO(NOTFSS,KCALC)
      DIMENSION X1(70),X2(70)
      COMMON /CXZERO/X2
      READ (34) N
      READ (34) (X1(I),I=1,N)
      IF(KCALC.EQ.5) GO TO 200
      READ (34) N
      READ (34) (X2(I),I=1,N)
      DO 100 I=1,N
  100 X2(I)=X1(I)-X2(I)
      IF(NOTFSS.EQ.0) GO TO 103
  102 READ(34) N
      READ (34) (X1(I),I=1,N)
  103 WRITE(3,101) (X2(I),I=1,N)
  101 FORMAT(1H1,28HINITIAL STATE VECTOR (XZERO)///,(10(2X,1PE10.3)))
      RETURN
  200 IF(NOTFSS.EQ.0) RETURN
      READ(3,201) (X2(I),I=1,N)
  201 FORMAT(9E8.4)
      GO TO 103
      END
```

```
$IBFTC DET.    DECK
      FUNCTION DET(B,N,A)
C  NOTE DET IS SCALED BY FACTORS OF 1.0E5 TO AVOID OVERFLOWS
C  SCALING IS NOT PRINTED OR FLAGGED
      DIMENSION B(70,70),A(N,N)
C     CALCULATES DETERMINANT OF MATRIX B
C     MATRIX A USED FOR SCRATCH
      NLIM=N-1
      D=1.0
      DO 10 I=1,N
      DO 10 J=1,N
   10 A(I,J)=B(I,J)
      DO 120 I=1,NLIM
```

```
      LOW=I+1
      TEST=ABS(A(I,I))
      JROW=I
      SGN=1.0
      DO 30 J=LOW,N
      IF(ABS(A(J,I)).LE.TEST) GO TO 30
      JROW=J
      TEST=ABS(A(J,I))
   30 CONTINUE
      IF(A(JROW,I).EQ.0.0) GO TO 140
      IF(JROW.EQ.I) GO TO 90
   40 SGN=-1.0
      DO 50 J=I,N
      TEMP=A(I,J)
      A(I,J)=A(JROW,J)
   50 A(JROW,J)=TEMP
   90 D=D*A(I,I)*SGN
      IF(ABS(D).GT.1.0E25) D=D/1.0E5
      DO 110 J=LOW,N
      DO 100 K=LOW,N
  100 A(J,K)=A(J,K)-A(I,K)*A(J,I)/A(I,I)
  110 CONTINUE
  120 CONTINUE
  130 DET=D*A(N,N)
      RETURN
  140 DET=0.0
      RETURN
      END


$IBFTC INPUB.  DECK,SDD
CINPUTB
C  SUBROUTINE TO TREAT INPUT DATA FOR EIGENSYSTEM CALCS
C  INPUT DATA ON UN34 FROM PRIOR CALCS
      SUBROUTINE INPUTB
      COMMON /EIGCOM/ AA(70,70),R(70),RI(70),N,K,MATFAC,VECT(140)
      COMMON /CCHAR/ A(70),B(70),BP(70),GP(71),FORM
      DIMENSION DUM(70,70)
      EQUIVALENCE (DTNT,R(1))
      MATFAC=0
      NP=N
      M=N-1
      NN=N+1
      NORM=FORM
      DO 6 L=1,N
    6 BP(L)=1.0
      IP=N+K
      IF(NORM.EQ.4) GO TO 35
    1 IF(NORM.EQ.1) GO TO 10
C  TRIDIAGONAL MATRIX
      READ(34)  (A(I),I=1,N),(B(I),I=1,M),(BP(I),I=1,M)
      WRITE (3,317)
      WRITE (3,318)              (A(I),I=1,N)
      WRITE(3,319) (B(I),I=1,M)
      WRITE(3,320) (BP(I),I=1,M)
      DO 200 J=1,N
      DO 200 L=1,N
  200 AA(J,L)=0.
      DO 201 J=1,M
      AA(J,J)=A(J)
      AA(J+1,J)=BP(J)
  201 AA(J,J+1)=B(J)
      AA(N,N)=A(N)
      DTNT=DET(AA,N,DUM)
      GO TO 20
C     OPERATE ON GENERAL NXN MATRIX
   10 READ(34)  ((AA(I,J),J=1,N),I=1,N)
   12 WRITE (3,321)
      DO 11 L=1,N
   11 WRITE (3,322)              (AA(L,J),J=1,N)
C     MATRIX ARRANGED BY ROWS
      DTNT=DET(AA,N,DUM)
   13 DPROD=AA(1,1)
      DO 18 I=2,N
      DPROD=DPROD*AA(I,I)
      IF(DPROD.GT.1.0E15) GO TO 14
   18 CONTINUE
      GO TO 19
   14 MATFAC=MATFAC+1
      DO 15 I=1,N
      DO 15 J=1,N
   15 AA(I,J)=AA(I,J)/8.
      GO TO 13
   19 CONTINUE
   20 TRACE=0.0
      DO 120 I=1,N
  120 TRACE=TRACE+AA(I,I)
      TRACE=TRACE*8.**MATFAC
      WRITE(3,311) TRACE,DTNT
      IF(K.EQ.0) GO TO 4
      DO 103 I=1,K
      NI=N+I
   40 READ(34)  (AA(J,NI),J=1,N)
  103 CONTINUE
      WRITE(3,309) ((AA(J,NI),J=1,N),NI=NN,IP)
    4 WRITE(3,310) FORM,N,K
      RETURN
C     BAND MATRIX
   35 WRITE(3,31)
   31 FORMAT(17H TRIED BAND INPUT)
      CALL EXIT
      RETURN
  100 FORMAT(6E12.5)
  301 FORMAT (7F10.5)
  302 FORMAT (7F10.5)
  309 FORMAT(37H1B MATRIX  (NON-AUTONOMOUS RELATIONS)//,(1P7E16.5))
  310 FORMAT(//7H FORM =,F6.1,5H  N =,I3,5H  K =,I3//)
  311 FORMAT(//30X,7HTRACE =,1PE15.7/,24X,13HDETERMINANT =,E15.7)
  317 FORMAT(1H1,24HTRIDIAGONAL INPUT MATRIX///)
```

```
  318 FORMAT( 2H A,1P7E15.5/,(2X,7E15.5))
  319 FORMAT(/2H B,1P7E15.5/,(2X,7E15.5))
  320 FORMAT(/2H C,1P7E15.5/,(2X,7E15.5))
  321 FORMAT(1H1,29HA MATRIX  (AUTONOMOUS SYSTEM)///)
  322 FORMAT(/(1P7E16.5))
      END


$IBFTC INPUT.  DECK,SDD
CINPUT
C  SUBROUTINE TO TREAT INPUT DATA FOR EIGENSYSTEM CALCS
C  INPUT DATA ON CARDS
      SUBROUTINE INPUT
      COMMON /EIGCOM/ AA(70,70),R(70),RI(70),N,K,MATFAC,VECT(140)
      COMMON /CCHAR/ A(70),B(70),BP(70),GP(71),FORM
      DIMENSION DUM(70,70)
      EQUIVALENCE (DTNT,R(1))
      MATFAC=0
      NP=N
      M=N-1
      NN=N+1
      NORM=FORM
      DO 6 L=1,N
    6 BP(L)=1.0
      IP=N+K
      IF(NORM.EQ.4) GO TO 35
      IF(NORM.GT.4) GO TO 32
    1 IF(NORM.EQ.1) GO TO 10
C  TRIDIAGONAL MATRIX
      READ(2,301) (A(I),I=1,N),(B(I),I=1,M),(BP(I),I=1,M)
      WRITE (3,317)
      WRITE (3,318)              (A(I),I=1,N)
      WRITE(3,319) (B(I),I=1,M)
      WRITE(3,320) (BP(I),I=1,M)
      DO 200 J=1,N
      DO 200 L=1,N
  200 AA(J,L)=0.
      DO 201 J=1,M
      AA(J,J)=A(J)
      AA(J+1,J)=BP(J)
  201 AA(J,J+1)=B(J)
      AA(N,N)=A(N)
      DTNT=DET(AA,N,DUM)
      GO TO 20
C     OPERATE ON GENERAL NXN MATRIX
   10 READ (2,302)            ((AA(I,J),J=1,N),I=1,N)
   12 WRITE (3,321)
      DO 11 L=1,N
   11 WRITE (3,322)              (AA(L,J),J=1,N)
C     MATRIX ARRANGED BY ROWS
      DTNT=DET(AA,N,DUM)
   13 DPROD=AA(1,1)
      DO 18 I=2,N
      DPROD=DPROD*AA(I,I)
      IF(DPROD.GT.1.0E15) GO TO 14
   18 CONTINUE
      GO TO 19
   14 MATFAC=MATFAC+1
      DO 15 I=1,N
      DO 15 J=1,N
   15 AA(I,J)=AA(I,J)/8.
      GO TO 13
   19 CONTINUE
   20 TRACE=0.0
      DO 120 I=1,N
  120 TRACE=TRACE+AA(I,I)
      TRACE=TRACE*8.**MATFAC
      WRITE(3,311) TRACE,DTNT
      IF(K.EQ.0) GO TO 4
      DO 103 I=1,K
      NI=N+I
    3 IF(NORM.NE.5) GO TO 40
      READ(2,100) (AA(J,NI),J=1,N)
      GO TO 103
   40 READ(2,301) (AA(J,NI),J=1,N)
  103 CONTINUE
      WRITE(3,309) ((AA(J,NI),J=1,N),NI=NN,IP)
    4 WRITE(3,310) FORM,N,K
      RETURN
   32 DO 34 I=1,N
   34 READ(2,100) (AA(I,J),J=1,N)
      GO TO 12
C     BAND MATRIX
   35 WRITE(3,31)
   31 FORMAT(17H TRIED BAND INPUT)
      CALL EXIT
      RETURN
  100 FORMAT(6E12.5)
  301 FORMAT (7F10.5)
  302 FORMAT (7F10.5)
  309 FORMAT(37H1B MATRIX  (NON-AUTONOMOUS RELATIONS)//,(1P7E16.5))
  310 FORMAT(//7H FORM =,F6.1,5H  N =,I3,5H  K =,I3//)
  311 FORMAT(//30X,7HTRACE =,1PE15.7/,24X,13HDETERMINANT =,E15.7)
  317 FORMAT(1H1,24HTRIDIAGONAL INPUT MATRIX///)
  318 FORMAT( 2H A,1P7E15.5/,(2X,7E15.5))
  319 FORMAT(/2H B,1P7E15.5/,(2X,7E15.5))
  320 FORMAT(/2H C,1P7E15.5/,(2X,7E15.5))
  321 FORMAT(1H1,29HA MATRIX  (AUTONOMOUS SYSTEM)///)
  322 FORMAT(/(1P7E16.5))
      END
```

```
$IBFTC QREIG.  DECK,DD
C QR ALGORITHM OF B. PARLETT - NINE SUBROUTINES
      SUBROUTINE QREIG(P,NN,R,RI,NPR,ND  )
      DIMENSION P(ND  ,ND  ),R(NN),RI(NN)
      DIMENSION A(70,70),V(70),D(70),L(70),F(70),G(70),VR(70),VI(70),
     2COND(70)
      INTEGER EQUIL,CONDS
C  TO SAVE SPACE WHEN CONDS = 0,  EQUIVALENCE (L,F,G,VR,VI,COND)
      DATA EQUIL,NPERM,CONDS,NPRINT/1,1,1,1/
      N=NN
      NDIM=70
   10 DO 20 I=1,N
      DO 20 J=1,N
   20 A(J,I)=P(J,I)
C VALU(N,2) CONTAINS ROOTS AS 2 VECTORS
C CONDS = 0 OR 1    1 FOR CONDITION NUMBERS
C      EQUIL,NPERM,AND NPRINT MUST BE 0 OR 1.
C       IF EQUIL =1 THE MATRIX WILL BE BALANCED.
C       IF NPERM =1, MATRIX COLUMNS ARE ORDERED SO THEIR LENGTHS DECREASE
C       IF NPRINT =0 ONLY THE EIGENVALUES ARE PRINTED.
C
      NPRINT=NPR
      IF(NPR.EQ.0) GO TO 40
      PRINT 8000,EQUIL,NPERM,CONDS
   40 CONTINUE
      CALL TIME(T)
      CALL SPCTRM(A,R,RI,NN,NDIM,V,D,ANORM,SPURA,SPURB,EQUIL,NPERM,
     2 CONDS,NPRINT,L,F,G,VR,VI,COND)
      IF(NPR.EQ.0) GO TO 70
      CALL TIME(S)
      TT=S-T
      SUM=0.0
      DO 65 J=1,N
   65 SUM=SUM+V(J)
      AV=SUM/FLOAT(N)
      PRINT 7000, SPURA,SPURB,AV,TT,ANORM
      PRINT 6000,(R(I),RI(I),V(I),COND(I),I=1,N)
   70 RETURN
 6000 FORMAT (7X,9HREAL PART 9X,10HIMAG. PART 19X  9HCONDITION //
     1(1X2E18.9,F6.0,E19.4))
 7000 FORMAT (//21HTRACE OF THE MATRIX =E17.9/20HSUM OF EIGENVALUES = E1
     17.9/20HITS PER EIGENVALUE = F6.2/ 18HTIME TAKEN (MIN) = E15.4/
     26HNORM = E17.9)
 8000 FORMAT(1H1,20X 67HTHE QR ALGORITHM APPLIED TO A REAL MATRIX WITH
     1EQUIL,NPERM,CONDS = ,3I3//)
      END


$IBFTC SPCTR.  DECK,SDD
      SUBROUTINE SPCTRM(A,VALR,VALI,NSUB,NDIM,V,D,ANORM,SPURA,SPURB,
     1 EQUIL,NPERM,CONDS,NPRINT,L,F,G,VR,VI,COND)
      DIMENSION A(NDIM,NDIM),VALR(NDIM),VALI(NDIM),V(NDIM),D(NDIM),
     1 L(NDIM), F(NDIM), G(NDIM), VR(NDIM), VI(NDIM), COND(NDIM)
      INTEGER EQUIL,CONDS
      DATA EPS,ZERO/1.0E-11,1.0E-36/
C
C PERMUTE ROWS AND COLS IF DESIRED. REDUCE TO HESSENBERG FORM
C AND THEN USE THE QR TRANSFORMATION.
C
      N=NSUB
      DO 1 J=1,N
    1 D(J)=1.
      IF (EQUIL.EQ.0) GO TO 5
      CALL BALANC(A,VALR,VALI,V,D,NDIM,N,N,0)
    5 CONTINUE
      SPURA=0.
      DO 10 J=1,N
      SPURA=SPURA+A(J,J)
      V(J)=0.
      DO 10 I=1,N
   10 V(J)=V(J)+A(I,J)**2
C
      IF (NPERM.NE.1) GO TO 70
   20 DO 60 J=1,N
      T=0.
      DO 40 I=J,N
      IF (V(I).LE.T) GO TO 40
   30 T=V(I)
      JMAX=I
   40 CONTINUE
      IF (T.LE.4.*V(J)) GO TO 60
   50 CALL XCHANG(A,N,NDIM,J,JMAX)
      T=V(J)
      V(J)=V(JMAX)
      V(JMAX)=T
   60 CONTINUE
   70 CALL SUBDIA(A,N,NDIM,VALI,VALR)
      ANORM=0.
      DO 80 J=1,N
   80 ANORM=ANORM+V(J)
      ANORM=SQRT(ANORM)
      DEL=EPS*ANORM
      CALL QRMETH(A,VALR,VALI,N,NDIM,V,DEL,NPRINT,CONDS)
      IF(CONDS.EQ.0) GO TO 85
      CALL CONDIT(A,VALR,VALI,N,NDIM,DEL,ZERO,L,F,G,VR,VI,COND)
   85 CONTINUE
      SPURB=0.
      DO 90 J=1,N
   90 SPURB=SPURB+VALR(J)
      RETURN
      END


