A Generalized Model for the Dynamic Behavior of a Distillation Column

N. J. TETLOW, D. M. GROVES, and C. D. HOLLAND
Texas A&M University, College Station, Texas

The generalized model accounts for the effects of channeling, transfer lag, mixing, and mass transfer that occur on each plate of a column in the process of separating a multicomponent mixture at unsteady state operation. The equations required to describe the model were tested by solving a wide variety of numerical examples. Selected numerical results are presented to demonstrate certain characteristics and uses of the generalized model.

Presented herein is the formulation of a more general model for the unsteady state operation of a distillation column than has been available previously. Suitable numerical methods for solving the equations required to describe the model are also presented. The reliability of the proposed numerical methods was established by solving a wide variety of problems (*18*). To demonstrate some of the characteristics of the model as well as possible uses, such as the analysis of various control schemes, selected numerical results are presented in a subsequent section.

In general, the models proposed for distillation columns in unsteady state operation may be divided into two groups: one group consists of those models used to obtain analytical and analog computer solutions; and the other group consists of those models used to obtain numerical solutions by use of digital computers. Analytical and analog models generally require many simplifying assumptions, such as linear equilibrium relationships, the lumping together of plates, and the treatment of multicomponent mixtures as binary mixtures. In the past these models have proved to be useful for the broad understanding of the operation of distillation columns (*6*) and are presently being used successfully as a basis for column control (*9*). Models of the second group used to obtain numerical solutions on digital computers need not contain many of the simplifying assumptions generally used for the simpler analytical and analog models. Models of the second group, which give an accurate description of column operation, have been proposed by Rosenbrock (*15*), who cited reasons for their superiority over the approximate models of the first group. Peiser et al. (*13*) proposed a model of the second group and used it in the solution of a plant problem involving the flooding of a section of a distillation column. As pointed out by Peiser et al., no information pertaining to a problem of this type could be obtained from the usual steady state model or a simplified unsteady state model that did not contain fluid dynamic relationships. Moczek et al. (*12*) used a variation of the model proposed by Rosenbrock to test simpler models of the first group.

Previous models have neglected the combination of mixing effects on the plates and in the downcomers, and in most models the mixing effects in the holdups of the reflux drum and transfer lines have been neglected also. The present model includes the effect of mixing in all of these holdups. Liquid passing through a column exhibits some degree of mixing in the direction of bulk flow. The mixing effects of a liquid in bulk flow, without dead volume, on a plate and its downcomer are bounded by those for the three limiting cases: perfect mixing, plug flow, and channeling. The third limiting case was introduced to account for bypass flow such as the weeping of liquid through plates. Over a given period of time, the mixing effects of a binary liquid mixture (under the flow conditions enumerated) may be accounted for by use of a linear combination of the three modes. Thus, it was elected to approximate the mixing effects of a multicomponent liquid mixture on a plate and its downcomer, which was not in contact with vapor, in the same manner as shown in Figure 1. To describe the mass transfer that occurs on each plate, the mass transfer section is employed. In this section, mass is transferred according to the relationship:

$$y_{ji} = E_{ji}K_{ji}x_{ji} \tag{1}$$

The mass transfer section has the capacity for effecting the same amount of mass transfer as that observed on the

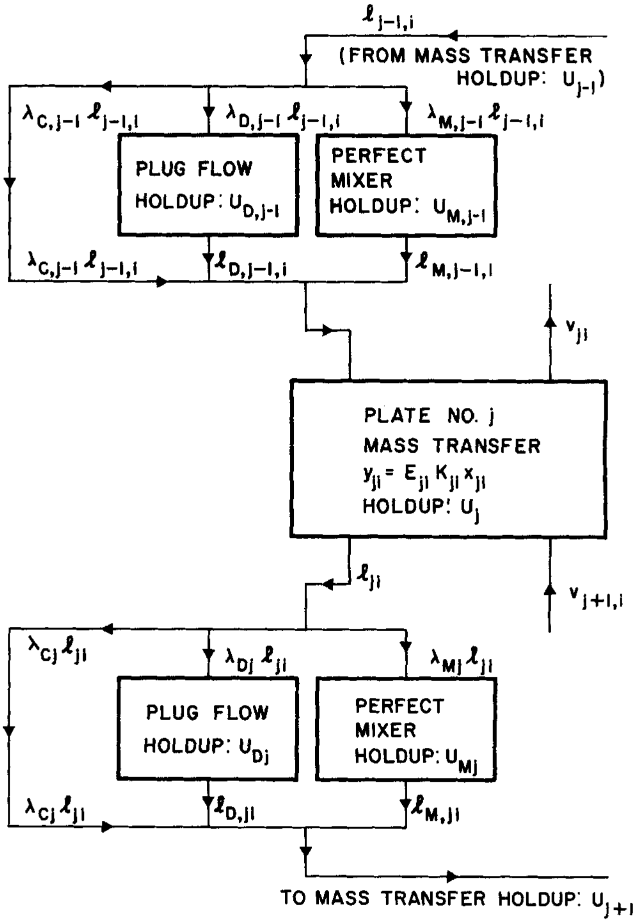

Fig. 1. Model for a typical plate *j*.

N. J. Tetlow is at Texas Instruments, Dallas, Texas. D. M. Groves is at Humble Oil and Refining Company, Baytown, Texas.

actual plate. More precisely, it is supposed that the mean mole fraction $(x_{ji})_m$ of each component i in the holdup of this section is equal to the mole fraction x_{ji} of component i in the liquid leaving plate j at any instant. Furthermore, the mole fraction of component i in the vapor leaving the mass transfer section is equal to its mean value in the vapor entering plate $j - 1$; that is, $V_j y_{ji} = v_{ji}$, the vapor flow rate at which component i enters plate $j - 1$. Thus, if the liquid in contact with vapor on the actual plate were perfectly mixed, the vapors above plate j were likewise perfectly mixed, and the vapor path through the liquid were of infinite extent, then Equation (1) reduces to the well-known equilibrium relationship $y_{ji} = K_{ji} x_{ji}$ or $E_{ji} = 1$. Thus, the vaporization efficiency (*8*) accounts for both mixing and rate effects and may be regarded as the fractional deviation of the mass transfer section from an equilibrium section.

Thus, by the proposed model shown in Figure 1, the liquid stream passes alternately through weighted mixers and mass transfer sections. More precisely, as shown in Figure 1, the total holdup associated with each plate j is divided into three parts, denoted by U_{Dj}, U_{Mj}, and U_j. The holdup U_{Dj} represents that part of plate j that contains liquid which is in plug flow but not in contact with a vapor stream. The liquid entering the holdup U_{Mj} is perfectly mixed with the contents of U_{Mj} without contacting a vapor stream. In the holdup U_j, mass transfer occurs between the vapor V_{j+1} entering plate j and the liquid in the holdup U_j. The positive multipliers $\lambda_{C,j-1}$, $\lambda_{D,j-1}$, $\lambda_{M,j-1}$, whose sum is unity, are the fractions of the stream L_{j-1} that proceed to plate j by channeling, plug flow, and by passing through the perfect mixer, respectively. Note that when $\lambda_{Cj} = 1$ for all j, the present model reduces to one similar to those used by Waggoner et al. (*20*) and Peiser et al. (*13*).

The holdups in mass (or volumetric) units corresponding to the molal holdups U_{Dj}, U_{Mj}, and U_j are denoted by $\mathcal{M}_{Dj}$, $\mathcal{M}_{Mj}$, and $\mathcal{M}_j$, respectively. A new set of holdups was computed at the end of each trial of each time period by use of fluid dynamic relationships. The relationships between the inputs and outputs to the respective holdups $\mathcal{M}_{Dj}$ and $\mathcal{M}_{Mj}$ are needed in the subsequent statements of material and enthalpy balances.

RELATIONSHIPS BETWEEN THE INPUTS AND OUTPUTS TO THE PLUG FLOW AND PERFECT MIXER HOLDUPS

Throughout these developments, it is supposed that the liquid mixtures are ideal solutions in the sense that the volume of the mixture is equal to the sum of the volumes of the individual components. Then, at any time t the average molecular weight (or average molal volume) of the liquid leaving the mass transfer holdup U_j has the form

$$M_j = \sum_{i=1}^{c} M_i x_{ji} \tag{2}$$

where M_i denotes the molecular weight of component i or molal volume (at the conditions of the liquid leaving the holdup U_j). Since the total mass (or volumetric) flow rate at any time t is given by the product $L_j M_j$, the mass (or volumetric) flow rates for channeling, plug flow, and perfect mixing are given by $\lambda_{Cj} L_j M_j$, $\lambda_{Dj} L_j M_j$, and $\lambda_{Mj} L_j M_j$, respectively. The total molal holdup of the mass transfer section at the end of each trial for a given time is then computed in the usual way, $U_j = \mathcal{M}_j / M_j$. Similarly, for a perfect mixer j, the total molal holdup is computed by use of the relationship $U_{Mj} = \mathcal{M}_{Mj} / M_{Mj}$. The residence time or contact time of the liquid in the perfect mixer is computed in an obvious manner; namely $t_{Mj} = U_{Mj} / L_{Mj}$.

An expression relating the inlet mass (or volumetric) flow rate $\lambda_{Mj} L_j M_j$ to the outlet mass (or volumetric) flow rate $L_{Mj} M_{Mj}$ is obtained by use of the following material balance that encloses the perfect mixer of plate j.

$$\int_{t_n}^{t_{n+1}} [\lambda_{Mj} L_j M_j - L_{Mj} M_{Mj}] \, dt = \mathcal{M}_{Mj}\Big|_{t_{n+1}} - \mathcal{M}_{Mj}\Big|_{t_n} \tag{3}$$

When the integral is approximated by use of the implicit method, as described by Waggoner et al. (*20*) and the resulting expression solved for $L_{Mj} M_{Mj}$, the following result is obtained

$$L_{Mj} M_{Mj} = \lambda_{Mj} L_j M_j + \sigma [\lambda_{Mj} L_j^0 M_j^0 - L_{Mj}^0 M_{Mj}^0] - \left[\frac{\mathcal{M}_{Mj} - \mathcal{M}_{Mj}^0}{\mu \Delta t} \right] \tag{4}$$

The superscript 0 denotes the value of a variable at time t_n, the beginning of the time period under consideration. The absence of a superscript means the value of the variable at time t_{n+1}, the end of the time period. The absence of a superscript is also used to denote the instantaneous value of a variable. When the meaning of the symbol without a superscript is not clear from the context, the precise time at which the variable is to be evaluated is indicated.

The component flow rates to and from the perfect mixer of plate j are related by the following component–material balance that encloses the perfect mixer.

$$\int_{t_n}^{t_{n+1}} (\lambda_{Mj} l_{ji} - l_{Mji}) \, dt = u_{Mji}\Big|_{t_{n+1}} - u_{Mji}\Big|_{t_n} \tag{5}$$

Approximation of the integral on the left-hand side by use of the implicit method, followed by rearrangement, yields

$$l_{Mji} = a_j l_{ji} + b_j l_{ji}^0 + c_j l_{Mji}^0 \tag{6}$$

and summation of each member of this expression over all components gives

$$L_{Mj} = a_j L_j + b_j L_j^0 + c_j L_{Mj}^0 \tag{7}$$

where

$$a_j = \frac{\lambda_{Mj}}{1 + \tau_{Mj}/\mu}; \quad b_j = \sigma a_j; \quad c_j = \left[\frac{\tau_{Mj}^0}{\mu} - \sigma \right] \frac{a_j}{\lambda_{Mj}};$$

$$\sigma = (1 - \mu)/\mu; \quad \tau_{Mj} = t_{Mj}/\Delta t; \quad \tau_{Mj}^0 = t_{Mj}^0/\Delta t$$

The development of the formula for l_{Dji} as a function of l_{ji} follows. By plug flow is meant that the concentration of each component i [in moles per unit mass (or volume)] leaving the holdup $\mathcal{M}_{Dj}$ at time t_{n+1} is equal to the concentration of the liquid entering $\mathcal{M}_{Dj}$ at time $t_{n+1} - t_{Dj}$; that is

$$C_{Dji}\Big|_{t_{n+1}} = C_{ji}\Big|_{t_{n+1} - t_{Dj}} \tag{8}$$

where t_{Dj} is the time required for the contents of $\mathcal{M}_{Dj}$ to be swept out once. If it is supposed that concentration varies linearly with time over each time period and that $t_{Dj} < \Delta t$, then the concentration at time $t_{n+1} - t_{Dj}$ is given by

$$C_{ji}\Big|_{t_{n+1} - t_{Dj}} = C_{ji}\Big|_{t_{n+1}} - t_{Dj} \left(\frac{C_{ji}\Big|_{t_{n+1}} - C_{ji}\Big|_{t_n}}{\Delta t} \right) \tag{9}$$

To obtain the desired formula for l_{Dji} from this expression, note that an equivalent statement of Equation (8) is

$$\frac{l_{Dji}}{L_{Dj} M_{Dj}}\Bigg|_{t_{n+1}} = \frac{l_{ji}}{L_j M_j}\Bigg|_{t_{n+1} - t_{Dj}} \tag{10}$$

Then from Equations (9) and (10), it follows that

$$l_{Dji} = d_j l_{ji} + e_j \overset{0}{l}_{ji} \tag{11}$$

and that

$$L_{Dj} = d_j\, L_j + e_j\, \overset{0}{L}_j \tag{12}$$

where

$$d_j = \frac{L_{Dj}\, M_{Dj}}{L_j\, M_j}\left(1 - \frac{t_{Dj}}{\Delta t}\right); \quad e_j = \frac{L_{Dj}\, M_{Dj}\, t_{Dj}}{\Delta t\, \overset{0}{L}_j\, \overset{0}{M}_j}$$

The outlet mass (or volumetric) flow rate $L_{Dj} M_{Dj}$ is found by use of a mass (or volumetric) balance analogous to the one given by Equation (4).

$$L_{Dj}\, M_{Dj} = \lambda_{Dj}\, L_j\, M_j + \sigma\left[\lambda_{Dj}\, \overset{0}{L}_j \overset{0}{M}_j - \overset{0}{L}_{Dj}\, \overset{0}{M}_{Dj}\right] - \frac{\mathcal{M}_{Dj} - \overset{0}{\mathcal{M}}_{Dj}}{\Delta t} \tag{13}$$

The formula for the residence time t_{Dj} is developed as follows. Since t_{Dj} is the time required to sweep out the holdup $\mathcal{M}_{Dj}$ one time, it follows that

$$\mathcal{M}_{Dj} = \int_{t_{n+1} - t_{Dj}}^{t_{n+1}} \lambda_{Dj}\, L_j\, M_j\, dt \tag{14}$$

If it is supposed that the flow rate $L_j M_j$ varies linearly with time between t_n and t_{n+1} and $t_{Dj} < \Delta t$, then Equation (14) reduces to

$$\mathcal{M}_{Dj} = \lambda_{Dj}\, t_{Dj}\left[L_j\, M_j - \frac{t_{Dj}}{2}\left(\frac{L_j\, M_j - \overset{0}{L}_j \overset{0}{M}_j}{\Delta t}\right)\right] \tag{15}$$

The residence time t_{Dj} is found from this expression by use of the quadratic formula. If $\overset{0}{L}_j \overset{0}{M}_j \cong L_j\, M_j$, Equation (15) reduces approximately to

$$t_{Dj} = \frac{\mathcal{M}_{Dj}}{\lambda_{Dj}\, L_j\, M_j}$$

For the case where $t_{Dj} > \Delta t$, the development is carried out in a manner analogous to that shown above by supposing that C_{ji} and $L_j M_j$ vary linearly over each time period (*18*).