$IBFTC BALNC.  DECK
      SUBROUTINE BALANC(A,VALR,VALI,COUNT,D,NDIM,NIN,NOUT,IS)
      DIMENSION A(NDIM,NDIM),VALR(NDIM),VALI(NDIM),D(NDIM),COUNT(NDIM)
C
C     BALANCE THE MATRIX BY DIAGONAL SIMILARITY TRANSFORMATIONS.
```

```
C
       N=NIN
       NOUT=NIN
      IF (IS .NE. 0) GOTO 2
      DO 1 J=1,N
      D(J)=1.0
    1 CONTINUE
    2 DO 7 J=1,N
    3  ROW=0.0
       COL=0.0
      DO 4 K=1,N
      IF (J .EQ. K) GOTO 4
      IF(ABS(A(J,K)).GT.ROW)ROW=ABS(A(J,K))
      IF(ABS(A(K,J)).GT.COL)COL=ABS(A(K,J))
    4 CONTINUE
       IF (ROW.NE.0. .AND. COL.NE.0.) GO TO 5
      IF (J .GT. NOUT) GOTO 8
      CALL XCHANG(A,N,NDIM,J,NOUT)
      VALR(NOUT)=A(N,N)
      VALI(NOUT)=0.
      COUNT(NOUT)=0.
      NOUT=NOUT-1
      GOTO 3
    5 CONTINUE
      Q=COL/ROW
      Q=0.5*ALOG(Q)/ALOG(2.0)
       IF (Q.LT.0.)M=Q-0.5
       IF (Q.GE.0.)M=Q+0.5
      D(J)=D(J)*(2.**M)
      IF (M .EQ. 0) GOTO 7
      DO 6 K=1,N
      A(J,K)=A(J,K)*(2.**M)
      A(K,J)=A(K,J)/(2.**M)
    6 CONTINUE
    7 CONTINUE
    8 DO 9 K=1,NOUT
      D(K)=D(K)/D(NOUT)
    9 CONTINUE
   10 RETURN
      END


$IBFTC XCHNG.  DECK
      SUBROUTINE XCHANG(A,N,NDIM,I,K)
      DIMENSION A(NDIM,NDIM)
C     INTERCHANGE ROWS AND COLUMNS I AND K OF NXN MATRIX A
      ENTRY XCHAN2
       IF (I.EQ.K) GO TO 3
   10 NSUB=N
      DO 1 L=1,NSUB
      T=A(I,L)
      A(I,L)=A(K,L)
    1 A(K,L)=T
      DO 2 L=1,NSUB
      T=A(L,I)
      A(L,I)=A(L,K)
    2 A(L,K)=T
    3 RETURN
C
C
      END


$IBFTC HESS.  DECK
      SUBROUTINE SUBDIA(A,NSUB,NDIM,QVEC,WVEC)
      DIMENSION A(NDIM,NDIM),QVEC(NDIM),WVEC(NDIM)
C
C     HOUSEHOLDER REDUCTION OF REAL MATRIX TO UPPER HESSENBERG FORM
C
      EQUIVALENCE  (SUM,SCALAR) ,(TEMP,DIV)
C
      N=NSUB
      DO 200 I=1,N
C
C     REDUCE COLUMN OF MATRIX
C
      WVEC(I)=0.0
      I1=I+1
      I2=I1+1
      SUM=0.0
      DO 70 J=I2,N
   70 SUM=SUM+A(J,I)**2
       IF (SUM.EQ.0.) GO TO 200
   75 J=I1
      TEMP=A(J,I)
      SUM=SQRT(SUM+ TEMP  **2)
      A(J,I )=-SIGN(SUM, TEMP  )
      WVEC(J)=SQRT( 1.0+ABS( TEMP)/SUM)
      DIV=SIGN(    WVEC(J )*SUM, TEMP  )
      DO 85 J=I2,N
   85 WVEC(J)=A(J,I)/DIV
      SCALAR=0.0
      DO 95 J=I1,N
      QVEC(J)=0.0
      DO 90 K=I1,N
   90 QVEC(J)=QVEC(J)+A(K,J)*WVEC(K)
      SCALAR=SCALAR +QVEC(J)*WVEC(J)
   95 CONTINUE
      SCALAR=SCALAR/2.0
      DO 120 J=I1,N
      QVEC(J)= QVEC(J)-SCALAR*WVEC(J)
      DO 120 K=I1,N
      A(K,J)=A(K,J)-WVEC(K)*QVEC(J)
  120 CONTINUE
      DO 180 K=1,N
      QVEC(K)=-SCALAR*WVEC(K)
      DO 170 J=I1,N
  170 QVEC(K)=QVEC(K)+A(K,J)*WVEC(J)
```

```
      DO 180 J=I1,N
      A(K,J)=A(K,J)-QVEC(K)*WVEC(J)
  180 CONTINUE
C
  200 CONTINUE
C
      RETURN
      END


$IBFTC QRMET.  DECK
      SUBROUTINE QRMETH(A,VALR,VALI,NSUB,NDIM,COUNT,EPS,NPRINT,CONDS)
      DIMENSION A(NDIM,NDIM),VALR(NDIM),VALI(NDIM),COUNT(NDIM)
C
C      THIS SUBROUTINE FINDS THE EVALUES BY ITERATING WITH THE DOUBLE
C      QR ALGORITHM . IT CALCULATES THE SHIFTS FOR THE ALGORITHM
C      AND CALLS THE DETERMINANT SHIFT IF NECESSARY.
C
      INTEGER CONDS
      INTEGER P,Q
      IF (NPRINT.EQ.0) GO TO 5
      PRINT500
    5 N=NSUB
      P=1
      M=0
      DO 10 I=1,N
   10 COUNT(I)=0.
      CALL QQR2(A,N,NDIM,NSUB,EPS,SIG,RHO,Q,P,M,S,CONDS)
       SIG=0.
       RHO=0.
   20 NM1=N-1
         IF (NM1) 170,120,30
   30 NOSHIF=0
      Q=1
       OLDXR=0.
       OLDXI=0.
       OLDYR=0.
       OLDYI=0.
   40  IF (ABS(A(N,NM1)).LE.EPS) GO TO 120
      ANN=A(N,N)
      AN1N1=A(NM1,NM1)
      ADI=A(NM1,N)*A(N,NM1)
      DIF=.5*(AN1N1-ANN)
      DISC=DIF**2+ADI
      D=SQRT(ABS(DISC))
      SUM=DIF+ANN
      PROD=AN1N1*ANN-ADI
      IF (DISC.LE.0.0) GO TO 50
      XR=SUM+SIGN(D,SUM)
      YR=PROD/XR
       XI=0.
       YI=0.
      IF (ABS(ANN-XR).GE.ABS(AN1N1-XR)) GO TO 60
      DIF=XR
      XR=YR
      YR=DIF
      GO TO 60
   50 XR=SUM
      YR=XR
      XI=D
      YI=-D
   60    IF (N.EQ.2.OR.ABS(A(NM1,N-2)).LE.EPS) GO TO 130
      IF (ABS(SUM).LT.100.*EPS.AND.ABS(PROD).LT.100.*EPS) GO TO 90
      X2=XR**2+XI**2
      Y2=YR**2+YI**2
      DX=(XR-OLDXR)**2+(XI-OLDXI)**2
      DY=(YR-OLDYR)**2+(YI-OLDYI)**2
         IF(DX.GE.0.25*X2) GO TO 80
         IF(DY.GE.0.25*Y2) GO TO 70
      SIG=SUM*2.
      RHO=PROD
      GO TO 100
   70 SIG=2.*XR
      RHO=XR**2
      GO TO 100
   80    IF (DY.GE.0.25*Y2) GO TO 90
      SIG=2.*YR
      RHO=YR**2
      GO TO 100
   90 NOSHIF=NOSHIF+1
      IF (NOSHIF.LT.(N-Q+1).AND.NOSHIF.LT.10) GO TO 100
      CALL DTSHIF(A,N,NDIM,Q,SIG,RHO,EPS,VALI)
      NOSHIF=0
  100    IF (NPRINT.EQ.0) GO TO 107
      ANNM1=ABS(A(N,NM1))
      AN1N2=ABS(A(NM1,N-2))
         PRINT 1000,Q,P,M,N,NOSHIF,S,SIG,RHO,ANNM1,AN1N2
  107 CALL QR2
      COUNT(N)=COUNT(N)+1.0
  110 OLDXR=XR
      OLDXI=XI
      OLDYR=YR
      OLDYI=YI
       IF( COUNT(N)-50.) 40,150,150
  120 VALR(N)=A(N,N)
      VALI(N)=0.
      N=N-1
      GO TO 140
  130 VALR(NM1)=XR
      VALI(NM1)=XI
      VALR(N)=YR
      VALI(N)=YI
      N=N-2
  140    IF (N.LE.2.OR.NOSHIF.EQ.0) GO TO 20
      SIG=A(N-1,N-1)+A(N,N)
      RHO=A(N-1,N-1)*A(N,N)-A(N-1,N)*A(N,N-1)
      GO TO 20
  150 PRINT 2000
      DO 160 J=Q,N
```

```
      PRINT 3000,((A(J,L),L=Q,N)
      VALR(J)=3.E+10*EPS
  160 VALI(J)=3.E+10*EPS
      N=Q-1
      GO TO 140
  170 RETURN
  500 FORMAT (/5X 1HQ 4X 1HP 4X 1HM 4X 27H N NOSHIFT SMALLEST SUBDIAG
     15X 5HSIGMA 10X 3HRHO 10X 2HV1 15X 2HV2 //)
 1000 FORMAT(1X,5I5,5X,5E15.3/)
 2000 FORMAT(//51H AFTER 50 ITERATIONS THIS SUBMATRIX IS NOT RESOLVED//)
 3000 FORMAT(1H0,7E17.8)
      END


$IBFTC QRTWO.  DECK
      SUBROUTINE QQR2(A,NSUB,NDIM,NIN,DEL,SIG,RHO,Q,P,M,S,NC)
      DIMENSION A(NDIM,NDIM),GAM(3),PSI(2)
      EQUIVALENCE (GAM,GK,DENOM), (GAM(2),PSI,DIF), (GAM(3),A10),
     1            (KAP,A21), (ALF,A11,A22), (ETA,A12,A32), (I1,L)
C
C       ONE DOUBLE QR ITERATION IS EXECUTED IN THIS SUBROUTINE.
C
      INTEGER P,Q,Q1
      REAL KAP
       RETURN
       ENTRY QR2
      N=NSUB
      N1=N-1
       P=N1-1
       N2=N1-1
      N3=N2-1
       S=3.E+10*DEL
      DO 50 I1=1,N3
      I=N2-I1
   20 A10=A(I+1,I)
      IF (ABS(A10)-DEL) 60, 60, 30
   30 A12=A(I+1,I+2)
      A21=A(I+2,I+1)
      A11=A(I+1,I+1)
      DIF=A11-SIG
      DENOM=DIF*A11+A12*A21+RHO
       IF (DENOM.EQ.0.) GO TO 40
   35 A32=ABS(A(I+3,I+2))
      A22=A(I+2,I+2)
      IF (ABS(A10*A21*(ABS(A22+DIF)+A32)/DENOM)-DEL) 60, 60, 40
   40 P=I
   50 CONTINUE
   60 DO 100 I1=1,P
      I=P+1-I1
      IF (ABS(A(I+1,I))-DEL) 110, 110, 90
   90 Q=I
  100 CONTINUE
  110 DO 300 I=P,N1
       IF (I.NE.P) GO TO 130
  120 DIF=A(I,I)-SIG
      GAM(1)=DIF*A(I,I)+A(I,I+1)*A(I+1,I)+RHO
      GAM(2)=A(I+1,I)*(DIF+A(I+1,I+1))
      GAM(3)=A(I+1,I)*A(I+2,I+1)
      A(I+2,I)=0.0
      GO TO 150
  130 GAM(1)=A(I,I-1)
      GAM(2)=A(I+1,I-1)
      GAM(3)=A(I+2,I-1)
       IF (I.NE.N1) GO TO 150
  140 GAM(3)=0.0
  150 KAP=SIGN(SQRT(GAM(1)**2+GAM(2)**2+GAM(3)**2),GAM(1))
      GK=GAM(1)+KAP
       IF (GK.NE.0.) GO TO 170
  160 ALF=-2.0
      GK=ALF
      GO TO 180
  170 ALF=-GK/KAP
  180 PSI(1)=GAM(2)/GK
      PSI(2)=GAM(3)/GK
       IF (I.EQ.Q) GO TO 220
  190  IF (I.NE.P) GO TO 210
  200 A(I,I-1)=-A(I,I-1)
      GO TO 220
  210 A(I,I-1)=-KAP
         IF (ABS(KAP).GT.S) GO TO 220
         S=ABS(KAP)
         M=I
  220 NX=N+NC*(NIN-N)
      DO 250 J=I,NX
      ETA=ALF*(A(I,J)+PSI(1)*A(I+1,J)+PSI(2)*A(I+2,J))
      A(I,J)=ETA+A(I,J)
      A(I+1,J)=A(I+1,J)+PSI(1)*ETA
      A(I+2,J)=A(I+2,J)+PSI(2)*ETA
  250 CONTINUE
      L=I+2
      IF(L-N) 270, 270, 260
  260 L=N
  270 Q1=Q-NC*(Q-1)
      DO 280 J=Q1,L
      ETA=ALF*(A(J,I)+PSI(1)*A(J,I+1)+PSI(2)*A(J,I+2))
      A(J,I)=ETA+A(J,I)
      A(J,I+1)=A(J,I+1)+PSI(1)*ETA
      A(J,I+2)=A(J,I+2)+PSI(2)*ETA
  280 CONTINUE
      IF (I-N2) 290, 300, 300
  290 ETA=ALF*PSI(2)*A(I+3,I+2)
      A(I+3,I)=ETA
      A(I+3,I+1)=A(I+3,I)*PSI(1)
      A(I+3,I+2)=A(I+3,I+2)+PSI(2)*ETA
  300 CONTINUE
      ANN1=ABS(A(N,N1))
      IF (ANN1.GT.S) GO TO 310
      M=N
      S=ANN1
```