A discussion of the assignment of the holdups follows. No holdup is assigned for the bypass or channeling stream, which implies that the bypass reaches the next plate in zero time. The holdups $\mathcal{M}_{Dj}$ and $\mathcal{M}_{Mj}$ are selected such that they are proportional to the corresponding flow rates ($\lambda_{Dj}\, L_j\, M_j$ and $\lambda_{Mj}\, L_j\, M_j$) of the streams entering these holdups. That is

$$\mathcal{M}_{Dj} = \frac{\lambda_{Dj}}{\lambda_{Dj} + \lambda_{Mj}}\begin{bmatrix}\text{total mass (or volume)}\\ \text{holdup assigned to the}\\ \text{mixer between plates } j\\ \text{and } j+1\end{bmatrix} \tag{16}$$

$$\mathcal{M}_{Mj} = \frac{\lambda_{Mj}}{\lambda_{Dj}}\, \mathcal{M}_{Dj} \tag{17}$$

In the problems solved, the holdups of the mixers were taken equal to the holdups of the downcomers. However, if desired, part of the liquid near the entrance of plate j may be considered as a part of the downcomer holdup of plate $j - 1$, and part of the liquid near the exit of plate j may be considered as part of the downcomer holdup of plate j.

In the model for the condenser–accumulator section, the accumulator was regarded as the mixer between the condenser and the top plate of the column. For the case of a total condenser, the liquid distillate was withdrawn between the mixer and the top plate and possessed the same composition as the reflux stream L_R to the column. For the case of a partial condenser, the vapor distillate was withdrawn from the condenser. Then for a column with a total condenser, the molal reflux rate is given by

$$L_R = \lambda_{C0}\, L_0 + L_{D0} + L_{M0} - D \tag{18}$$

where L_0 is the flow rate of liquid from the condenser to the accumulator. The volumetric reflux rate $L_R M_R$ is given by

$$L_R M_R = \lambda_{C0}\, L_0\, M_0 + L_{D0}\, M_{D0} + L_{M0}\, M_{M0} - D M_R \tag{19}$$

The holdups $\mathcal{M}_{D0}$ and $\mathcal{M}_{M0}$ are related as indicated by Equation (17), and the holdup for mass transfer $\mathcal{M}_0$ is fixed relative to the other holdups.

COMPONENT–MATERIAL BALANCES

More than one equivalent method for writing the component–material balances exists (*18*). In the following statement of these balances, only the holdup for mass transfer U_j is enclosed by each balance (see Figure 1). The set of integral-difference equations so obtained is converted to a set of algebraic equations by use of the implicit method in a manner analogous to that described by Waggoner et al. (*20*). The algebraic equations have the following representation:

$$\begin{bmatrix}
-\rho_{0i} & 1 & 0 & 0 & 0 \ldots\ldots 0 & & \\
\delta_{0i} & -\rho_{1i} & 1 & 0 & 0 \ldots\ldots 0 & & \\
 & \delta_{1i} & -\rho_{2i} & 1 & 0 \ldots\ldots 0 & & \\
\ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\
0 \ldots\ldots & & & 0 & \delta_{N-1,i} & -\rho_{Ni} & 1 \\
0 \ldots\ldots & & & 0 & 0 & \delta_{Ni} & -\rho_{N+1,i}
\end{bmatrix}
\begin{bmatrix} v_{0i} \\ v_{1i} \\ v_{2i} \\ \ldots\ldots \\ v_{Ni} \\ v_{N+1,i} \end{bmatrix}
=
\begin{bmatrix} -P_{0i} \\ -P_{1i} \\ -P_{2i} \\ \ldots\ldots \\ -P_{Ni} \\ -P_{N+1,i} \end{bmatrix} \tag{20}$$

where

$$\rho_{ji} = 1 + A_{ji}(1 + \tau_j/\mu)$$

$$\delta_{ji} = [\lambda_{Cj} + a_j + d_j]\ A_{ji}$$

$$P_{ji} = \sigma\left[\overset{0}{z}_{ji} + \overset{0}{v}_{j+1,i} + \lambda_{C,j-1}\overset{0}{l}_{j-1,i} + \overset{0}{l}_{D,j-1,i} + \overset{0}{l}_{M,j-1,i} - \overset{0}{v}_{ji} - \overset{0}{l}_{ji}\right] + \frac{\overset{0}{\tau}_j}{\mu}\overset{0}{l}_{ji} + [b_{j-1} + e_{j-1}]\, l_{j-1,i} + c_{j-1} l_{M,j-1,i} + z_{ji}$$

$$P_{N+1,i} = \sigma\left[\lambda_{C,N}\overset{0}{l}_{Ni} + \overset{0}{l}_{D,Ni} + \overset{0}{l}_{M,Ni} - \overset{0}{v}_{N+1,i} - \overset{0}{l}_{N+1,i}\right] + \frac{\overset{0}{\tau}_{N+1}}{\mu}\overset{0}{l}_{N+1,i} + [b_N + e_N]\, l_{Ni} + c_N l_{M,Ni}$$

$z_{ji} = 0(j \neq f - 1, f)$. $z_{f-1,i} = v_{Fi}$, $z_{fi} = l_{Fi}$. For bubble point liquid and subcooled feeds, $l_{Fi} = FX_i$ and $v_{Fi} = 0$. For dew point vapor and superheated feeds $v_{Fi} = FX_i$ and $l_{Fi} = 0$.

Equation (20) applies for a column with a partial condenser; however, it is readily modified to describe a column with a total condenser (*18*).

THE θ METHOD OF CONVERGENCE

The θ method of convergence is developed for the two general types of specifications considered. These two sets of specifications differ in that in the first set, one of the specifications is a product rate B (or D), whereas, in the second set, the reboiler duty Q_R is specified instead of a product rate.

Specifications: L_R/D (or L_R, or L_o), B (or D) $\mathcal{M}_O$ and $\mathcal{M}_{N+1}$

The specifications of B (or D) and the two holdups give rise to the multipliers θ_{-1}, θ_0, and θ_{N+1}, defined as follows:

$$\left.\begin{aligned} \left(\frac{b_i}{d_i}\right)_{co} &= \theta_{-1}\left(\frac{b_i}{d_i}\right)_{ca} \\ \left(\frac{u_{0i}}{d_i}\right)_{co} &= \theta_0\left(\frac{u_{0i}}{d_i}\right)_{ca} \\ \left(\frac{u_{N+1,i}}{d_i}\right)_{co} &= \theta_{N+1}\left(\frac{u_{N+1,i}}{d_i}\right)_{ca} \end{aligned}\right\} \tag{21}$$

Actually, multipliers also exist for the perfectly mixed and plug flow sections of the condenser–accumulator holdups. However, in the interest of speed and simplicity, these multipliers are taken equal to the respective θ's for the mass transfer sections. Multipliers for the holdups on plates $1 \leqq j \leqq N$ do not exist, because these holdups are determined from fluid dynamic relationships rather than being specified. For these holdups, the approximate relationship $(u_{ji}/d_i)_{co} = \theta_{-1}(u_{ji}/d_i)_{ca}$ was used to relate the corrected and calculated holdups.

The multipliers θ_{-1}, θ_0, θ_{N+1} consist of that set of positive numbers that makes $g_{-1} = g_0 = g_{N+1} = 0$, simultaneously, where

$$\left.\begin{aligned} g_{-1}(\theta_{-1}, \theta_0, \theta_{N+1}) &= \sum_{i=1}^{c} (b_i)_{co} - B \\ g_0(\theta_{-1}, \theta_0, \theta_{N+1}) &= \sum_{i=1}^{c} (u_{0i}) - U_0 \\ g_{N+1}(\theta_{-1}, \theta_0, \theta_{N+1}) &= \sum_{i=1}^{c} (u_{N+1,i})_{co} - U_{N+1} \end{aligned}\right\} \tag{22}$$

where the holdups for plates $j = 0$ and $j = N + 1$ are computed as follows:

$$U_j = \frac{\mathcal{M}_j \sum_{i=1}^{c} (u_{ji})_{co}}{\sum_{i=1}^{c} (u_{ji})_{co} M_i} \tag{23}$$

Although g_0 and g_{N+1} could have been stated in terms of the sum of the holdups for mass transfer, plug flow, and perfect mixing, simplicity is achieved by use of the holdups for mass transfer alone.