```
  310 RETURN
C
C
      END


$IBFTC DTSHF.  DECK
      SUBROUTINE DTSHIF(A,NSUB,NDIM,M,SIG,RHO,EPS,V)
      DIMENSION  A(NDIM,NDIM),V(NDIM)
C
C THE PRINCIPAL SUBMATRIX CONTAINING A(M,M) THROUGH A(NSUB,NSUB) IS
C SUPPOSED TO HAVE EIGENVALUES OF EQUAL MODULUS.  SHIFT BY THIS MOD.
C
      N=NSUB
      NM1=N-1
      V(M)=1.0
      T=0.
      DO 15 J=M,N
      T=T+A(J,J)
      S=0.
      DO 10 K=M,J
   10 S=S+A(K,J)*V(K)
      IF (J.GE.N) GO TO 18
   15 V(J+1)=-S/A(J+1,J)
   18 DO 20 J=M,NM1
   20 S=S*A(J+1,J)
      IF (ABS(T).GE.EPS) GO TO 23
      T=S
   23 IF (N-M-3) 25,27,30
   25  S=ABS(S)**(1.0/3.0)
      GO TO 35
   27 S=SQRT(SQRT(ABS(S)))
      GO TO 35
   30  S=ABS(S)**(1./FLOAT(N-M+1))
   35 SIG=SIGN(S+S,T)
      RHO=S**2
      RETURN
      END


$IBFTC CONDN.  DECK
      SUBROUTINE CONDIT(A,VALR,VALI,NSUB,NDIM,EPS,ZERO,L,F,G,VR,VI,COND)
      DIMENSION A(NDIM,NDIM),VALR(NDIM),VALI(NDIM),L(NDIM),F(NDIM),
     1 G(NDIM),VR(NDIM),VI(NDIM),COND(NDIM)
C
C THE NSUBXNSUB MATRIX A IS THE FINAL BLOCK TRIANGULAR RESULT OF THE QR
C TRANSFORMATION. THIS PROGRAM FINDS THE CONDITION NUMBERS OF THE EIGEN-
C VALUES (VALU) AND STORES THEM IN COND. EPS IS THE CRITERION FOR ZERO
C FOR A AND ZERO IS APPROXIMATELY THE SMALLEST FLOATING PT. NUMBER WHOSE
C RECIPROCAL DOES NOT CAUSE OVERFLOW
C
      N=NSUB
C
C USE PLANE ROTATIONS TO STANDARDIZE A SO THAT COMPLEX EIGENVALUES COME
C FROM 2X2 SUBMATRICES WITH EQUAL DIAGONAL ELEMENTS AND REAL EIGENVALUES
C COME FROM 1X1 ISOLATED SUBMATRICES
C
      J=2
   10 JM1=J-1
      IF (ABS(A(J,JM1)).LT.EPS) GO TO 45
      DMA=A(J,J)-A(JM1,JM1)
      AJJ1=A(J,JM1)
      AJ1J=A(JM1,J)
      IF ((.5*DMA)**2+AJJ1*AJ1J.GE.0.) GO TO 15
C COMPLEX CASE
      BPC=AJJ1+AJ1J
      T=SQRT(BPC**2+DMA**2)
      C=SQRT(.5*(1.+ABS(BPC)/T))
      S=SIGN(DMA/(2.*C*T),-BPC*DMA)
      GO TO 20
C REAL CASE
   15 T=.5*(DMA+SIGN(VALR(JM1)-VALR(J),DMA))/AJJ1
      S=SIGN(SQRT(1./(1.+T**2)),T)
      C=S*T
C COLUMN OPERATION
   20 DO 25 K=1,J
      AKJ1=A(K,JM1)
      AKJ=A(K,J)
      A(K,JM1)=C*AKJ1-S*AKJ
   25 A(K,J)=S*AKJ1+C*AKJ
C ROW OPERATION
      DO 30 K=JM1,N
      AJ1K=A(JM1,K)
      AJK=A(J,K)
      A(JM1,K)=C*AJ1K-S*AJK
   30 A(J,K)=S*AJ1K+C*AJK
C
C REORDER EIGENVALUES,RECORD ROW LINKAGE L AND UNITARY MATRIX (1 I*F)
C                                                            (I*F 1)*G
C
      IF (ABS(A(J,JM1)).LT.EPS) GO TO 35
      VALI(JM1)=ABS(VALI(JM1))
      VALI(J)=-VALI(JM1)
      L(JM1)=1
      L(J)=-1
      F(J)=VALI(JM1)/A(JM1,J)
      F(JM1)=VALI(JM1)/A(JM1,J)
       G(JM1)=1./SQRT(1.-A(J,JM1)/A(JM1,J))
       G(J)=1./SQRT(1.-A(J,JM1)/A(JM1,J))
      GO TO 40
   35 VALR(JM1)=A(JM1,JM1)
      VALR(J)=A(J,J)
       L(JM1)=0.
       L(J)=0.
       F(JM1)=0.
       F(J)=0.
       G(JM1)=1.
       G(J)=1.
```

```
   40 J=J+2
      GO TO 50
   45  L(J-1)=0.
       F(J-1)=0.
      G(J-1)=1.
      J=J+1
   50 IF (J-N-1) 10,45,55
C
C THE COLUMN AND ROW EIGENVECTORS ARE FOUND BY BACK-SOLVING THE COMPLEX
C TRIANGULAR MATRIX B OBTAINED FROM A
C
   55 CONTINUE
      DO 110 I=1,N
      VALUR=VALR(I)
      VALUI=VALI(I)
      VR(I)=1.
      VI(I)=0.
C NC=0 COMPUTE COLUMN VECTOR,NC=1 COMPUTE ROW VECTOR
      NC=0
   60 VNORM2=1.
      J=I+2*NC-1
   65 IF ( J.LT.1.OR. J.GT.N) GO TO 100
       SR=0.
       SI=0.
      KS=J+1+NC*(I-J-1)
      KF=I+NC*(J-I-1)
      LJ=L(J)
      FJ=F(J)
      GJ=G(J)
      DO 80 K=KS,KF
      LK=L(K)
       INDX1=J+LJ
       INDX2=K+L(K)
      IF (NC.EQ.1) GO TO 70
      BR=G(K)*(A(J,K)+FJ*F(K)*A(INDX1,INDX2))
      BI=G(K)*(F(K)*A(J,INDX2)-FJ*A(INDX1,K))
      GO TO 75
   70 BR=G(K)*(A(K,J)+FJ*F(K)*A(INDX2,INDX1))
      BI=G(K)*(FJ*A(K,INDX1)-F(K)*A(INDX2,J))
   75 SR=SR+GJ*(BR*VR(K)-BI*VI(K))
      SI=SI+GJ*(BR*VI(K)+BI*VR(K))
   80 CONTINUE
      DR=VALUR-VALR(J)
      DI=VALUI-VALI(J)
      D2=DR**2+DI**2
      IF (D2.LT.ZERO*(SR**2+SI**2)) GO TO 85
      IF (D2.EQ.0.) GO TO 90
      VR(J)=(SR*DR+SI*DI)/D2
      VI(J)=(SI*DR-SR*DI)/D2
      GO TO 95
   85 COND(I)=SQRT(1./ZERO)
      GO TO 110
   90  VR(J)=0.
       VI(J)=0.
   95 VNORM2=VNORM2+VR(J)**2+VI(J)**2
      J=J+2*NC-1
      GO TO 65
  100 IF (NC.EQ.1) GO TO 105
      CNORM2=VNORM2
      NC=1
      GO TO 60
  105 COND(I)=SQRT(CNORM2*VNORM2)
  110 CONTINUE
      RETURN
      END
```

```
$IBFTC EIVEC.  DECK,SDD
C SUBROUTINE TO DETERMINE EIGENVECTORS BY INVERSE ITERATION
C COMPLEX DOUBLE PRECISION VERSION
C  COMPLEX CONJUGATE DETERMINED BY DEFINITION
      SUBROUTINE EIGVEC(R,RI,I,E)
      DIMENSION UR(70),UI(70),VR(70),VI(70),B(70,70),V1(70),V2(70)
      DIMENSION ER(70),EI(70),JPR(70)
      COMMON /EIGCOM/ A(70,70),RT(70),RTI(70),N,K,MATFAC,VECT(140)
      DOUBLE PRECISION SR,SI,TR,TI,UR,UI,VR,VI
      DOUBLE PRECISION VMR,VMI,SN,ER,EI,CMR,CMI,CDR,CDI
      INTEGER E
      COMPLEX B,TC,V1,V2
      EQUIVALENCE (V1,UR),(V2,VR)
      CMR(C,TR,TI)=DBLE(REAL(C))*TR-DBLE(AIMAG(C))*TI
      CMI(C,TR,TI)=DBLE(REAL(C))*TI+DBLE(AIMAG(C))*TR
      CDR(TR,TI,C)=(TR*DBLE(REAL(C))+TI*DBLE(AIMAG(C)))/(DBLE(REAL(C))
     2**2+DBLE(AIMAG(C))**2)
      CDI(TR,TI,C)=(TI*DBLE(REAL(C))-TR*DBLE(AIMAG(C)))/(DBLE(REAL(C))
     2**2+DBLE(AIMAG(C))**2)
      DATA TST,RIEN,ZERO/1.0E-8,1.0E-15,1.0E-32/
      DATA CON1,CON2/1.0E-5,1.0E-10/
      ITRANS=1
   10 DO 25 J=1,N
      DO 20 L=1,N
      GO TO (18,19),ITRANS
C  RIGHT EIGENVECTOR
   18 B(J,L)=CMPLX(A(J,L),0.)
      GO TO 20
C  LEFT EIGENVECTOR
   19 B(J,L)=CMPLX(A(L,J),0.)
   20 CONTINUE
   25 B(J,J)=B(J,J)-CMPLX(R,RI)
C FACTOR B BY GAUSSIAN ELIMINATION
C ALGORITHM OF WILKINSON, ALG. EIG. PROB., P. 220
   29 JMAX=1
   31 DO 30 J=2,N
   30 IF(ABS(REAL(B(J,1))).GT.ABS(REAL(B(JMAX,1)))) JMAX=J
      NM1=N-1
      DO 80 J=1,NM1
      JPR(J) = JMAX
      IF (JMAX.EQ.J) GO TO 40
      DO 35 L=1,N
      TC=B(J,L)
      B(J,L)=B(JMAX,L)
   35 B(JMAX,L)=TC
   40 JP1=J+1
      JMAX=J+1
      DO 70 JS=JP1,N
      IF (CABS(B(J,J)).LT.ZERO) GO TO 90
      B(JS,J)=B(JS,J)/B(J,J)
      DO 60 JT=JP1,N
   60 B(JS,JT)=B(JS,JT)-B(JS,J)*B(J,JT)
   70 IF(ABS(REAL(B(JS,J+1))).GT.ABS(REAL(B(JMAX,J+1)))) JMAX=JS
   80 CONTINUE
  100 IF(CABS(B(N,N)).GT.TST) GO TO 200
C END GAUSSIAN ELIMINATION
C BEGIN BACK SUBSTITUTION FOR EIGENVECTOR
C  USED ONLY WHEN LAST PIVOT IS VERY SMALL
      VR(N)=1.0
      VI(N)=0.0
      DO 130 J=2,N
      JI=N-J+1
      VR(JI)=0.0
      VI(JI)=0.0
      SR=0.0
      SI=0.0
      JIP1=JI+1
      DO 110 L=JIP1,N
      SR=SR-CMR(B(JI,L),VR(L),VI(L))
  110 SI=SI-CMI(B(JI,L),VR(L),VI(L))
      IF (CABS(B(JI,JI)).GE.ZERO) GO TO 120
      VR(JI) = 1.0
      VI(JI) = 0.0
      GO TO 130
  120 VR(JI) = CDR(SR,SI,B(JI,JI))
      VI(JI)=CDI(SR,SI,B(JI,JI))
  130 CONTINUE
C END BACK SUBSTITUTION
      GO TO 300
   90 WRITE(3,1) I,ITRANS,J,B(J,J)
    1 FORMAT(7H VECTOR,I3,I3,15H DIAG. ELEMENT ,I3,2H =,1P2E12.4,20X,
     225HVECTOR NOT CALCULATED****)
      GO TO 400
C BEGIN INVERSE ITERATION
  206 IF (DABS(VR(N)).LT.1.0E5) GO TO 95
      DO 204 J=1,N
      VR(J)=VR(J)/1024.
  204 VI(J)=VI(J)/1024.
      GO TO 206
C  ARRANGE RIGHT SIDE ACCORDING TO ROW SHIFTS IN TRIANGULARIZATION
   95 DO 98 J=1,NM1
      IF (JPR(J) .EQ. J) GO TO 96
      JMAX = JPR(J)
      TR = VR(J)
      VR(J) = VR(JMAX)
      VR(JMAX) = TR
      TI = VI(J)
      VI(J) = VI(JMAX)
      VI(JMAX) = TI
   96 JP1 = J + 1
      DO 97 JS=JP1,N
      TR = VR(J)*DBLE(REAL(B(JS,J))) - VI(J)*DBLE(AIMAG(B(JS,J)))
      TI = VI(J)*DBLE(REAL(B(JS,J))) + VR(J)*DBLE(AIMAG(B(JS,J)))
      VR(JS) = VR(JS) - TR
      VI(JS) = VI(JS) - TI
   97 CONTINUE
   98 CONTINUE
      GO TO 205
  200 CON = CON1
      LIM1 = 3
```