To find the formula for $(d_i)_{co}$, the following overall component-material balance,

$$\int_{t_n}^{t_{n+1}} [FX_i - d_i - b_i]\, dt = \sum_{j=0}^{N+1} \left[u_{T,ji}\Big|_{t_{n+1}} - u_{T,ji}\Big|_{t_n} \right] \tag{24}$$

is reduced to algebraic form by use of the implicit method and solved for $(d_i)_{co}$ by use of Equation (21) to give

After Equation (20) has been solved for the v_{ji}'s, the molal holdups at time t_{n+1} that appear in Equation (25) are readily computed. The l_{ji}'s are given by the relationship $l_{ji} = A_{ji}\, v_{ji}$, and the l_{Mj}'s and l_{Dj}'s are calculated by use of Equations (6) and (11), respectively. Then

$$u_{Mji} = \frac{U_{Mj}}{L_{Mj}}\, l_{Mj} = t_{Mj} l_{Mji} \tag{26}$$

since the mole fraction of component i in the output from the perfect mixer is the same as it is within the mixer. The holdup u_{Dji} is found by converting the component-material balance enclosing U_{Dj} to algebraic form by the implicit method to give

$$u_{Dji} = u^0_{Dji} + \Delta t \Big[\mu(\lambda_{Dj}\, l_{ji} - l_{Dji}) + (1 - \mu)\left(\lambda_{Dj}\, l^0_{ji} - l^0_{Dji}\right)\Big] \tag{27}$$

The desired set of θ's (that set of θ's > 0 that makes $g_{-1} = g_0 = g_{N+1} = 0$, simultaneously) was found by the Newton–Raphson procedure (*8*). The values of the partial derivatives needed in the Newton–Raphson method were found by use of the analytical expressions for the derivatives.

The corrected d_i's given by Equation (25) were used to calculate the mole fractions x_{ji} and y_{ji} by use of Equations (18) and (19) of reference *20*. On the basis of the x_{ji}'s (or y_{ji}'s) so obtained, the temperatures for the next trial are found by use of the K_b method (*8*). These temperatures and compositions are used in the enthalpy and total material balances to compute the total flow rates for the next trial for the time period under consideration.

Specifications: L_R (or $L_R\ M_R$, L_R/D, or L_o), Q_R $\mathcal{M}_O$, and $\mathcal{M}_{N+1}$

For this set of specifications, the θ's are again defined by Equation (21) and the expressions for the g's are the same as those given by Equation (22). It should be acknowledged that the use of the θ method for the specification of Q_R does not represent so direct a procedure as does its use for the specification of B (or D), since the function g_{-1} treats B (or D) as the specified value. For the case where Q_R is specified, B is seen to be a derived rather than a direct specification.

ENTHALPY AND TOTAL MATERIAL BALANCES

For any plate j ($j \neq 0, f - 1, f, N + 1$), the enthalpy balance enclosing the holdup U_j (see Figure 1) is represented as follows:

$$\int_{t_n}^{t_{n+1}} [V_{j+1} H_{j+1} + \lambda_{C,j-1} L_{j-1} h_{j-1} + L_{D,j-1} h_{D,j-1} + L_{M,j-1} h_{M,j-1} - V_j H_j - L_j h_j]\, dt = U_j h_j\Big|_{t_{n+1}} - U_j h_j\Big|_{t_n} \tag{28}$$

which may be reduced by use of the implicit method to algebraic form. From the expression so obtained, the terms $L_{M,j-1} h_{M,j-1}$ and $L_{D,j-1} h_{D,j-1}$ are eliminated by use of the following expressions, which are consistent with the approximations represented by Equations (6) and (11), respectively.

$$(d_i)_{co} = \frac{FX_i + \sigma\left[F^0_i X^0_i - d^0_i - b^0_i\right] + \sum_{j=1}^{N+1} u^0_{T,ji}}{1 + \theta_{-1}\left(\frac{b_i}{d_i}\right)_{ca} + \left(\frac{1}{\mu\Delta t}\right)\left[\theta_0\left(\frac{u_{T,0i}}{d_i}\right)_{ca} + \theta_{N+1}\left(\frac{u_{T,N+1,i}}{d_i}\right)_{ca} + \theta_{-1}\sum_{j=1}^{N}\left(\frac{u_{Tji}}{d_i}\right)_{ca}\right]} \tag{25}$$

where

$$u_{Tji} = u_{ji} + u_{Dji} + u_{Mji}$$

$$L_{D,j-1}\, h_{D,j-1} = d_{j-1} L_{j-1} h_{j-1} + e_{j-1} L^0_{j-1} h^0_{j-1} \tag{29}$$

$$L_{M,j-1}\,h_{M,j-1} = a_{j-1}L_{j-1}h_{j-1} + b_{j-1}L^0_{j-1}h^0_{j-1} + c_{j-1}L^0_{M,j-1}h^0_{M,j-1}$$

Then, $V_{j+1}H_{j+1}$ is eliminated by use of the constant-composition method (*8*), and the U_j's $(1 \leqq j \leqq N)$ by use of Equations (2) and (34) are shown by Tetlow (*18*). In a similar manner, the expressions for the enthalpy balances for plates $j = f - 1, f$, and the reboiler are developed. The enthalpy balances so obtained may be represented by the functional notation $G_{2j} = 0$ $(1 \leqq j \leqq N)$ $G_{2N+3} = 0$ for a total of $N + 1$ functions.

The total material balance enclosing each holdup U_j $(j \neq f - 1, f)$ is given by

$$\int_{t_n}^{t_{n+1}} [V_{j+1} + \lambda_{C,j-1}L_{j-1} + L_{D,j-1} + L_{M,j-1} - V_j - L_j]\,dt - U_j\big|_{t_{n+1}} + U_j\big|_{t_n} = 0 \quad (30)$$

After this expression has been converted to algebraic form by use of the implicit method, $L_{M,j-1}$ and $L_{D,j-1}$ are eliminated by use of Equations (7) and (12). Also, the holdups U_j at time t_{n+1} are eliminated by use of Equations (2) and (34). The final expression so obtained is denoted by $G_{2j+1} = 0$ $(0 \leqq j \leqq N)$ and $G_{2N+2} = 0$ for a total of $N + 2$ functions.

The enthalpy and total material balances consist of a set of $2N + 3$ simultaneous equations in $2N + 5$ independent variables (the L_j's, V_j's, and Q_R). Any two of these may be either specified or obtained from other equivalent specifications for a given problem. This system of equations may be solved by use of the Newton–Raphson method to give the V_j's, L_j's, and Q_R. After these quantities have been determined, the condenser duty Q_c is obtained directly from the enthalpy balance enclosing the condenser.