```
      LIM2=10
  201 DO 202 J=1,N
      VR(J) = 1.0
      VI(J)=0.0
      UR(J) = 1.0
  202 UI(J)=0.0
      NPAS=1
      JMAX=0
      ITER=1
  205 IF (CABS(B(N,N)).GE.ZERO) GO TO 207
      GO TO 257
C  BACK SUBSTITUTION
  207 TR=VR(N)
      VR(N)=CDR(VR(N),VI(N),B(N,N))
      VI(N)=CDI(TR,VI(N),B(N,N))
  257 DO 210 J=2,N
      JI=N-J+1
      JIPL1=JI+1
      SR=VR(JI)
      SI=VI(JI)
      DO 208 L=JIPL1,N
      SR=SR-CMR(B(JI,L),VR(L),VI(L))
  208 SI=SI-CMI(B(JI,L),VR(L),VI(L))
      IF(CABS(B(JI,JI)).LT.ZERO) GO TO 210
  261 VR(JI) = CDR(SR,SI,B(JI,JI))
      VI(JI)=CDI(SR,SI,B(JI,JI))
  210 CONTINUE
      IF(JMAX.GT.0) GO TO 211
  265 JMAX = 1
      DO 209 J=2,N
  209 IF(DSQRT(VR(J)**2+VI(J)**2).GT.DSQRT(VR(JMAX)**2+VI(JMAX)**2))
     2 JMAX=J
C  DIVIDE BY LARGEST ELEMENT AND GENERATE NEW VECTOR
  211 JOK=0
      SN=DSIGN(1.,UR(JMAX))
      GO TO (212,213),NPAS
  212 VMR=VR(JMAX)*SN
      VMI=VI(JMAX)*SN
      GO TO 214
  213 VMR=(VR(JMAX)+UR(JMAX))*SN
      VMI=(VI(JMAX)+UI(JMAX))*SN
  214 TR=VMR**2+VMI**2
      DO 218 J=1,N
      IF(NPAS.EQ.1) GO TO 215
      VR(J)=VR(J)+UR(J)
      VI(J)=VI(J)+UI(J)
  215 TI=VR(J)
      VR(J)=(VR(J)*VMR+VI(J)*VMI)/TR
      VI(J)=(VI(J)*VMR-TI*VMI)/TR
C  CONVERGENCE CHECK
      IF(DABS(VR(J)).LT.RIEN) GO TO 216
      IF(DABS((VR(J)-UR(J))/VR(J)).GE.CON) GO TO 217
  216 IF(DABS(VI(J)).LT.RIEN) GO TO 218
      IF(DABS((VI(J)-UI(J))/VI(J)).LT.CON) GO TO 218
  217 JOK=JOK+1
  218 CONTINUE
  219 CONTINUE
      IF(JOK.EQ.0) GO TO (225,300),NPAS
      IF(NPAS.EQ.2.AND.ITER.EQ.LIM2) GO TO 240
      GO TO (220,230),NPAS
  220 IF(ITER.EQ.LIM1) GO TO 225
      ITER=ITER+1
  221 DO 222 J=1,N
      UR(J)=VR(J)
  222 UI(J)=VI(J)
      IF(ITER.GT.LIM1/2) CON=CON1*10.
      GO TO 206
C  FIRST TIME THAT NPAS = 2
  225 NPAS=2
      ITER=0
      CON=CON2
  230 DO 235 J=1,N
      SR=UR(J)
      SI=UI(J)
      UR(J)=VR(J)
      UI(J)=VI(J)
      DO 232 L=J,N
      SR=SR-CMR(B(J,L),VR(L),VI(L))
  232 SI=SI-CMI(B(J,L),VR(L),VI(L))
      VR(J)=SR
  235 VI(J)=SI
      ITER=ITER+1
      IF(ITER.GT.LIM2/2) CON=CON2*10.
      GO TO 206
  240 CONTINUE
  241 WRITE(3,2) I,ITRANS
    2 FORMAT(36H ****FAILED TO CONVERGE ON VECTOR  (,I2,I2,1H))
C END INVERSE ITERATION
C BEGIN NORMALIZATION TO UNIT LENGTH
  300 CONTINUE
  301 GO TO (305,325),ITRANS
  305 SR=0.0
      DO 310 J=1,N
  310 SR=SR+VR(J)**2+VI(J)**2
      SR=DSQRT(SR)
      DO 320 J=1,N
      ER(J)=VR(J)/SR
      EI(J)=VI(J)/SR
  320 V1(J)=CMPLX(SNGL(ER(J)),SNGL(EI(J)))
      WRITE(34) (V1(J),J=1,N)
      ITRANS=2
      GO TO 10
C FORM ORTHONORMAL TRANSPOSE EIGENVECTOR
  325 SR=0.0
      SI=0.0
      DO 340 J=1,N
      SR=SR+ER(J)*VR(J)-EI(J)*VI(J)
  340 SI=SI+ER(J)*VI(J)+EI(J)*VR(J)
      DO 350 J=1,N
      TR=VR(J)
```

```
      VR(J)=(VR(J)*SR+VI(J)*SI)/(SR**2+SI**2)
      VI(J)=(VI(J)*SR-TR*SI)/(SR**2+SI**2)
  350 V2(J)=CMPLX(SNGL(VR(J)),SNGL(VI(J)))
      WRITE(34) (V2(J),J=1,N)
      GO TO (400,360),E
C  FIND COMPLEX CONJUGATE VECTORS (RIGHT AND LEFT)
  360 DO 370 J=1,N
      V1(J)=CMPLX(SNGL(ER(J)),SNGL(EI(J)))
      V1(J)=CONJG(V1(J))
  370 V2(J)=CONJG(V2(J))
      WRITE(34) (V1(J),J=1,N)
      WRITE(34) (V2(J),J=1,N)
  400 RETURN
      END



$IBFTC VECIO.  DECK,SDD
C  PRINT EIGENVECTORS AND CHECK
      SUBROUTINE VECIO(NVEC)
      COMMON /CXZERO/ XZERO(70)
      COMMON /EIGCOM/ AA(70,70),R(70),RI(70),N,K,MATFAC,VECT(140)
      DATA ZERO/1.0E-30/
      DIMENSION VM(35,70),VC(35,70),V(70),CFF(70),COEFF(70)
      DOUBLE PRECISION SUMR,SUMI,SUMD,SUME
      COMPLEX VM,VC,CFF,COEFF
      EQUIVALENCE (CFF,COEFF)
      LIM=N
C  VECTORS ON UN34, READ AND PRINT
C  U = VM, V = VC
      DO 39 I=1,NVEC
      READ(34) (VM(I,J),J=1,N)
      READ(34) (VC(I,J),J=1,N)
      ITRAN=1
      IF(ABS(RI(I)).GT.ZERO) GO TO 38
      DO 37 J=1,LIM
   37 V(J)=REAL(VM(I,J))
      WRITE(3,316) R(I)
  761 DO 660 JD=1,LIM,7
      JUP=JD+6
      IF(JUP.GT.LIM) JUP=LIM
      WRITE (3,416) (VECT(J),J=JD,JUP)
      WRITE(3,417) (V(J),J=JD,JUP)
  660 CONTINUE
      GO TO (762,39),ITRAN
  762 DO 661 J=1,LIM
  661 V(J)=REAL(VC(I,J))
      WRITE(3,662)
      ITRAN=2
      GO TO 761
   38 WRITE(3,315) R(I),RI(I)
  763 DO 664 JD=1,LIM,3
      JUP=JD+2
      IF(JUP.GT.LIM) JUP=LIM
      WRITE(3,415) (VECT(J),J=JD,JUP)
      GO TO (764,775),ITRAN
  764 WRITE(3,418) (VM(I,J),J=JD,JUP)
      GO TO 664
  775 WRITE(3,418) (VC(I,J),J=JD,JUP)
  664 CONTINUE
      GO TO (776,39),ITRAN
  776 WRITE(3,662)
      ITRAN=2
      GO TO 763
   39 CONTINUE
C  END PRINTING OF EIGENVECTORS
C  FUNDAMENTAL CHECK OF EIGENVECTORS BY (A - RI)*V
      WRITE(3,700)
  700 FORMAT(1H1,41HCHECK OF PREVIOUS VECTORS BY (A-RI)*V = 0)
  704 TEST=1.0E-6
      DO 710 I=1,NVEC
      IST=0
      ITRAN=1
  701 DO 705 J=1,LIM
      SUMD=0.0
      SUME=0.0
      GO TO (765,766),ITRAN
  765 DO 702 L=1,LIM
      SUMD=SUMD+AA(J,L)*REAL(VM(I,L))
  702 SUME=SUME+AA(J,L)*AIMAG(VM(I,L))
      COEFF(J)=CMPLX(SNGL(SUMD),SNGL(SUME))-CMPLX(R(I),RI(I))*VM(I,J)
      GO TO 767
  766 DO 703 L=1,LIM
      SUMD=SUMD+AA(L,J)*REAL(VC(I,L))
  703 SUME=SUME+AA(L,J)*AIMAG(VC(I,L))
      COEFF(J)=CMPLX(SNGL(SUMD),SNGL(SUME))-CMPLX(R(I),RI(I))*VC(I,J)
  767 IF(ABS(REAL(COEFF(J))).GT.TEST.OR.ABS(AIMAG(COEFF(J))).GT.TEST
     1) IST=1
  705 CONTINUE
      IF(IST.EQ.0) GO TO (709,710),ITRAN
      WRITE(3,706) I
      WRITE(3,707) (COEFF(J),J=1,LIM)
      GO TO (709,710),ITRAN
  709 ITRAN=2
      IST=0
      GO TO 701
  710 CONTINUE
  706 FORMAT(//7H VECTOR,I3,41H YIELDS NONZERO PRODUCT VECTOR AS FOLLOWS
     2)
  707 FORMAT((1X,5(1PE9.2,2H +,E9.2,3HI  )))
  170 CONTINUE
C CHECK FOR CONSISTENCY BY U(T)*V
  210 WRITE(3,327)
  212 DO 74 I=1,NVEC
      DO 72 J=1,NVEC
      SUMR=0.0
      SUMI=0.0
      DO 75 L=1,LIM
```

```
      SUMR=SUMR+REAL(VC(I,L))*REAL(VM(J,L))
      SUMR=SUMR-AIMAG(VC(I,L))*AIMAG(VM(J,L))
      SUMI=SUMI+REAL(VC(I,L))*AIMAG(VM(J,L))
   75 SUMI=SUMI+AIMAG(VC(I,L))*REAL(VM(J,L))
   72 CFF(J)=CMPLX(SNGL(SUMR),SNGL(SUMI))
   73 WRITE(3,328) I,CFF(I),(CFF(J),J=1,NVEC)
   74 CONTINUE
      IF(NVEC.LT.LIM) GO TO 206
C  CHECK FOR CONSISTENCY BY V*U(T), ONLY WHEN NVEC = N
  201 WRITE(3,290)
  203 DO 205 I=1,N
      DO 204 J=1,N
      SUMR=0.0
      SUMI=0.0
      DO 207 L=1,NVEC
      SUMR=SUMR+REAL(VM(L,J))*REAL(VC(L,I))
      SUMR=SUMR-AIMAG(VM(L,J))*AIMAG(VC(L,I))
      SUMI=SUMI+REAL(VM(L,J))*AIMAG(VC(L,I))
  207 SUMI=SUMI+AIMAG(VM(L,J))*REAL(VC(L,I))
  204 CFF(J)=CMPLX(SNGL(SUMR),SNGL(SUMI))
      WRITE(3,328) I,CFF(I),(CFF(J),J=1,NVEC)
  205 CONTINUE
C  STORE EIGENVECTORS AND EIGENVALUES ON UN34 FOR RESPONSE CALCS
C  VC = V, VM = U
  206 REWIND 34
      WRITE(34) NVEC,N,K
      WRITE(34) (R(I),RI(I),I=1,NVEC),((VC(I,J),I=1,NVEC),J=1,N),
     2((VM(I,J),I=1,NVEC),J=1,N),(XZERO(I),I=1,N),(VECT(I),I=1,N)
      RETURN
  290 FORMAT(30H1NORMALIZATION CHECK.   V*U(T),///)
  327 FORMAT(63H1ORTHOGONALITY CHECK.  DIAGONAL ELEMENTS NORMALIZE V.
     1 U(T)*V,///)
  328 FORMAT(/14H DIAG. ELEMENT,I3,3H = ,2(1PE15.5)/(1X,5(E9.2,2H +,
     1E9.2,3HI   )))
  315 FORMAT(///1H ,1PE11.4,2H +,E11.4,2H I,7X,23HEIGENVECTOR OF MATRIX
     2A)
  316 FORMAT(///1H ,5X,1PE12.5,16X,23HEIGENVECTOR OF MATRIX A)
  662 FORMAT(/34X,34HEIGENVECTOR OF MATRIX A TRANSPOSED)
  415 FORMAT(44X,A4,2(25X,A4))
  416 FORMAT(36X,7(A4,8X))
  417 FORMAT(32X,1P7E12.4//)
  418 FORMAT(33X,3(1PE11.4,2H +,E11.4,5H I   )///)
      END
```

```
$IBFTC SKIP.   DECK,SDD
      SUBROUTINE SKIP
C  PROGRAM TO SPACE PLOT DATA TAPE BEYOND PREVIOUS RECORDS
C  USES DECK OF CARDS PUNCHED BY RESPNS IN PREVIOUS CALCS
C           SAME AS DATA USED FOR PLOTTING
C  LAST CARD FOR SKIP MUST BE BLANK
C  PLACE ALL CARDS FOR PLOT DATA TAPE AHEAD OF FIRST INPUT VECTOR
C  INCLUDE FIRST CONTROL CARD WITH NV NONZERO
C  SKIP CALLED FROM RESPNS WHEN NPLOT = 3 (SET BY DEBUG AT RESPNS 800)
      COMMON /CRESP/ VC(35,70),VM(35,70),R(70),RI(70),X(70),VECT(70),
     2NVEC,N,K,P(70,70)
      COMMON /CEIG/ VTST,NSEN,JOPT
      COMPLEX VC,VM
      DATA NCNT/0/
      NCNT=NCNT+1
      IF(NCNT.GT.1) RETURN
      MTIM=1
      REWIND 6
      READ 01,  (ILCH,J=1,4),NV,ILCH,ILCH
      IF(NV.EQ.0) RETURN
   01 FORMAT(7I2)
      READ (6) (ZILCH,J=1,123),TIM
   50 READ 02, KPLOT,JR,ILCH,ILCH,NZ,NT,ILCH,ZILCH,TIMA,ILCH
   02 FORMAT(7I4,A6,F7.2,I10)
   55 IF(KPLOT.EQ.0) RETURN
      IF(ABS(TIM-TIMA).LT.0.01) GO TO 100
      IF(MTIM.EQ.1) GO TO 130
      READ (6) (ZILCH,J=1,123),TIM
      IF(ABS(TIM-TIMA).GT.0.01) GO TO 140
  100 MTIM=2
      READ (6) (ZILCH,J=1,10)
      JRESP=JR+1
      GO TO (110,110,120),JRESP
  110 DO 115 I=1,NT
  115 READ (6) ZILCH,(ZILCH,J=1,NZ)
      GO TO 50
  120 DO 125 I=1,NT
  125 READ(6) ZILCH,(ZILCH,ZILCH,J=1,NZ)
      GO TO 50
  130 REWIND 6
  140 READ 03, KPLOT
   03 FORMAT(I4)
      IF(KPLOT.NE.0) GO TO 140
      PRINT 04
   04 FORMAT (//47H ERROR IN PLOT DATA TAPE OR DATA CARD.  SR SKIP///)
      RETURN
      END
```

```
$IBFTC SENTY.  DECK,SDD
C      CALCULATION OF EIGENVALUE SENSITIVITIES
C     USES DERIVATIVE MATRICES STORED ON UNIT 4
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      SUBROUTINE SENTY
      COMMON /CRESP/ VC(35,70),VM(35,70),R(70),RI(70),X(70),VECT(70),
     2NVEC,N,K,P(70,70)
      COMMON /CEIG/ VTST,NSEN,JOPT
      DIMENSION SEN(35,30),C(30),DA(70,70),NPAR(35),MUL(35)
      COMPLEX SUM,BOT,TOP,SEN
      COMPLEX VC,VM
      EQUIVALENCE (DA,VC)
      DATA ZERO,RIEN /1.0E-6,1.0E-25/
C     NO. OF PARAMETERS (OR GROUPS) GIVEN BY NSEN
      IF(NSEN.LE.0) GO TO 290
      READ(4) N
      DO 280 ISEN=1,NSEN
C  PARAMETER IDENT
      READ(4) NPAR(ISEN),MUL(ISEN)
      MULT=MUL(ISEN)
      IF(MULT.EQ.1) GO TO 250
C  MULTIPLE PARAMETER SENSITIVITY ,.SUM DERIV MATRICES
      DO 200 I=1,N
      DO 200 J=1,N
  200 DA(I,J)=0.0
  210 DO 240 ITIM=1,MULT
      READ(4) ((P(I,J),I=1,N),J=1,N)
  220 DO 230 I=1,N
      DO 230 J=1,N
  230 DA(I,J)=DA(I,J)+P(I,J)
  240 CONTINUE
      GO TO 260
C  SINGLE PARAM SENS
  250 READ(4) ((DA(I,J),I=1,N),J=1,N)
C  STORE SUM OF DERIV MATRICES ON UN34
  260 WRITE(34) ((DA(I,J),I=1,N),J=1,N)
  280 CONTINUE
C  READ VECTORS, ETC FOR RESPNS CALC FROM 34
  290 REWIND 34
      READ(34) NVEC,N,K
      READ(34) (R(I),RI(I),I=1,NVEC),((VC(I,J),I=1,NVEC),J=1,N),
     2((VM(I,J),I=1,NVEC),J=1,N),(X(I),I=1,N),(VECT(I),I=1,N)
      IF(NSEN.LE.0) RETURN
C  BEGIN SENSITIVITY CALC
      WRITE(3,10)
   10 FORMAT(1H1,38X,43HEIGENVALUE SENSITIVITY TO SYSTEM PARAMETERS////,
     26X,10HEIGENVALUE,34X,13HSENSITIVITIES,5X,11H(P/R)*DR/DP)
      DO 160 NTIM=1,NSEN
      READ(34) ((P(I,J),I=1,N),J=1,N)
      DO 150 I=1,NVEC
      BOT=(0.0,0.0)
      TOP=(0.0,0.0)
      DO 130 L=1,N
      SUM=(0.,0.)
      DO 120 J=1,N
  120 SUM=SUM+CMPLX(P(L,J),0.)*VM(I,J)
      SUM=SUM*VC(I,L)
      TOP=TOP+SUM
  130 BOT=BOT+VM(I,L)*VC(I,L)
  150 SEN(I,NTIM)=(TOP/BOT)/CMPLX(R(I),RI(I))
      CALL TIMREM(TIM)
      IF (TIM .LT. 0.2) GO TO 162
  160 CONTINUE
C  PRINT SENSITIVITIES
  162 DO 180 J=1,NSEN,5
      JUP=J+4
      IF(JUP.GT.NSEN) JUP=NSEN
      WRITE(3,20) (NPAR(ISEN),MUL(ISEN),ISEN=J,JUP)
      WRITE(3,21)
   20 FORMAT(///24X,5(5X,I4,1H(,I2,1H),5X))
   21 FORMAT(/)
      DO 170 L=1,NVEC
      IF(ABS(RI(L)).GT.RIEN) GO TO 165
      DO 161 ISEN=J,JUP
  161 C(ISEN)=REAL(SEN(L,ISEN))
      WRITE(3,30) R(L),(C(ISEN),ISEN=J,JUP)
      GO TO 170
  165 WRITE(3,40) R(L),RI(L),(SEN(L,ISEN),ISEN=J,JUP)
  170 CONTINUE
  180 CONTINUE
   30 FORMAT(6X,1PE10.3,2X,5(11X,0PF7.4))
   40 FORMAT(1X,1PE10.3,1X,E10.3,5(3X,0PF7.4,1X,F7.4))
      RETURN
      END
```

```
$IBFTC RESPN.  DECK,SDD
CRESPNS
      SUBROUTINE RESPNS(LABELS,NINCR,MODEL,KCALC,NOTFSS)
C     CALCULATES RESPONSE OF SYSTEM TO DISTURBANCE
C     INPUT REQUIRES XZERO,ROOTS, U AND V EIGENVECTORS
      COMMON /CRESP/ V(35,70),U(35,70),R(70),RI(70),X(70),VECT(70),NV,N,
     2K,P(70,70)
      COMMON /CEIG/ VTST,NSEN,JOPT
      DIMENSION W(35),LABELS(48),ICJG(35),XZ(70),B(70,10),D(15),F(70),
     2C(35),XI(70),Y(70),ANG(70),PLUS(70),TMP(70)
      DIMENSION MSGA(2),MSGD(24),NRESP(25),MSGC(10)
      DIMENSION CAPA(70),TAW(70),GAM(70),PSI(70),EPS(70),DELT(70),
     2SIGHT(70),SIG(70),ZI(70),ETA(70),EE(70),PP(70),VV(70),AL(70)
     3,ZETA(70)
      COMPLEX U,V
      EQUIVALENCE (B,P),(XZ,ANG,P(701)),(F,P(771)),(XI,P(841)),(Y,P(911))
     2),(W,P(981)),(ICJG,P(1016)),(C,P(1051)),(PLUS,P(1086)),
     3(TMP,P(1156))
      EQUIVALENCE (CAPA,P(1226)),(TAW,P(1296)),(GAM,P(1366)),
     2(PSI,P(1436)),(EPS,P(1506)),(DELT,P(1576)),(SIGHT,P(1646)),
     3(SIG,P(1716)),(ZI,P(1786)),(ETA,P(1856)),(EE,P(1926))
     4,(PP,P(1996)),(VV,P(2066)),(AL,P(2136)),(ZETA,P(2206))
      DATA LP,LL,LV/2H P,2H L,2H V/
      DATA ZERO,NPLOT,NOFR/1.0E-25,2,1/
      DATA  MSGD            /144H FEED FLOW RATE    FEED TEMPERATURE  FEE
```

```
     2D COMPOSITION  REFLUX FLOW RATE  STEAM TEMPERATURE COOLANT TEMP.
     3   2 OR MORE INPUTS NSE                /
      DATA  MSGA          /12H   COMPUTED /,MSGB/6HMODEL /, MSGC
     2   /60H  RESPONSE TO A DISTURBANCE IN                AUTONOMOUS RESP
     30/,MSGE/6H MODES/
C  SET UP TAPE ON UNIT 06 (SYSUT6) TO RECEIVE PLOT DATA
C  SET KPLOT VIA DEBUG TO GET DATA ONTO UNIT06 IN RESPNS
C  NPLOT = 1, SET BY DEBUG, ON FIRST CALL TO REWIND DATA TAPE
C  NPLOT = 3, SET BY DEBUG, ON FIRST CALL SKIPS PREVIOUS DATA ON TAPE
C           -  SUPPLY PLOT DATA CARDS FOR DATA ON TAPE
C  NPLOT = 2 FOR ALL SUBSEQUENT CALLS
C  KPLOT DESIGNATES KIND OF PLOT
C     = 1 FOR TRANSIENT RESPONSE
C     = 2 FOR FREQUENCY RESPONSE  (SET NOFR=2)
C     = 3 FOR BOTH OF ABOVE  (SET NOFR=2)
C  SET NOFR = 2 VIA DEBUG FOR FREQ. RESPONSE CALC.  (AT RESPN. 800)
      KPLOT = 0
      IF(MODEL.NE.1) GO TO 800
      REWIND 41
      READ (41) (ZILCH,J=1,3450)
      READ (41) NWDS,NS,N1,N2,DEE,VAPHT,UCP,XMU
      READ(41) (CAPA(J),TAW(J),GAM(J),PSI(J),EPS(J),DELT(J),SIGHT(J),
     2SIG(J),ZI(J),ETA(J),EE(J),ZETA(J),J=1,NS)
      REWIND 41
  800 CONTINUE
      IF(KPLOT.EQ.0) GO TO 810
      GO TO (815,816,817),NPLOT
  817 CALL SKIP
      GO TO 818
  815 REWIND 6
  818 NPLOT = 2
  816 CALL DATE(DAT)
      CALL TIME(TIM)
      WRITE(6) (LABELS(J),J=1,48),(MSGA(J),J=1,2),DAT,MSGB,MODEL,(VECT(J
     2),J=1,70),TIM
  801 FORMAT(7I4,A6,F7.2)
  810 KTYP=1
      IF(KCALC.EQ.5) KTYP=2
      GO TO (100,99),KTYP
   99 CONTINUE
      READ(4) ((B(I,J),J=1,K),I=1,N)
C  NRESP = 0 - 7 TO INDICATE KIND OF DISTURBANCE VECTORS WHICH FOLLOW
C  PROVIDE VECTOR OF NRESP,  VALUES INTERPRETED AS FOLLOWS
C  MAX OF 10 DISTURBANCES PER RESPONSE CALCULATION
C      1  FEED FLOW RATE
C      2  FEED TEMPERATURE
C      3  FEED COMPOSITION
C      4  REFLUX FLOW RATE
C      5  REBOILER STEAM TEMP
C      6  CONDENSER COOLING WATER TEMP
C      7  2 OR MORE INPUTS
      READ(2,09) (NRESP(J),J=1,25)
   09 FORMAT(25I2)
      JRESP=1
      IF(NRESP(1).EQ.0) RETURN
C  BEGIN RESPONSE CALC
  600 READ(2,08) (D(I),I=1,K)
   08 FORMAT(9E8.4)
  100 NMODES=N
      IF(N.GT.35) NMODES=35
      IF(NV.LE.N) NMODES=NV
      DO 101 J=1,N
  101 XZ(J)=X(J)
      IF(NMODES.GT.NV) NMODES = NV
      DO 103 I=1,NMODES
      ICJG(I)=1
      IF(ABS(RI(I)).LT.ZERO) ICJG(I)=0
  103 CONTINUE
      IF(ICJG(NMODES ).EQ.1.AND.ABS(R(NMODES)-R(NMODES-1)).GT.ZERO)
     2 NMODES=NMODES-1
      DO 153 I=1,NMODES
  153 W(I)=0.
      IF(KCALC.EQ.5.AND.NOTFSS.EQ.0) GO TO 200
C  BEGIN AUTONOMOUS ACTIVATION CALC
      WRITE(3,01) (LABELS(I),I=1,48),NMODES,MODEL
   01 FORMAT(1H1,45X,29HRESPONSE OF AUTONOMOUS SYSTEM,///4(30X,12A6//),
     2 46X,20HCALCULATION INCLUDES,I3,6H MODES/,57X,5HMODEL,I2///////,
     317X,7HMODE(S),15X,10HEIGENVALUE,14X,13HTIME CONSTANT,13X,
     4 9HWEIGHT(S)///)
C     FIRST CALCULATE ALL WEIGHTING FACTORS
  804 JR=0
      NOPLOT = 2
      IF(KPLOT.EQ.0.OR.KPLOT.EQ.2) GO TO 102
      NOPLOT = 1
      NRESP(1)=0
C  PLOT LABELS WRITTEN ON 6
      WRITE(6) (MSGC(I),I=6,10),(MSGD(I),I=22,24),NMODES,MSGE
      JRESP=1
  102 I=1
  104 IF(I.GT.NMODES) GO TO (410,200),KTYP
      IF(ICJG(I).EQ.1) GO TO 106
      DO 105 J=1,N
  105 W(I)=W(I)+X(J)*REAL(V(I,J))
      TAU=-1./R(I)
      WRITE(3,02) I, R(I), TAU, W(I)
      I=I+1
   02 FORMAT(18X,I3,18X,1PE10.3,15X,E10.3,15X,E10.3)
      GO TO 104
  106 DO 107 J=1,N
      W(I)=W(I)+2.*X(J)*REAL(V(I,J))
  107 W(I+1)=W(I+1)-2.*X(J)*AIMAG(V(I,J))
      TAU=-1./R(I)
      IP1=I+1
      WRITE(3,03) I,IP1,R(I),RI(I),TAU,W(I),W(I+1)
   03 FORMAT(15X,I3,2X,I3,8X,1PE10.3,3H + ,E10.3,2H I,8X,E10.3,8X,E10.3,
     24X,E10.3)
      I=I+2
      GO TO 104
  200 IHI=NRESP(JRESP)*3
      ILO=IHI-2
```

```
C  BEGIN STEP RESPONSE ACTIVATION CALC
      WRITE(3,201) (MSGD(I),I=ILO,IHI),(LABELS(I),I=1,48),NMODES,MODEL,
     2(D(I),I=1,K)
      WRITE(3,225)
  201 FORMAT(1H1,31X,38HRESPONSE OF SYSTEM TO A DISTURBANCE IN,3A6,///
     14(30X,12A6//),
     246X,20HCALCULATION INCLUDES,I3,6H MODES/,57X,5HMODEL,I2,///,19H DI
     3STURBANCE VECTOR,1X,1P10E10.2)
  225 FORMAT(//////3X,7HMODE(S),15X,10HEIGENVALUE,14X,13HTIME CONSTANT,
     214X,9HWEIGHT(S),21X,2HXI///)
  805 NOPLOT = 1
      IF(KPLOT.EQ.0.OR.KPLOT.EQ.2) NOPLOT=2
      GO TO (802,803),NOPLOT
  802 WRITE(6) (MSGC(I),I=1,5),(MSGD(I),I=ILO,IHI),NMODES,MSGE
      JR=1
C     CALCULATE ALL C(I)
  803 KBAK=1
  202 DO 403 I=1,N
      IF(NOTFSS.EQ.0) XZ(I)=0.
      XI(I)=0.
      F(I)=0.
      C(I)=0.
      DO 203 J=1,K
  203 F(I)=F(I)+B(I,J)*D(J)
  403 CONTINUE
      I=1
C  BEGIN CALC OF WEIGHTING FACTORS
  204 IF(I.GT.NMODES) GO TO (410,301),KBAK
      IF(ICJG(I).EQ.1) GO TO 206
      DO 205 J=1,N
  205 C(I)=C(I)+F(J)*REAL(V(I,J))
      GO TO (210,211),KBAK
  210 TAU=-1./R(I)
      XI(I)=-C(I)/R(I)
      WRITE(3,215) I,R(I),TAU,C(I),XI(I)
  215 FORMAT(4X,I3,18X,1PE10.3,15X,E10.3,15X,E10.3,17X,E10.3)
  211 I=I+1
      GO TO 204
  206 DO 207 J=1,N
      C(I)=C(I)+2.*F(J)*REAL(V(I,J))
  207 C(I+1)=C(I+1)+2.*F(J)*AIMAG(V(I,J))
      GO TO (212,213),KBAK
  212 XI(I)=-(C(I)*R(I)+C(I+1)*RI(I))/(R(I)**2+RI(I)**2)
      XI(I+1)=-(C(I+1)*R(I)-C(I)*RI(I))/(R(I)**2+RI(I)**2)
      TAU=-1./R(I)
      IP1=I+1
      WRITE(3,208) I,IP1,R(I),RI(I),TAU,C(I),C(I+1),XI(I),XI(I+1)
  208 FORMAT(1X,I3,2X,I3,8X,1PE10.3,3H + ,E10.3,2H I,8X,E10.3,9X,E10.3,
     22X,E10.3,5X,E10.3,2X,E10.3)
  213 I=I+2
      GO TO 204
  410 WRITE(3,04)
   04 FORMAT(1H1,55X,8HRESPONSE,///3X,4HTIME,53X,12HSTATE VECTOR///)
      TLIM=-4./R(1)
      IF(R(1).GE.0.) GO TO 135
      T=0.
      IF(NINCR.EQ.0) NINCR=30
      TINCR=TLIM/FLOAT(NINCR)
      NT=0
      GO TO 113
C
C     BEGIN LOOP FOR RESPONSE AT TIME T
  111 IF(T.GE.2.*TINCR) GO TO 112
      T=T+TINCR/10.
      GO TO  113
  112 T=T+TINCR
      IF(T.GT.TLIM) GO TO 135
  113 I=1
      GO TO (116,216),KTYP
  116 DO 114 J=1,N
  114 X(J)=-XZ(J)
      GO TO 115
  216 DO 214 J=1,N
  214 X(J)=0.
C
C     BEGIN LOOP FOR RESPONSE OF MODE I
  115 IF(I.GT.NMODES) GO TO 125
      E=EXP(R(I)*T)
      IF(ICJG(I).EQ.1) GO TO 120
      DO 118 J=1,N
      GO TO (117,217),KTYP
  217 X(J)=X(J)+REAL(U(I,J))*(XI(I)*(1.-E)+W(I)*E)
      GO TO 118
  117 X(J)=X(J)+W(I)*E*REAL(U(I,J))
  118 CONTINUE
      I=I+1
      GO TO 115
  120 WA=(W(I)*COS(RI(I)*T)+W(I+1)*SIN(RI(I)*T))*E
      WB=(W(I+1)*COS(RI(I)*T)-W(I)*SIN(RI(I)*T))*E
      GO TO (121,220),KTYP
  220 WA=WA+XI(I)*(1.-E*COS(RI(I)*T))-XI(I+1)*E*SIN(RI(I)*T)
      WB=WB-XI(I+1)*(1.-E*COS(RI(I)*T))-XI(I)*E*SIN(RI(I)*T)
  121 DO 122 J=1,N
  122 X(J)=X(J)+WA*REAL(U(I,J))+WB*AIMAG(U(I,J))
      I=I+2
      GO TO 115
C  END LOOP FOR RESPONSE OF MODE I
  125 IF(MODEL.NE.1) GO TO 1125
C  FOR MODEL 1 CALC L, V, AND P AT EACH STAGE
      DO 425 J=1,NS
      JH=J-1
      JX=J-1+N1
      JT=J-1+N1+NS
      IF(J.EQ.NS) GO TO 424
      PP(J)=ETA(J)*X(JX)/EE(J)-ETA(J)*(1.-EE(J))*X(JX+1)/EE(J)
     2 +PSI(J)*X(JT)
      VV(J)=ZI(J)*X(JH+1)+TAW(J)*X(JX)+SIG(J)*X(JX+1)+SIGHT(J)*X(JX+2)
     2 +DELT(J)*X(JT)+EPS(J)*X(JT+1)
      IF(J.EQ.N1.AND.NRESP(JRESP).GE.6) VV(J)=VV(J)-PSI(NS)*DEE*D(6)
      IF(J.EQ.1) GO TO 425
```