To demonstrate the application of the Newton-Raphson method, suppose that the output L_{N+1} (or B) from the reboiler and the reflux ratio R are specified. For this case, the Newton–Raphson equations take the form

$$\begin{bmatrix}
C_1 & D_1 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
B_2 & C_2 & D_2 & 0 & 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
A_3 & B_3 & C_3 & D_3 & 0 & 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
0 & A_4 & B_4 & C_4 & D_4 & 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
\vdots & & & & & & & & & & & \vdots \\
0 & 0 & A_{2j} & B_{2j} & C_{2j} & D_{2j} & 0 & 0 & \cdots & \cdots & \cdots & 0 \\
0 & 0 & 0 & A_{2j+1} & B_{2j+1} & C_{2j+1} & D_{2j+1} & 0 & \cdots & \cdots & \cdots & 0 \\
\vdots & & & & & & & & & & & \vdots \\
0 & \cdots & \cdots & \cdots & \cdots & 0 & A_{2N} & B_{2N} & C_{2N} & D_{2N} & 0 & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & A_{2N+1} & B_{2N+1} & C_{2N+1} & D_{2N+1} & 0 \\
0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & 0 & A_{2N+2} & B_{2N+2} & C_{2N+2} & D_{2N+2} \\
0 & \cdots & \cdots & \cdots & \cdots & 0 & 0 & 0 & 0 & A_{2N+3} & B_{2N+3} & C_{2N+3}
\end{bmatrix}
\begin{bmatrix}
\Delta L_0 \\ \Delta V_1 \\ \Delta L_1 \\ \Delta V_2 \\ \vdots \\ \Delta V_j \\ \Delta L_j \\ \vdots \\ \Delta V_N \\ \Delta L_N \\ \Delta V_{N+1} \\ \Delta Q_R
\end{bmatrix}
=
\begin{bmatrix}
-G_1 \\ -G_2 \\ -G_3 \\ -G_4 \\ \vdots \\ -G_{2j} \\ -G_{2j+1} \\ \vdots \\ -G_{2N} \\ -G_{2N+1} \\ -G_{2N+2} \\ -G_{2N+3}
\end{bmatrix} \quad (31)$$

The coefficients in this matrix equation are defined as follows.

Enthalpy balances (even functions)	Total material balances (odd functions)
$A_{2j} = \dfrac{\partial G_{2j}}{\partial V_{j-1}}$	$A_{2j+1} = \dfrac{\partial G_{2j+1}}{\partial L_{j-1}}$
$B_{2j} = \dfrac{\partial G_{2j}}{\partial L_{j-1}}$	$B_{2j+1} = \dfrac{\partial G_{2j+1}}{\partial V_j}$
$C_{2j} = \dfrac{\partial G_{2j}}{\partial V_j}$	$C_{2j+1} = \dfrac{\partial G_{2j+1}}{\partial L_j}\ (j \neq N+1)$
$D_{2j} = \dfrac{\partial G_{2j}}{\partial L_j}\ (j \neq N+1)$	$D_{2j+1} = \dfrac{\partial G_{2j+1}}{\partial V_{j+1}}$

$$D_{2N+2} = \frac{\partial G_{2N+2}}{\partial Q_R} \qquad C_{2N+3} = \frac{\partial G_{2N+3}}{\partial Q_R}$$

It should be noted that if a function, say G_{2j}, does not contain a variable, say V_{j-1}, then $\partial G_{2j}/\partial V_{j-1}$ is, of course, equal to zero. Equation (31) is readily solved for the ΔV_j's, ΔL_j's, and ΔQ_R by use of Crout's method or the recursion formulas stated by Tetlow (*18*). These recursion formulas are readily obtained from the original matrix equation by Gaussian elimination.

FLUID DYNAMIC RELATIONSHIPS

Before and after the total flow rates have been determined as described above, the mass (or volumetric) holdups are computed by use of fluid dynamic relationships. Peiser et al. (*13*) were the first workers to include these relationships in an unsteady state model.

Many correlations for estimating the holdup of liquid on the plates and downcomers of a distillation column exist. The particular set selected should not be regarded as being the best available, but instead as being fairly typical of those in use. For example, the effects of liquid foam, the constriction of the wall on the Francis formula for the flow over a chord type weir, and the friction within the downcomer are neglected. Also, the effect of unsteady state operation on the fluid dynamic relationships has been neglected. A single-pass plate with bubble caps was selected for analysis. The following formulas appear in the literature (*1*) and most texts (*3, 11, 14, 17*) that consider the dynamics of plates of distillation columns.

The height $\mathcal{H}_j$ of liquid in the downcomer of plate j is given by

$$\mathcal{H}_j = (\mathcal{H}_{wj} + \mathcal{H}_{0w,j}) + (\mathcal{H}_{w,j+1} + \mathcal{H}_{0w,j+1}) + \mathcal{H}_{dj} + \mathcal{H}_{rj} - x \quad (32)$$

where

$$\mathcal{H}_{0w,j} = 0.45\left[\frac{L_j M_j}{l_{wj}}\right]^{2/3}; \quad \mathcal{H}_{dj} = \frac{3}{2}\left(\frac{u^2_{dj}}{g}\right)$$

$$\mathcal{H}_{rj} = \frac{3.5}{g}(u_{r,j+1})^2 \frac{\rho^V_{j+1}}{\rho^L_j}$$

The height of the weir $\mathcal{H}_{wj}$ and the height x of the top of the slot in the cap above the floor of the plate are fixed by the designer. In the formula for $\mathcal{H}_{0w,j}$, the term $L_j M_j$ has the units of cu.ft./sec. The definition of the remaining symbols and their appropriate units are given in the Notation. After $\mathcal{H}_j$ has been computed by use of Equation (32), the sum of the holdups for the perfect mixer and the plug flow section is given by

$$\mathcal{M}_{Dj} + \mathcal{M}_{Mj} = \mathcal{H}_j \mathcal{A}_{dj} \quad (33)$$

and that of the mass transfer section by

$$\mathcal{M}_j = (\mathcal{H}_{wj} + \mathcal{H}_{0w,j})\mathcal{A}_{dj} \quad (34)$$

where $\mathcal{A}_{dj}$ is the cross-sectional area (sq.ft) of the downcomer, and $\mathcal{A}_{pj}$ is the area of the floor of plate j bounded by the downcomers and the walls of the column. The individual holdups $\mathcal{M}_{Dj}$ and $\mathcal{M}_{Mj}$ are found by use of Equations (16) and (17), respectively.

To accommodate different types of fluid dynamics, Equations (32) through (34) may be replaced by the desired expressions.

CALCULATIONAL PROCEDURE

The order of performing the calculations follows closely the order of presentation of the equations. Initially, at time $t = 0$, it is necessary that the values of all variables throughout the column be known. At time $t = 0+$, it is supposed that the column is at steady state initially. The procedure is initiated by finding the transient values of the variables at the end of the first time period.

Step 1: Assume a set of temperatures, L_j's and V_j's for the end of the time period.

Step 2: Evaluate all terms appearing in the expressions for δ_{ji}, ρ_{ji}, and P_{ji} of Equation (20). Note that for steady state operation at $t = 0$, $\overset{0}{l}_{Dji}$ and $\overset{0}{l}_{Mji}$ have the same composition as $\overset{0}{l}_{ji}$ (for the first time period after the upset). Furthermore, $\lambda_{Dj} \overset{0}{L_j} = \overset{0}{L}_{Dj}$ and $\lambda_{Mj} \overset{0}{L_j} = \overset{0}{L}_{Mj}$. Compute the first set of assumed values for $\mathcal{M}_{Dj}$, $\mathcal{M}_{Mj}$, and $\mathcal{M}_j$ at the end of the period as described after Equation (32). Compute the first set of assumed values for U_j and U_{Mj} at the end of the time period as discussed after Equation (2).

Step 3: Solve Equation (20) for the v_{ji}'s for each component.

Step 4: Determine θ_{-1}, θ_0, θ_{N+1} and $(d_i)_{co}$ for each component.

Step 5: Compute the x_{ji}'s and y_{ji}'s by use of Equations (18) and (19) of Waggoner et al. (*20*), respectively.

Step 6: Determine the temperatures by the K_b method (*8*).

Step 7: Recompute the values of $\mathcal{M}_{Dj}$, $\mathcal{M}_{Mj}$, $\mathcal{M}_j$, U_j, U_{Dj}, U_{Mj}, and the a_j's . . ., e_j's, based upon the most recent values of the T_j's, L_j's, V_j's, and x_j's. Solve the enthalpy and total material balances for the L_j's and V_j's. Compute the L_{Dj}'s and L_{Mj}'s by use of Equations (12) and (7), respectively. Repeat this step until the change between successive sets of calculated rates is less than some preassigned number.