```
      AL(J)=GAM(J)*(X(JH)+CAPA(J)*VV(J-1))
  424 PP(J)=PSI(NS)*VAPHT*VV(N1)/UCP+ETA(NS)*(ZETA(N1)*X(JX)/EE(N1)
     2 -ZETA(N1)*(1.-EE(N1))*X(JX)/EE(N1)+XMU*X(JT))
      IF(NRESP(JRESP).GE.6) PP(J)=PP(J)+PSI(NS)*D(6)
  425 CONTINUE
C     PRINT RESPONSE AT TIME T FOR ALL STATE VARIABLES
 1125 DO 130 L=1,N,6
      JD=L+5
      IF(JD.GT.N) JD=N
      IF(L.GT.1) GO TO 126
      WRITE(3,05) T,(VECT(J),X(J),J=L,JD)
      GO TO 130
  126 WRITE(3,06) (VECT(J),X(J),J=L,JD)
  130 CONTINUE
      IF(MODEL.EQ.1) WRITE(3,66) (LP,J,PP(J),J=1,NS),(LL,J,AL(J),
     2J=2,N1),(LV,J,VV(J),J=1,N1)
   66 FORMAT((12X,6(2X,A2,I2,3H = ,1PE9.2)))
  820 GO TO (811,812),NOPLOT
  811 WRITE(6) T,(X(J),J=1,N)
  812 NT=NT+1
   05 FORMAT(1H0,1PE9.2,2X,6(2X,A4,3H = ,1PE9.2))
   06 FORMAT((12X,6(2X,A4,3H = ,1PE9.2)))
      GO TO 111
C  END LOOP FOR RESPONSE AT TIME T
  135 CONTINUE
      IF(NOPLOT.EQ.1) PUNCH 801,KPLOT,JR,MODEL,NRESP(JRESP),N,NT,NMODES,
     2DAT,TIM
      GO TO (136,300),KTYP
  136 WRITE(3,07)
      WRITE(3,06) (VECT(J),XZ(J),J=1,N)
   07 FORMAT(///30X,57HINITIAL STATE VECTOR  (DEVIATION FROM FINAL STEAD
     2Y STATE)//)
      RETURN
C
C     BEGIN FREQUENCY RESPONSE
C  ****** NOT DEBUGGED *****
C
  300 GO TO (345,361),NOFR
  361 WRITE(3,370)
  370 FORMAT(1H1,51X,18HFREQUENCY RESPONSE,////2X,9HFREQUENCY,4X,
     232X,38HRESPONSE - PHASE (DEG), MAGNITUDE (DB)///)
  806 NOPLOT=2
      IF(KPLOT-1.GT.0) NOPLOT=1
      GO TO (807,808),NOPLOT
  807 JR=2
      WRITE(6) (MSGC(I),I=1,5),(MSGD(I),I=ILO,IHI),NMODES,MSGE
  808 DO 302 J=1,K
  302 IF(D(J).NE.0.) D(J)=1.0
      KBAK=2
      GO TO 202
  301 TLIM=-10.*R(NMODES)
      T=0.
      TINCR=-R(1)/1000.
      SLOW=0.5
      DO 303 J=1,N
      XI(J)=0.
  303 ANG(J)=0.0
      NT=0
      GO TO 313
C     BEGIN LOOP FOR RESPONSE AT FREQUENCY T
  311 TINCR=TINCR*2.
      T=T+TINCR
      SLOW=0.5
      IF(T.GT.TLIM) GO TO 340
  313 I=1
      DO 304 J=1,N
      Y(J)=0.
  304 X(J)=0.
C     BEGIN LOOP FOR MODE I
  320 IF(I.GT.NMODES) GO TO 330
      IF(ICJG(I).EQ.1) GO TO 325
      TM1=R(I)**2+T**2
      DO 321 J=1,N
      TMJ=C(I)*REAL(U(I,J))/TM1
      YINC=-T*TMJ
      XINC=-R(I)*TMJ
  341 X(J)=X(J)+XINC
  321 Y(J)=Y(J)+YINC
      I=I+1
      GO TO 320
  325 TM1=R(I)**2+(T-RI(I))**2
      TM2=R(I)**2+(T+RI(I))**2
      DO 326 J=1,N
      TMJ=C(I)*REAL(U(I,J))-C(I+1)*AIMAG(U(I,J))
      TAJ=C(I+1)*REAL(U(I,J))+C(I)*AIMAG(U(I,J))
      XINC=(-R(I)*TMJ+(T-RI(I))*TAJ)/TM1
      YINC=(-R(I)*TAJ-(T-RI(I))*TMJ)/TM1
  342 X(J)=X(J)+XINC
      Y(J)=Y(J)+YINC
      XINC=(-R(I)*TMJ-(T+RI(I))*TAJ)/TM2
      YINC=(R(I)*TAJ-(T+RI(I))*TMJ)/TM2
  343 Y(J)=Y(J)+YINC
  326 X(J)=X(J)+XINC
      I=I+2
      GO TO 320
  330 DO 331 J=1,N
      PLUS(J)=ANG(J)
      TEMP=ATAN(Y(J)/X(J))*57.29578
      IF(T.LT.ZERO.AND.X(J).LT.0.0) GO TO 328
      IF(ABS(TEMP-XI(J)+ANG(J)).LT.45.) GO TO 329
      IF(SIGN(1.,TEMP).EQ.SIGN(1.,(XI(J)-ANG(J)))) GO TO 500
      IF(ABS(TEMP-XI(J)+ANG(J)).LE.135.) GO TO 500
      IF(TEMP.GT.0.0) GO TO 328
      PLUS(J)=180.+ANG(J)
      GO TO 329
  328 PLUS(J)=-180.+ANG(J)
  329 TMP(J)=TEMP+PLUS(J)
  331 CONTINUE
      DO 360 J=1,N
      XI(J)=TMP(J)
```

```
      ANG(J)=PLUS(J)
  360 X(J)=20.*ALOG10(SQRT(X(J)**2+Y(J)**2))
C     PRINT FREQ RESPONSE FOR FREQ T
      DO 332 L=1,N,4
      JD=L+3
      IF(JD.GT.N) JD=N
      IF(L.GT.1) GO TO 333
      WRITE(3,335) T,(VECT(J),XI(J),X(J),J=L,JD)
      GO TO 332
  333 WRITE(3,336) (VECT(J),XI(J),X(J),J=L,JD)
  332 CONTINUE
  821 GO TO (813,814),NOPLOT
  813 WRITE(6) T,(XI(J),X(J),J=1,N)
  814 NT=NT+1
      GO TO 311
  335 FORMAT(1H0,1PE10.3,4(2X,A4,2H= ,1PE9.2,1H,,E9.2))
  336 FORMAT((11X,4(2X,A4,2H= ,1PE9.2,1H,,E9.2)))
  500 T=T-TINCR
      TINCR=TINCR*SLOW
      SLOW=SLOW*0.5
      T=T+TINCR
      GO TO 313
  340 CONTINUE
      IF(NOPLOT.EQ.1) PUNCH 801, KPLOT,JR,MODEL,NRESP(JRESP),N,NT,NMODES
     2,DAT,TIM
  345 JRESP=JRESP+1
      IF(JRESP.GT.25) GO TO 350
      IF(NRESP(JRESP).GT.0) GO TO 600
  350 RETURN
      END
```

```
$IBFTC PLOT.   DECK,SDD
C  PROGRAM FOR PREPARATION OF PLOT TAPE
      DIMENSION T(100),X(60,100),ANG(60,100),MAG(60,100),PLATE(60),
     2VECT(70),LA(48),LB(3),LC(2),LVER(2),LD(8),LE(2),LX1(4),LX2(5),
     3LX3(2),LY1(4),LY2(4),LY3(5)
      EQUIVALENCE (MAG,X)
      REAL MAG
      DATA IPX1,IPX2,IPX3,IPY1,IPY2,IPY3/24,30,12,24,24,30/,NGRPH/1/
      DATA  LX1(1)       /24HDIMENSIONLESS TIME,  T  /,LX2(1)       /30HD
     2IMENSIONLESS FREQUENCY,  W   /,LX3(1)     /12HPLATE NUMBER/, LY1(1
     3)       /24HCHANGE IN STATE VARIABLE/, LY2(1)    /24H   PHASE ANGL
     4E,  DEGREES/,LY3(1)   /30H    MAGNITUDE RATIO,  DECIBELS/, LVER(1)
     5       /12H   VERSUS   /
C ** PLOT TAPE MOUNTED ON UNIT UT6 (SETUP)
C ** DATA TAPE MOUNTED ON UNIT 8 (SETUP)
C ** TERMINATE DATA CARDS WITH ONE BLANK CARD **********************
C  FIRST CARD CONTROLS NO. OF CURVES AND TYPE OF PLOTS
C  CAN OVERRIDE PLOTTING OF ANY CURVE BY MAKING KSKIP NONZERO ON CARD
C  NO. OF PLOTS PER RESPONSE CALC. (MAY INCLUDE 2 CDS - T.R. AND F.R.) -
C        BASE NO. = 1,3,5,3 FOR KFR = 0,1,2,3, AND KTR=1 WHEN KPLOT = 3
C                 = 0,2,4,2 FOR FOR KFR = 0,1,2,3 WHEN KPLOT = 2
C                 = 0,1     FOR KTR = 0,1 WHEN KPLOT = 1
C        MULTIPLIER = 1 IF IDIF = 0, =(IX+IH+IT) IF IDIF = 1
      READ 01, IX,IH,IT,IDIF,NV,JFR,JTR
   01 FORMAT(7I2)
      CALL DATE(TODA)
      PRINT 10,  IX,IH,IT,IDIF,NV,JFR,JTR,TODA
   10 FORMAT(  1H1  //,22H PLOT TAPE PREPARATION//,6H IX = ,I2,7H  IH =
     2,I2,7H  IT = ,I2,9H  IDIF = ,I2,7H  NV = ,I3,8H  KFR = ,I2,8H  KTR
     3 = ,I2,10X,5HDATE ,A6////)
C  IX, IH, IT = 0 FOR OMISSION OF PLOT OF RESPECTIVE VARIABLE
C  IX, IH, IT = 1 FOR INCLUSION
C  IDIF = 0 IF ALL 3 TYPES OF VARIABLE (ABOVE) GO ON ONE PLOT
C  IDIF = 1 IF EACH TYPE OF VARIABLE TO GO ON SEPARATE PLOT
C  NV = 1 FOR INCLUSION OF ALL OF EACH TYPE OF STATE VARIABLE
C     = 2 FOR INCLUSION OF ALTERNATE PLATES
C     = 3 FOR INCLUSION OF EVERY THIRD PLATE
C     = 4 FOR INCLUSION OF ONLY BOTTOM,MIDDLE, TOP
C   FOR NV .GT. 10, SUBTRACT 10 AND PLOT ONLY THE PLATE NUMBER
C    INDICATED BY (NV-10),   COUNT REBOILER AS PLATE 1
C  KFR = 0 FOR NO FREQUENCY RESPONSE
C      = 1 FOR FREQUENCY RESPONSE ONLY
C      = 2 FOR ORDINARY FREQ. RESP. AND FREQ. RESP. VERSUS TRAY NUMBER
C      = 3 FOR FREQ. RESP. VERSUS TRAY NUMBER ONLY
C  KTR = 0,1 FOR NO TRANSIENT RESP. OR TRANSIENT RESP. CALCULATION
      REWIND 8
      MTIM=1
      READ(8) (LA(J),J=1,48),(LB(J),J=1,3),(LC(J),J=1,2),(VECT(J),J=1,70
     2),TIM
   50 READ 02, KPLOT,JR,MOD,NIL,N,NT,NIL,DAT,TIMA,KSKIP
   02 FORMAT(7I4,A6,F7.2,I10)
      KFR=JFR
      KTR=JTR
      IF(KPLOT.EQ.1) KFR=0
      IF(KPLOT.EQ.2) KTR=0
```