Step 8: After convergence has been achieved, predict a new set of temperatures and flow rates at the end of the next time period. The final values at the end of the present time period are adequate or the point-slope predictor as shown by Waggoner et al. may be used (*20*). Then proceed with step 2 and repeat the procedure described above.

CHARACTERISTICS AND USES OF THE GENERALIZED MODEL

The proposed convergence method and calculational procedure for the generalized model were tested by solving a large variety of examples. The results obtained for eight selected examples that involved a three-component, five-plate column, an eleven-component, twelve-plate column, and a nine-component, twenty-four-plate column were recorded by Tetlow (*18*). The proposed convergence method and calculational procedure gave satisfactory results for all problems considered.

To demonstrate some of the characteristics and uses of the generalized model, example 1 (stated in Table 1) was solved in several different ways. First, as cases I, II, and III, problems were solved to demonstrate the behavior of a column operating at each of the limiting conditions of channeling ($\lambda_{Cj} = 1$), plug flow ($\lambda_{Dj} = 1$), and perfect mixers ($\lambda_{Mj} = 1$) between all stages. The effect of the mixing model selected on the percentage of heavies

TABLE 1. STATEMENT OF EXAMPLE 1

Conponent	Initial feed (at time $t = 0$) l°_{Fi}, moles/min.	v°_{Fi}, moles/min.	Upset in feed (at time $t = 0+$) l_{Fi}, moles/min.	v_{Fi}, moles/min.
C_3H_8	1.364	0.636	1.519	0.481
i-C_4H_{10}	1.177	0.323	1.263	0.237
n-C_4H_{10}	1.224	0.276	1.299	0.201
n-C_5H_{12}	2.703	0.297	3.159	0.241
n-C_6H_{14}	1.899	0.101	2.506	0.094

Other conditions (at time $t = 0$ and $t = 0+$)

Number of stages = 25 (including a total condenser and a reboiler). Column pressure = 300 lb./sq. in. abs. Reflux rate = 10 moles/min. Initially the column is at steady state operation, and the partially vaporized feed shown enters at 201°F. at the column pressure. For time $t = 0+$, the feed shown enters at 258°F. at the column pressure. The equilibrium and the enthalpy data for the hydrocarbons were taken from Tables A-4 and A-8 of reference *8*. Other physical properties of the hydrocarbons were obtained from *Engineering Data Book*, 7 ed., Natural Gasoline Association, Tulsa, Oklahoma, 1957.

Column dimensions: Diameter of column = 5 sq. ft., plate floor area = 15.2 sq. ft., cross-sectional area of downcomers = 2.2 sq. ft., length of overflow weir = 3.75 ft., height of overflow weir = 0.25 ft., height of inlet weir = 0.23 ft., spacing between plates = 2 ft. The plates were taken to be of the sieve type that had a dry plate pressure drop equivalent to 0.06 ft. of liquid at a vapor flow rate of 15 moles/min. The holdup of the condenser was 2 cu. ft., the reflux drum was 100 cu. ft., the reboiler was 200 cu. ft., and the transfer line at the base of the column was 10 cu. ft. The mass $\mathcal{M}_s$ of steam in the reboiler tubes was 1.5 lb. The heat transfer rate constant (UA) for the reboiler was 4,500 B.t.u./(min.)(°F.). The steam line pressure was 265 lb./sq. in. abs.

Problems: For case I ($\lambda_{Cj} = 1$), case II ($\lambda_{Dj} = 1$), case III ($\lambda_{Mj} = 1$), and for cases I through IV $Q_R = 1.011 \times 10^5$ B.t.u./min. For case V, the temperature of plate 22 was controlled with a set point of 349.5°F. For cases IV and V, the λ's were weighted as stated in the text. For case V, the volumes in the accumulator and reboiler were controlled at 100 cu. ft. and 200 cu. ft. by proportional reset controllers; full-scale volumes were taken as 150 and 250 cu. ft., respectively. The settings on these controllers was $s = 1.0$ and $r = 0.2$. The settings of the temperature controller were $s = 0.3$ and $r = 0.2$, and the range of the controller was 100°F. All control valves were semilogarithmic with $K = 0.2$.

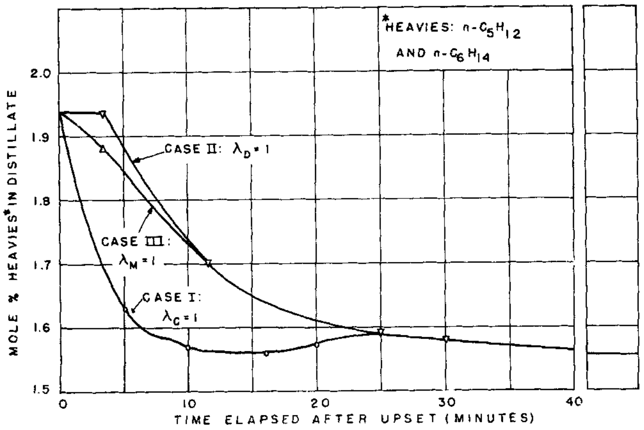

Fig. 2. Effect of each mixing model ($\lambda_{Cj} = 1$, $\lambda_{Dj} = 1$, $\lambda_{Mj} = 1$) on the distillate composition, example 1, cases I, II, and III.

(n-C_5H_{12} and n-C_6H_{14}) in the distillate is displayed in Figure 2. The results obtained for the limiting conditions of perfect mixers and plug flow models differ most during the first few minutes after the upset.*

The dead time obtained for the limiting case of plug flow corresponds approximately to the time required to sweep out the contents of the accumulator one time. In the problems solved, the holdups of the mixers between stages were taken equal to the actual volume occupied by liquid in the downcomers. Thus, in these particular examples, the accumulator played a significant role because its holdup of 100 cu.ft. was considerably larger than the sum of the holdups of the interstage mixers (approximately 46 cu.ft.).

The limiting case of channeling ($\lambda_{Cj} = 1$) might appear at first to be unrealistic, but further consideration shows that it might indeed be approached in actual operation. For example, suitably close locations of the inlets and outlets of the accumulator could easily produce results approaching the case of perfect channeling in the accumulator. In any event, it is evident that the generalized model may be used to test the effect of various design and operating variables on the dynamic behavior of a column as well as the reliability of simplified models for particular installations.

USE OF THE GENERALIZED MODEL IN THE ANALYSIS OF CONTROL SYSTEMS

The generalized model described may be used to demonstrate the behavior that can be expected of a column when its operation is governed by any one of the control systems that have been proposed for distillation columns. Over the last couple of decades, a variety of control systems for a variety of separations has been employed in the operation of a continuous distillation column (*2, 7, 9, 10, 16, 19, 21, 22*). The various control systems may be analyzed in a manner analogous to the one that follows for the system presented in Figure 3.

In this control system, the volumetric flow rate of the reflux is fixed independently of the values of all other variables and maintained at this value by the flow controller (FC). The distillate rate is regulated by use of the liquid level controller (LC) on the accumulator. The steam rate is controlled by use of the temperature controller (TC). The bottoms rate B is controlled by use of a liquid level controller (LC) on the reboiler. The pressure at the top of the column is assumed to be controlled at a fixed value in the scheme shown in Figure 3, by the rate of removal of noncondensables from the column.