```
      IF(KSKIP.EQ.0) PRINT 11
   11 FORMAT(1H1)
      IF(KPLOT.NE.0) GO TO 55
   52 CALL CCEND
      STOP
   55 PRINT 12, KPLOT,JR,MOD,N,NT,DAT,TIMA,KSKIP
   12 FORMAT(9H KPLOT = ,I2,7H  JR = ,I2,8H  MOD = ,I2,6H  N = ,I3,7H  N
     2T = ,I3,3X,A6,3X,F8.2,10H  KSKIP = ,I3//)
C  JR = 0,1,2 FOR AUTON. RESP., FORCED RESP, FREQ. RESP.
C  NT = NUMBER OF TIME STEPS
      IF(ABS(TIM-TIMA).LT.0.01) GO TO 100
      IF(MTIM.EQ.1) GO TO 520
      READ(8) (LA(J),J=1,48),(LB(J),J=1,3),(LC(J),J=1,2),(VECT(J),
     2J=1,70),TIM
      IF(ABS(TIM-TIMA).GT.0.01) GO TO 520
  100 MTIM=2
      READ(8) (LD(J),J=1,8),(LE(J),J=1,2)
      JRESP=JR+1
      IF(MOD.EQ.4) NS=N
      IF(MOD.EQ.3) NS=(N+2)/2
      IF(MOD.EQ.2) NS=N/2
      IF(MOD.EQ.1) NS=(N+2)/3
      NVAR=NV
      IF(NV.EQ.4) NVAR=NS/2
      M=NT
      GO TO (110,110,120),JRESP
  110 DO 115 I=1,NT
  115 READ(8) T(I),(X(J,I),J=1,N)
      IF(KTR.EQ.0.OR.KSKIP.NE.0) GO TO 50
      KCURV=1
      GO TO 130
  120 DO 125 I=1,NT
  125 READ(8) T(I),(ANG(J,I),MAG(J,I),J=1,N)
      IF(KFR.EQ.0.OR.KSKIP.NE.0) GO TO 50
      GO TO (127,300,127),KFR
  127 KCURV=2
C  BEGIN PLOT PREPARATION
C  PRINT PLOT SUMMARY
  130 PRINT 03, LA,LD,LC,LE,LB,NT
   03 FORMAT( //4(10X,12A6/),10X,8A6/,10X,A6,I2,30X,I3,A6/,10X,3A6,20X,
     2I4,7H POINTS////)
  132 REWIND 9
      NCURV=1
      J=1
      IF(MOD.EQ.4.OR.MOD.EQ.2) GO TO 150
      IF(IH.EQ.0) GO TO 145
C  HOLDUP RESPONSE
      IF(NVAR.GT.11) J=NVAR-12
  135 JRIT=1
      GO TO (201,202,203),KCURV
  136 IF(NVAR.GT.11) GO TO 140
      IF(J.EQ.NS-2) GO TO 140
      NCURV=NCURV+1
      J=J+NVAR
      IF(J.GT.NS-2) J=NS-2
      GO TO 135
C  COMPOSITION RESPONSE
  140 IF(IDIF.EQ.1.OR.IX+IT.EQ.0) GO TO 142
      NCURV=NCURV+1
      GO TO 150
  142 KBAK=1
      GO TO 500
  145 J=NS-1
  150 IF(IX.EQ.0) GO TO 170
      JRPT=1
  152 JLIM=J+NS-1
      J1=J
      IF(NVAR.GT.10) J=J+NVAR-11
  155 JRIT=2
      GO TO (201,202,203),KCURV
  156 IF(NVAR.GT.10) GO TO 160
      IF(J.EQ.JLIM) GO TO 160
      NCURV=NCURV+1
      IF(J.EQ.J1.OR.J.EQ.JLIM-1) GO TO 157
      J=J+NVAR
      IF(J.GT.JLIM-1) J=JLIM-1
      GO TO 155
  157 J=J+1
      GO TO 155
  160 IF(IDIF.EQ.1.OR.IT.EQ.0) GO TO 162
C  TEMPERATURE RESPONSE
      NCURV=NCURV+1
      GO TO (170,180),JRPT
  162 KBAK=2
      GO TO 500
  165 GO TO (170,190),JRPT
  170 IF(IT.EQ.0) GO TO 190
      IF(MOD.GT.2) GO TO 190
  175 IF(MOD.EQ.2) J=NS+1
      IF(MOD.EQ.1) J=2*NS-1
      JRPT=2
      GO TO 152
  180 NCURV=NCURV-1
  185 KBAK=3
      GO TO 500
  190 GO TO (50,195,200),KCURV
  195 KCURV=3
      GO TO 132
  200 GO TO (50,300,300),KFR
  201 PRINT 04 ,VECT(J),X(J,M)
      WRITE(9) M,(T(I),X(J,I),I=1,M)
      GO TO (136,156),JRIT
  202 MID=M/2
      PRINT 08, VECT(J),ANG(J,MID),T(MID)
      L=M-1
      WRITE (9) L,(T(I),ANG(J,I),I=2,M)
      GO TO (136,156),JRIT
  203 MID=M/2
      PRINT 08, VECT(J),MAG(J,MID),T(MID)
      L=M-1
```

```
   08 FORMAT(10X,A4,10X,11HMIDPOINT = ,1PE11.4,8H AT W = ,E11.4)
      WRITE(9) L,(T(I),MAG(J,I),I=2,M)
      GO TO (136,156),JRIT
   04 FORMAT (10X,A4,10X,13HLAST POINT = ,1PE11.4)
  300 KCURV=4
C  PLOT OF PHASE OR MAGNITUDE VS PLATE NO.
  301 REWIND 9
      NCURV=1
      J=1
      IF(MOD.EQ.1.OR.MOD.EQ.3) J=NS-1
      DO 305 I=1,NS
      IP=J+I-1
  305 PLATE(IP)=FLOAT(I)
      LIM=J+NS-1
      ITINC=NT/10
      KBAK=4
  310 IT=1
  312 IF(KCURV.EQ.5) GO TO 315
      PRINT 05 , T(IT),ANG(LIM,IT)
      WRITE(9) NS,(PLATE(I),ANG(I,IT),I=J,LIM)
      GO TO 320
  315 PRINT 05, T(IT),MAG(LIM,IT)
   05 FORMAT(10X,4HW = ,1PE11.4,4X,13HLAST POINT = ,E11.4)
      WRITE(9) NS,(PLATE(I),MAG(I,IT),I=J,LIM)
  320 IT=IT+ITINC
      IF(IT.GT.NT) GO TO 500
      NCURV=NCURV+1
      GO TO 312
  325 IF(KCURV.EQ.5) GO TO 50
      KCURV=5
      GO TO 310
C  FOLLOWING SECTION PLOTS APPROPRIATE GRAPH INCLUDING ALL LABELING
  500 GO TO (501,502,503,504,505),KCURV
  501 CALL GRAPH(9,NCURV,0,0,0,0,LX1,IPX1,LY1,IPY1)
      PRINT 06, LY1,LVER,LX1
   06 FORMAT(5X,9HGRAPH OF ,12A6)
      GO TO 510
  502 CALL GRAPH(9,NCURV,1,0,0,0,LX2,IPX2,LY2,IPY2)
      PRINT 06, LY2,LVER,LX2
      GO TO 510
  503 CALL GRAPH(9,NCURV,1,0,0,0,LX2,IPX2,LY3,IPY3)
      PRINT 06, LY3,LVER,LX2
      GO TO 510
  504 CALL GRAPH(9,NCURV,0,0,0,0,LX3,IPX3,LY2,IPY2)
      PRINT 06, LY2,LVER,LX3
      GO TO 510
  505 CALL GRAPH(9,NCURV,0,0,0,0,LX3,IPX3,LY3,IPY3)
      PRINT 06 , LY3,LVER,LX3
  510 PRINT 17,NGRPH
   17 FORMAT(11H FRAME NO. ,I2////)
      NGRPH=NGRPH+1
      CALL CCLTR(0.50,5.85,0.2,LD,48)
      YL=5.70
      XL=1.25
      DO 515 L=1,4
      LMAX=12*L
      LMIN=12*L-11
      WRITE(98,14) (LA(J),J=LMIN,LMAX)
   14 FORMAT(12A6)
      CALL CCLTR(XL,YL,0,1)
  515 YL=YL-0.15
      WRITE(98,15) LC
   15 FORMAT(A6,I2)
      CALL CCLTR(1.82,5.10,0,1)
      WRITE(98,16) LE
   16 FORMAT(I3,A6)
      CALL CCLTR(4.27,5.10,0,1)
      CALL CCLTR(6.50,5.10,0,1,LB,18)
      NCURV=1
      REWIND 9
      GO TO (145,165,190,325),KBAK
  520 PRINT 18, TIM,TIMA
   18 FORMAT(//49H DATA TAPE OR DATA CARD ERROR     EXEC. TERMINATED/
     2 7H TIM = ,F8.2,9H  TIMA = ,F8.2)
      GO TO 52
      END
```

```
$IBFTC GRAPH.  DECK
C  SUBROUTINE TO PREPARE DATA TAPE FOR CAL-COMP PLOTTER
C     SCALES DATA, PREPARES GRID, TICS, LABELS, AND PLOTS LINES
C  PROGRAM BY J. E. CRIDER
      OSUBROUTINE GRAPH(ITAPE,NCURV,LOGX,LOGY,IVERT,MMCALC,PRNTX,IPX,
     1PRNTY,IPY)
      ODIMENSION X(700),Y(700),DM(2,2),DCC(2,2),ITE(2),IR(2),DPL(2),
     1IRAN(2),DTS(2),IT(2),P(2),TL(2),FMI(1),FM(3),IW(2),NAX(2)
       COMMON /CCPOOL/XMIN,XMAX,YMIN,YMAX,CCXMIN,CCXMAX,CCYMIN,CCYMAX
       EQUIVALENCE (XMIN,DM(1,1)),(CCXMIN,DCC(1,1))
       LOGICAL L(2),LT,LCONT
       DATA QP,FM(1),LCONT/0164400000000,18H(F6.2)(F6.1)(F6.0),.FALSE./
       DATA NG,NAX/1,1HX,1HY/
      OSPACE(I) = AINT(ALOG10(AMAX0(1,IABS(I))))*7. + FLOAT((1-ISIGN(1,I)
      1)*2)
       DJ(DI) = AINT(DI) + SIGN(0.5,DI) - 0.5
       IF(LCONT)GO TO 98
       CALL CCBGN
       CALL FXMSET(0,I,-1,36)
       LCONT = .TRUE.
       GO TO 99
   98 CALL CCNEXT
       NG = NG+1
   99 REWIND ITAPE
       W = 0.
       L(1) = LOGX.NE.0
       L(2) = LOGY.NE.0
       CCXMIN = 100.
       CCYMIN = 200.
  100 IF(IVERT.NE.0)GO TO 101
       CCXMAX = 900.
       CCYMAX = 700.
       GO TO 102
  101 CCXMAX = 600.
       CCYMAX = 1000.
  102 IF(MMCALC.NE.0)GO TO 104
       READ(ITAPE)NPT,XMIN,YMIN
       REWIND ITAPE
       XMAX = XMIN
       YMAX = YMIN
       IF(NCURV.GT.0)GO TO 302
       PRINT 202,NG,NCURV,NG
 2020FORMAT(39HOERROR MESSAGE, SUBROUTINE GRAPH, GRAPH14//10X34HERROR I
     1N ARGUMENT LIST.  NCURV IS I6,22H, WHICH IS LESS THAN 1/10X5HGRAPH
     2I4,13H NOT PLOTTED.//)
       GO TO 167
C  FIND MAX AND MIN OF DATA
  302 DO 103 K = 1,NCURV
       READ(ITAPE)NPT,(X(I),Y(I), I = 1,NPT)
       DO 103 I = 1,NPT
       XMAX = AMAX1(XMAX,X(I))
       XMIN = AMIN1(XMIN,X(I))
       YMAX = AMAX1(YMAX,Y(I))
  103 YMIN = AMIN1(YMIN,Y(I))
       REWIND ITAPE
  104 DO 114 I = 1,2
       IF(L(I))GO TO 109
       IW(I) = 2
      OIF(DM(1,I).GT.0..AND.DM(1,I)/DM(2,I).LE..125.AND.MMCALC.EQ.0)
      1DM(1,I) = 0.
  204 TE = ALOG10(DM(2,I) - DM(1,I))
       ITE(I) = TE
       IF(TE.LT.0.)ITE(I) = ITE(I)-1
       PT = 10.**(-ITE(I)+1)
  105 DI = DM(2,I)*PT
       IF(DI.EQ.0.)DI = ABS(DI)
       XAM = DJ(DI) + SIGN(0.5,DI - DJ(DI) - QP) + 0.5
       DI = DM(1,I)*PT
       IF(DI.EQ.0.)DI = ABS(DI)
       XIM = DJ(DI) + SIGN(0.5,DI - DJ(DI) + QP - 1.) + 0.5
       IF(XIM.EQ.0.)XIM = -ABS(XIM)
       IR(I) = XAM - XIM
       IF(IR(I).LE.55)GO TO 106
       PT = PT/10.
       GO TO 105
  106 IF(IR(I).LE.10)GO TO 706
       ZIR = 2.
       IF(IR(I).GE.25)ZIR = 5.
       IF(XIM)206,406,306
  206 XIM = XIM - AMOD(ZIR - AMOD(ABS(XIM),ZIR),ZIR)
       GO TO 406
  306 XIM = XIM - AMOD(XIM,ZIR)
  406 IF(XAM)506,706,606
  506 XAM = XAM + AMOD(ABS(XAM),ZIR)
       GO TO 706
  606 XAM = XAM + AMOD(ZIR - AMOD(XAM,ZIR),ZIR)
  706 XIR = XAM - XIM
       IR(I) = XIR
       DPL(I) = AINT((DCC(2,I) - DCC(1,I))/XIR)
       DCC(2,I) = DCC(1,I) + DPL(I)*XIR
       DM(2,I) = XAM/PT
       DM(1,I) = XIM/PT
       RAN(I) = DM(2,I) - DM(1,I)
       DTS(I) = RAN(I)/XIR
       TL(I) = RAN(I)*10./(DCC(2,I) - DCC(1,I))
       IT(I) = 5
       P(I) = 10.**(-ITE(I))
       IF(IR(I).GT.11)GO TO 107
       DTS(I) = DTS(I)/5.
       IR(I) = IR(I)*5
       GO TO 208
  107 IF(IR(I).GT.22)GO TO 108
       DTS(I) = DTS(I)/2.
       DPL(I) = DPL(I)*2.
       IT(I) = 4
       IR(I) = IR(I)*2
       GO TO 208
  108 DPL(I) = DPL(I)*5.
  208 IF(IABS(ITE(I)).NE.1)GO TO 114
       IF(I.EQ.1)W = 7.*FLOAT(ITE(1))
```