For illustrative purposes, it is supposed that the controllers shown in Figure 3 are of the proportional reset type (*4, 5, 7*), which may be represented by

$$p\Big|_{t_{n+1}} - p\Big|_{t_n} = \frac{\epsilon}{s}\Bigg|_{t_{n+1}} - \frac{\epsilon}{s}\Bigg|_{t_n} + \frac{r}{s}\int_{t_n}^{t_{n+1}} \epsilon \, dt \quad (35)$$

where p = output of the controller for any given input x of the control variable, expressed as a fraction of the controller range; r = reset rate, a controller setting; s = proportional band width, a controller setting; $\epsilon = \pm\,(c - x)$; c = control point of the control variable, expressed as a fraction of the range of the input to the controller; x = value of the control variable at any time, also expressed as a fraction of the input range to the controller. Equation (35) may be reduced to the following algebraic form by use of the implicit method.

$$p - p^0 = \frac{\epsilon - \epsilon^0}{s} + \frac{r\Delta t}{s}\left[\mu\epsilon + (1-\mu)\epsilon^0\right] \quad (36)$$

The change in output $p - p^0$ of the controller may be stated in terms of the volumetric flow rate as follows. The volumetric flow rate through the control valve is given by

$$q = CA\sqrt{\frac{P_1 - P_2}{\rho}} = CA\sqrt{\Delta h} \quad (37)$$

For a semilogarithmic valve (*5*), the change in the output $p - p^0$ from the controller or the stem position of the control valve is given by

$$p - p^0 = K \log_e (A/A^0) \quad (38)$$

Thus, in view of the relationship given by Equation (37), Equation (38) may be stated as follows:

$$p - p^0 = K \log_e \left(\frac{q}{q^0}\right)\left(\sqrt{\frac{\Delta h}{\Delta h^0}}\right) \quad (39)$$

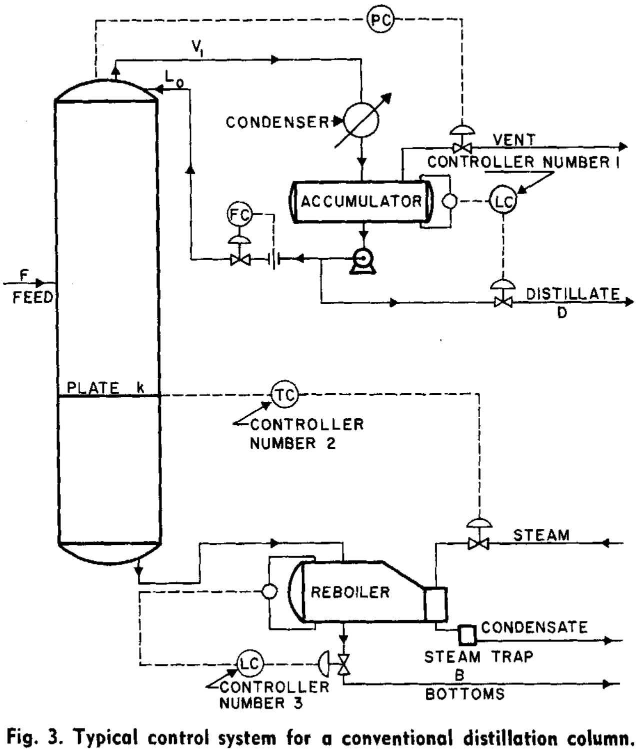

Fig. 3. Typical control system for a conventional distillation column.

---

[*] Tabular material has been deposited as document 9249 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for $2.50 for photoprints or $1.75 for 35-mm. microfilm.

The development of the controller equations for the control system shown in Figure 3 follows, after which the procedure for solving the equations so obtained simultaneously with the other equations is given. First consider the liquid level controller on the accumulator and the control valve on the distillate rate D. Elimination of $p - p^0$ from Equations (36) and (39) yields an expression involving the error

$$\epsilon - \epsilon^0 + r\Delta t\,[\mu\epsilon + (1-\mu)\epsilon^0] - Ks\log_e\left(\frac{q}{q^0}\right) = 0 \quad (40)$$

where q may be replaced by its equivalent DM_R for the accumulator and by BM_{N+1} for the reboiler. Also, the change in the pressure drop across the control valve has been neglected in Equation (40). The error ϵ is given by

$$\epsilon = \frac{h - h_c}{h_{\text{full}}} = \frac{\mathcal{M} - \mathcal{M}_c}{\mathcal{M}_{\text{full}}}$$

As shown by Tetlow (*18*), the equations for the temperature controller, the steam-control valve, and an enthalpy balance enclosing the steam side of the reboiler may be used to obtain the reboiler duty Q_R given by the temperature controller. The values of Q_R and the holdups $\mathcal{M}_0$ and $\mathcal{M}_{N+1}$ obtained from Equation (40) served as the specified values of these variables for the trial calculation under consideration. The points in the calculational procedure at which the controller equations were solved follows. Immediately preceding step 7 of the Calculational Procedure, Q_R was determined. The Q_R so obtained was used in the enthalpy balances of step 7 and the solution of the latter yielded the corresponding value of B. In the next trial, this value of B was used in the function g_{-1}. Equation (40) was solved within step 7 each time the $\mathcal{M}_j$'s $(0 \leqq j \leqq N+1)$ were computed. The $\mathcal{M}_j$'s so obtained were used to compute the U_j's for the next trial by use of Equation (23).

To demonstrate the use of the generalized model for the study of control systems such as the one shown in Figure 3, example 1 was solved in two other ways as cases IV and V. In case V the temperature of plate 22 was specified and the temperature controller on this plate determined the reboiler duty Q_R. In cases I through IV, the reboiler duty was fixed at 1.011×10^5 B.t.u./min. and the temperature controller on plate 22 was, of course, omitted. In cases IV and V, the following mixing model was employed.

Downcomers:

$$\lambda_C = 0.05, \quad \lambda_M = 0.45, \quad \lambda_D = 0.5$$

Accumulator:

$$\lambda_C = 0, \quad \lambda_M = 0.5, \quad \lambda_D = 0.5$$

Transfer line at base of tower:

$$\lambda_C = 0, \quad \lambda_M = 0, \quad \lambda_D = 1.0$$

Selected results are displayed in Figure 4 (more complete statements of these results are available elsewhere*). Improved purity was achieved through the use of the temperature controller, and the effect of the mixing model selected on the dynamic behavior of each control scheme is evident.

Thus, in conclusion, the generalized model and associated numerical methods for obtaining the dynamic behavior of a distillation column may be used to study mixing models, column designs, and control systems.

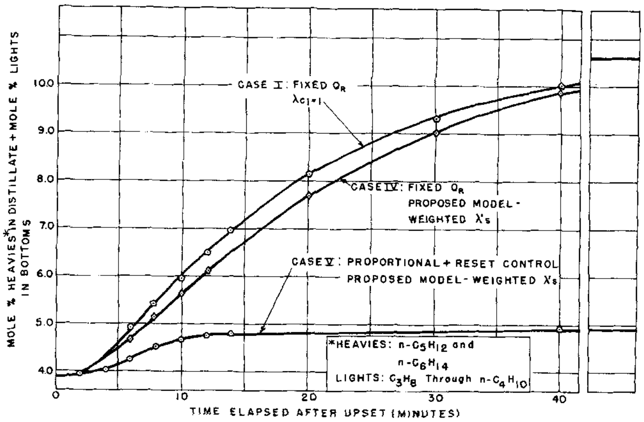

Fig. 4. Use of generalized model for simulation of control systems example 1, cases I, IV, and V.

ACKNOWLEDGMENT

The aid provided by the National Science Foundation; Texaco, Inc.; and Humble Oil and Refining Company in support of this research is gratefully acknowledged. The helpful suggestions of G. T. Atkins are appreciated.

NOTATION

a_j, b_j, c_j = coefficients used in the expression for l_{Mji}; defined below Equation (7)

A = area of opening of a valve, sq.in.; also used to denote the heat transfer area of the heat exchanger for the reboiler

A_{ji} = $L_j/(E_{ji}K_{ji}V_{ji})$

$\mathcal{A}_{dj}$ = cross-sectional area of the downcomer, sq.ft.