```
      IW(I) = 2+ITE(I)
      ITE(I) = 0
      P(I) = 1.
      GO TO 114
  109 IF(DM(1,I).GT.0.)GO TO 111
      PRINT 110,NG,NAX(I),DM(1,I)
 1100FORMAT(39H0ERROR MESSAGE, SUBROUTINE GRAPH, GRAPHI4//10X11HMINIMUM
     1 ON A1,8H AXIS IS1PE15.7,15H, NOT POSITIVE./10X49HAXIS IS CONVERTE
     2D FROM LOG TO LINEAR COORDINATES.//)
      L(I) = .FALSE.
      GO TO 204
  111 DI = ALOG10(DM(2,I))
      IF(DI.EQ.0.)DI = ABS(DI)
      DM(2,I) = DJ(DI) + SIGN(0.5,DI - DJ(DI) - QP) + 0.5
      DI = ALOG10(DM(1,I))
      IF(DI.EQ.0.)DI = ABS(DI)
      DM(1,I) = DJ(DI) + SIGN(0.5,DI - DJ(DI) + QP - 1.) + 0.5
      IF(DI.EQ.0.)DM(1,I) = -ABS(DM(1,I))
      RAN(I) = DM(2,I) - DM(1,I)
      IF(RAN(I).LE.5.)GO TO 113
      RAN(I) = 5.
      DM(1,I) = DM(2,I) - 5.
      PRINT 112,NG,NAX(I)
 1120FORMAT(21H0ERROR MESSAGE, GRAPHI4/34H ONLY THE 5 HIGHEST CYCLES ON
     1 THE A1,15H AXIS ARE USED.//)
  113 DCYC = AINT((DCC(2,I) - DCC(1,I))/RAN(I))
  114 CONTINUE
      IF(.NOT.(L(1).OR.L(2)))GO TO 115
     DIF(L(1).AND.L(2))DCYC = AINT(AMIN1( 800./AMAX1(RAN(1),RAN(2)),500.
     1/AMIN1(RAN(1),RAN(2))))
      IF(DCYC.LT.700.)GO TO 156
      JMX = 9
      JMS = 1
      GO TO 158
  156 IF(DCYC.LT.350.)GO TO 157
      JMX = 8
      JMS = 2
      GO TO 158
  157 JMX = 5
      JMS = 3
  158 IF(.NOT.L(2))GO TO 115
      CCYMAX = CCYMIN + DCYC*RAN(2)
      TL(2) = 10./DCYC
  115 X(1) = XMIN
      Y(1) = YMIN
      IF(L(1))GO TO 116
      ASSIGN 120 TO ITT
      IM = IR(1)-1
      GO TO 119
  116 CCXMAX = CCXMIN + DCYC*RAN(1)
      TL(1) = 10./DCYC
      IF(DCYC.LT.700.)GO TO 117
      ASSIGN 121 TO ITT
      IM = 64
      GO TO 119
  117 IF(DCYC.LT.350.)GO TO 118
      ASSIGN 122 TO ITT
      IM = INT(RAN(1))*18-1
      GO TO 119
  118 ASSIGN 123 TO ITT
      IM = INT(RAN(1))*9-1
  119 DO 125 I = 1,IM
      GO TO ITT,(120,121,122,123,221)
  120 T = XMIN + DTS(1)*FLOAT(I)
      LT = MOD(I,IT(1)).EQ.0
      GO TO 124
  121 IF(I.EQ.40)ASSIGN 221 TO ITT
      T = XMIN + ALOG10(1. + FLOAT(I)/10.)
      LT = MOD(I,10).EQ.0
      GO TO 124
  221 T = XMIN + ALOG10(5. + FLOAT(I-40)/5.)
      LT = MOD(I-40,5).EQ.0
      GO TO 124
  122 ILN = MOD(I-1,18)+3
      T = XMIN + ALOG10(FLOAT(ILN)/2.) + FLOAT((I-1)/18)
      LT = MOD(ILN,4).EQ.0
      GO TO 124
  123 ILN = MOD(I-1,9)+2
      T = XMIN + ALOG10(FLOAT(ILN)) + FLOAT((I-1)/9)
      LT = ILN.EQ.2.OR.MOD(ILN,5).EQ.0
C  TICS     X-AXIS    BOTTOM
  124 IX = I*3
      X(IX-1) = T
      X(IX) = T
      X(IX+1) = T
      Y(IX-1) = YMIN
      Y(IX) = YMIN + TL(2)
      IF(LT)Y(IX) = Y(IX) + TL(2)
  125 Y(IX+1) = YMIN
      X(IX+2) = XMAX
      Y(IX+2) = YMIN
      IF(L(2))GO TO 126
      ASSIGN 130 TO ITT
      IM = IR(2)-1
      GO TO 129
  126 IF(DCYC.LT.700.)GO TO 127
      ASSIGN 131 TO ITT
      IM = 64
      GO TO 129
  127 IF(DCYC.LT.350.)GO TO 128
      ASSIGN 132 TO ITT
      IM = INT(RAN(2))*18-1
      GO TO 129
  128 ASSIGN 133 TO ITT
      IM = INT(RAN(2))*9-1
  129 DO 135 I = 1,IM
      GO TO ITT,(130,131,132,133,231)
  130 T = YMIN + DTS(2)*FLOAT(I)
      LT = MOD(I,IT(2)).EQ.0
      GO TO 134
```

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  131 IF(I.EQ.40)ASSIGN 231 TO ITT
      T = YMIN + ALOG10(1. + FLOAT(I)/10.)
      LT = MOD(I,10).EQ.0
      GO TO 134
  231 T = YMIN + ALOG10(5. + FLOAT(I-40)/5.)
      LT = MOD(I-40,5).EQ.0
      GO TO 134
  132 ILN = MOD(I-1,18)+3
      T = YMIN + ALOG10(FLOAT(ILN)/2.) + FLOAT((I-1)/18)
      LT = MOD(ILN,4).EQ.0
      GO TO 134
  133 ILN = MOD(I-1,9)+2
      T = YMIN + ALOG10(FLOAT(ILN)) + FLOAT((I-1)/9)
      LT = ILN.EQ.2.OR.MOD(ILN,5).EQ.0
C  TICS  Y-AXIS  RIGHT
  134 IY = I*3+IX
      X(IY) = XMAX
      X(IY+1) = XMAX - TL(1)
      IF(LT)X(IY+1) = X(IY+1) - TL(1)
      X(IY+2) = XMAX
      Y(IY) = T
      Y(IY+1) = T
  135 Y(IY+2) = T
      IY = IY+3
      X(IY) = XMAX
      Y(IY) = YMAX
      IZ = IX+2
      T = YMAX + YMIN
C  TICS  X-AXIS  TOP
      DO 136 I = 1,IX
      JT = IY+I
      JB = IZ-I
      X(JT) = X(JB)
  136 Y(JT) = T - Y(JB)
      IZ = IX+IY
      IX = IY-IX-1
      IY = IY+1
      T = XMAX + XMIN
C  TICS  Y-AXIS  LEFT
      DO 137 I = 1,IX
      JT = IZ+I
      JB = IY-I
      X(JT) = T - X(JB)
  137 Y(JT) = Y(JB)
      WRITE(98,138)NG
  138 FORMAT(6H GRAPH,I4)
      CALL CCALTR(-250.,305.,1,2)
      IF(IPX)1438,1438,1138
 1138 T = (CCXMAX - CCXMIN)*.5 - FLOAT(IPX)*7.
      XP = 153.
      IF(L(1).OR.ITE(1).EQ.0)GO TO 1238
      T = T - DIM(140. - T,0.)
      IF(T.LT.-42.)XP = 133.
 1238 T = AMAX1(T,-42.)
C  LABEL X-AXIS
 1338 CALL CCALTR(CCXMIN + T,XP,0,2,PRNTX,MIN0(IPX,64))
 1438 IF(L(1))GO TO 140
      IF(ITE(1).EQ.0)GO TO 238
C  SCALE FACTOR X-AXIS
      CALL CCALTR(CCXMAX - 84.,153.,0,2,6H( 10 ),6)
      CALL CCALTR(CCXMAX - 66.,156.,0,1,1HX,1)
      WRITE(98,141)ITE(1)
      CALL CCALTR(CCXMAX - 42. + SPACE(ITE(1)),163.,0,1)
  238 IM = IR(1)/IT(1)+1
      DTS(1) = DTS(1)*FLOAT(IT(1))
      T = AMAX1(SPACE(INT(XMAX*P(1))),SPACE(INT(XMIN*P(1)))) - W
      IF(T.GT.21.)PRINT 2238,NG,NAX(1),XMIN,NAX(1),XMAX,NAX(1)
 2238FORMAT(39HOERROR MESSAGE, SUBROUTINE GRAPH, GRAPH14//10XA1,5HMIN =
     11PE15.7,2H, A1,5HMAX =E15.7,1H,/10X15HGRID LABELS ON A1,23H AXIS M
     2AY BE TRUNCATED.//)
      IF((T*2. + 56.)*FLOAT(IM-1).LE.CCXMAX - CCXMIN)GO TO 338
      DTS(1) = DTS(1)*2.
      DPL(1) = DPL(1)*2.
      IM = (IM-1)/2+1
  338 T = T + 39.
      I = IW(1)
      FMT = FM(I)
C  NUMBERS ON X-AXIS (LINEAR)
      DO 139 I = 1,IM
      XI = FLOAT(I-1)
      XP = (XMIN + DTS(1)*XI)*P(1)
      IF(ABS(XP).LE.QP)XP = QP
      WRITE(98,FMT)XP
      CALL CCALTR(T + DPL(1)*XI,173.,0,2)
  139 CONTINUE
      GO TO 151
C  NUMBERS ON X-AXIS (LOG)
  140 IM = RAN(1) + 1.
      DO 149 I = 1,IM
      XI = FLOAT(I-1)
      IX = XMIN + XI
      T = 95. + DCYC*XI
      IF(IX.EQ.0)GO TO 142
      CALL CCALTR(T - 14.,173.,0,2,2H10,2)
      IF(IX.EQ.1)GO TO 143
      WRITE(98,141)IX
  141 FORMAT(I3)
      CALL CCALTR(T + SPACE(IX),183.,0,1)
      GO TO 143
  142 CALL CCALTR(T,173.,0,2,1H1,1)
  143 IF(I.EQ.IM)GO TO 149
      DO 148 J = 2,JMX,JMS
      WRITE(98,147)J
  147 FORMAT(I1)
      CALL CCALTR(T + DCYC*ALOG10(FLOAT(J)),173.,0,2)
  148 CONTINUE
  149 CONTINUE
  151 IF(L(2))GO TO 153
      IM = IR(2)/IT(2)+1
      DTS(2) = DTS(2)*FLOAT(IT(2))
```

```
      I = IW(2)
      FMT = FM(I)
C  NUMBERS ON Y-AXIS (LINEAR)
      DO 152 I = 1,IM
      XI = FLOAT(I-1)
      XP = (YMIN + DTS(2)*XI)*P(2)
      IF(ABS(XP).LE.QP)XP = QP
      WRITE(98,FMT)XP
      CALL CCALTR(16.,193. + DPL(2)*XI,0,2)
  152 CONTINUE
      GO TO 260
  153 IM = RAN(2) + 1.
C  NUMBERS ON Y-AXIS (LOG)
      DO 160 I = 1,IM
      XI = FLOAT(I-1)
      IX = YMIN + XI
      T = 193. + DCYC*XI
      IF(IX.EQ.0)GO TO 154
      CALL CCALTR(52.,T,0,2,2H10,2)
      IF(IX.EQ.1)GO TO 155
      WRITE(98,141)IX
      CALL CCALTR(66. + SPACE(IX),T + 10.,0,1)
      GO TO 155
  154 CALL CCALTR(66.,T,0,2,1H1,1)
  155 IF(I.EQ.IM)GO TO 160
      DO 159 J = 2,JMX,JMS
      WRITE(98,147)J
      CALL CCALTR(66.,T + DCYC*ALOG10(FLOAT(J)),0,2)
  159 CONTINUE
  160 CONTINUE
  260 XI = CCYMAX + 13.
      IF(L(2).OR.ITE(2).EQ.0)GO TO 161
C  SCALE FACTOR Y-AXIS
      CALL CCALTR(16.,XI,0,2,6H( 10 ),6)
      CALL CCALTR(34.,XI + 3.,0,1,1HX,1)
      WRITE(98,141)ITE(2)
      CALL CCALTR(58. + SPACE(ITE(2)),XI + 10.,0,1)
  161 IF(L(2))GO TO 261
      W = 7.*FLOAT(IW(2) - 2)
      T = AMAX1(SPACE(INT(YMAX*P(2))),SPACE(INT(YMIN*P(2)))) - W
      IF(T.GT.21.)PRINT 2238,NG,NAX(2),YMIN,NAX(2),YMAX,NAX(2)
      IF(ITE(2).NE.0)T = 21.
      T = 44. - AMIN1(42.,T*2.)
      GO TO 361
  261 T = 38.
  361 IF(IPY)561,561,461
  461 XP = (CCYMAX - CCYMIN)*.5 - FLOAT(IPY)*7.
      XP = AMAX1(XP,-7.)
C  LABEL Y-AXIS
      CALL CCALTR(T,CCYMIN + XP,1,2,PRNTY,MIN0(IPY,64))
C
C  FOLLOWING TWO CARDS ARE A MODIFICATION BY R. E. LEVY
  561 CCXMAX=CCXMIN+(CCXMAX-CCXMIN)*(1.01*XMAX-XMIN)/(XMAX-XMIN)
      XMAX=1.01*XMAX
C
C  GRIDS AND TICS
      CALL CCPLOT(X,Y,JT)
      IF(NCURV.LE.0)GO TO 167
C  PLOT CURVES
      DO 166 K = 1,NCURV
      READ(ITAPE)NPT,(X(I),Y(I), I = 1,NPT)
      IF(.NOT.L(1))GO TO 163
      DO 162 I = 1,NPT
  162 X(I) = ALOG10(X(I))
  163 IF(.NOT.L(2))GO TO 165
      DO 164 I = 1,NPT
  164 Y(I) = ALOG10(Y(I))
  165 CALL CCPLOT(X,Y,NPT)
  166 CONTINUE
  167 RETURN
      END
```

G.10 Typical Input Data

The following are input data cards for a typical calculation: case A-10-1 with response to step changes in each of the six distillation inputs.

The following cards are read by EXEC.

```
5    1  48          1.0    +8
                    TEN-TRAY BUBBLE-CAP COLUMN
                    ACETONE-BENZENE SYSTEM
                    SUBCOOLED FEED AND REFLUX
```

The following cards are read by DISTM.

```
  2  12   1   2   1  30          2   2            4
-7.66+3 1.279+1                 1.1480+41.7260+11.237 -23.3080+4  2.76+
1.237-2 -6.16+3  9.79+                  0.9710+4  9.38+  2.105-23.1860+4
-4.69+ 2.105-02
 1.00-2  2.66-2  2.66-2  2.66-2  2.66-2  2.66-2  1.60-2  1.60-2  1.60-2
 1.60-2  1.60-2  1.60-2
 6.70+2  6.67+2  6.64+2  6.61+2  6.58+2  6.55+2  6.52+2  6.49+2  6.46+2
 6.43+2  6.40+2  6.40+2
  6
0.583 +3  1.25-2  1.25-2
1.0   -31.0   -39.0   +11.    +1                          1.1111+1
```

The following cards are read by EQUIL and DISTM.

```
 2.750+ 2.745 + 2.740 + 2.735 + 2.730 + 2.725 + 2.720 + 2.715 + 2.710 +
2.705 + 2.700 + 2.700 +
5.808 +17.34  +1-4.51 -27.811 +17.75  +1-4.16 -2
2.45  + 4.07  -13.00  -21.59  -11.    -33.0   -14.0   -1
2.68  -12.68  -12.68  -1       10.   -290.   -218.   -282.   -226.   -2
74.   -234.   -266.   -242.   -258.   -250.   -250.   -256.   -244.   -2
62.   -238.   -268.   -232.   -273.   -227.   -278.   -222.   -283.   -2
17.   -2
1.19  +56.95  +35.55  +46.95  +31.726 +12.47  -29.37  + 4.21  -22.16  +4
1.45  +12.215 +41.407 +17.33  + 5.65    5.60  +26.    + 6.0   +11.0   +1
.82  +05.82  + 6.17  + 1.66  +19.20  + 2.45   2
```

The following cards are read by RESPN.

```
 1 2 3 4 5 6
9.4   -3
       1.535 -2
              5.0   -3
                    1.0   -2
                          2.02   2
                                1.55  -2
```

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