$\mathcal{A}_{pj}$ = area of floor of plate j bounded by the downcomers, sq.ft.

b_i = molal flow rate of component i in the bottoms product

B = total molal flow rate of the bottoms product

c = control point of the control variable, dimensionless

C = constant for a given valve; defined by Equation (37)

C_{ji}, C_{Dj} = concentration of component i in the liquid leaving the mass transfer section of plate j, and the concentration of component i in the liquid leaving the plug flow holdup of plate j; moles per unit volume

d_j, e_j = coefficients in the expression for l_{Dji}; defined below Equation (12)

E_{ji} = vaporization efficiency for component i and mass transfer holdup j

F = total molal flow rate of the feed

g = acceleration of gravity, ft./sec.^{2}

g_{-1}, g_0, g_{N+1} = functions of θ_{-1}, θ_0, and θ_{N+1}; defined by Equation (22)

G_{2j}, G_{2j+1} = enthalpy and total material balance functions, respectively

h = height of liquid in either the accumulator or the reboiler

Δh = change in head across a valve; defined by Equation (37)

h_{Dj}, h_{Mj} = enthalpies of the liquid streams leaving the plug flow holdup U_{Dj} and the perfect mixer with holdup U_{Mj}, respectively; defined by Equation (29)

h_j = $\sum_{i=1}^{c} h_{ji}\, x_{ji}$

---

* See footnote on page 482.

$H_j = \sum_{i=1}^{c} H_{ji} x_{ji}$

$\mathcal{H}_j$ = total height of liquid in the downcomer of plate j, ft.

$\mathcal{H}_{dj}$ = head loss resulting from the flow of liquid under the downcomer of plate j, ft. of liquid

$\mathcal{H}_{ow,j}$ = height of liquid over the weir, ft.

$\mathcal{H}_{rj}$ = head loss resulting from the flow of liquid through the risers and caps, ft. of liquid

$\mathcal{H}_{wj}$ = heignt of weir, ft.

K = constant for a given valve; see Equation (38)

K_{ji} = equilibrium constant; evaluated at the temperature and pressure of the mass transfer holdup of plate j

l_{ji} = molal flow rate of component i in the liquid leaving the mass transfer holdup of plate j

l_{wj} = length of the weir of plate j, ft.

l_{Dji}, l_{Mji} = molal flow rate of component i in the liquid leaving the plug flow holdup and the perfect mixer of plate j, respectively; L_{Dj} and L_{Mj} represent the total molal flow rates of these respective streams

L_j = total molal flow rate of the liquid leaving the mass transfer holdup of plate j. L_R = reflux rate; defined by Equation (18)

$\lambda_{Cj} L_j$ = total molal flow rate at which liquid passes from the mass holdup on plate j to the mass transfer holdup on plate $j + 1$

L_{Dj} = total molal flow rate of liquid leaving the plug flow holdup of plate j

L_{Mj} = total molal flow rate of the liquid leaving the perfect mixer holdup of plate j

M_R = mean molal volume of the reflux

M_i = molecular weight (or molal volume) at the conditions of liquid leaving the mass transfer section of plate j

M_j = average molecular weight (or average molal volume) of the liquid leaving the mass transfer section of plate j

M_{Dj}, M_{Mj} = average molecular weights (or average molal volume) of the liquid streams leaving the plug flow holdup and the perfect mixer of plate j, respectively

$\mathcal{M}_j$, $\mathcal{M}_{Dj}$, $\mathcal{M}_{Mj}$ = holdups in mass (or volumetric) units of the mass transfer part, the plug flow part, and the perfect mixer part of plate j, respectively

p^0, p = valve positions at the beginning and end of a time period, respectively

P_1, P_2 = pressures on the upstream and downstream sides of a control valve

P_{ji} = constant that appears in the component–material balances for each plate j and each component i; definition follows Equation (20)

q = volumetric flow rate

Q_C, Q_R = condenser and reboiler duties, respectively

r = reset rate for the reset mode; see Equation (35)

s = proportional band width; see Equation (35)

t, Δt = time; t_n denotes the time of the beginning of the time period and t_{n+1} the time of the time period under consideration; $\Delta t = t_{n+1} - t_n$

t_{Dj} = time required for a slug of liquid to pass through the plug-flow holdup

t_{Mj} = residence time for the perfectly mixed holdup

T_j = temperature of the mass transfer holdup of plate j

u_{dj} = velocity of the liquid under the downcomer, ft./sec.

u_{rj} = maximum velocity of the vapor through the riser and cap of plate j, ft./sec.

u_{Tji} = sum of u_{ji}, u_{Dji}, and u_{Mji}

U_j, U_{Dj}, U_{Mj} = total molal holdups for the mass transfer part, the plug flow part, and the perfect mixer part of plate j; the lower case letters u_{ji}, u_{Dji}, and u_{Mji} represent the corresponding holdups for component i

U = overall heat transfer coefficient for the steam heated heat exchanger for the reboiler

w = mass flow rate

x = value of the control variable; dimensionless; also used to denote the distance from the floor of the plate to the top of the slot

x_{ji} = mole fraction of component i in the liquid leaving the mass transfer holdup of plate j

X_i = total mole fraction of component i in the feed

y_{ji} = mole fraction of component i in the vapor leaving the mass transfer holdup of plate j

(FC) = flow controller; see Figure 3

(LC) = liquid level controller; see Figure 3

(PC) = pressure controller; see Figure 3

(TC) = temperature controller; see Figure 3

Greek Letters

δ_{ji} = term that appears in the component–material balances for each plate j and each component i

ϵ = error in the control variable $\epsilon = \pm (c - x)$, dimensionless

λ_{Cj}, λ_{Dj}, λ_{Mj} = fractions of the liquid stream L_j that bypass, pass through the plug flow holdup, and the perfect mixer, respectively, corresponding holdups for component i

τ_{Mj}, $\tau^0{}_{Mj}$ = dimensionless times for the perfect mixer part of plate j; definitions follow Equation (7)

θ_{-1}, θ_0, θ_{N+1} = multipliers defined by Equation (21)

ρ_{ji} = term that appears in the component–material balances for each plate j and each component i

ρ_j^L, ρ_j^V = density of the vapor and liquid streams (lb.$_m$/cu.ft.) leaving the mass transfer section of plate j

σ = $(1 - \mu)/\mu$

Subscripts

c = control point

ca = calculated value

co = corrected value

full = total volume or height

i = component number

j = plate number

m = mean value

s = saturated steam

Superscripts

V, L = vapor and liquid, respectively

0 = value of a variable at the beginning of a time period

LITERATURE CITED

1. Bolles, W. L., *Hydrocarbon Process. Petrol. Refiner*, **25**, 613 (1946).
2. Boyd, D. M., Jr., *Hydrocarbon Process. Petrol. Refiner*, **27**, No. 10, 533 (1948); No. 11, 594.
3. Brown, G. G., and Associates, "Unit Operations," Wiley, New York (1953).
4. Cleaglske, N. H., "Automatic Process Control for Chemical Engineers," Wiley, New York (1961).
5. Eckman, D. P., "Principles of Industrial Process Control," 2 ed., Wiley, New York (1956).
6. Gilliland, E. R., and C. M. Mohr, *Chem. Eng. Progr.*, **58**, No. 9, 59 (1962).
7. Harriott, Peter, "Process Control," McGraw-Hill, New York (1964).
8. Holland, C. D., "Multicomponent Distillation," Prentice-Hall, Englewood Cliffs, N. J. (1963).

9. Lupfer, D. E., and J. R. Parsons, *Chem. Eng. Progr.*, **58**, No. 9, 37 (1962).
10. Luyben, W. L., and J. A. Gerster, *Ind. Eng. Chem. Process Design Develop.*, **3**, No. 4, 374 (1964).
11. McCabe, W. L., and J. C. Smith, "Unit Operations of Chemical Engineering," McGraw-Hill, New York (1956).
12. Moczek, J. S., R. E. Otto, and T. J. Williams, *Chem. Eng. Progr. Symp. Ser. No. 55*, **61**, 136 (1965).
13. Peiser, A. M., and S. S. Grover, *Chem. Eng. Progr.*, **58**, No. 9, 65 (1962).
14. Robinson, G. S., and E. R. Gilliland, "Elements of Fractional Distillation," 4 ed., McGraw-Hill, New York (1950).
15. Rosenbrock, H. H., *Brit. Chem. Eng.*, **3**, 364, 432, 491 (1958).
16. Shinskey, F. G., *Oil Gas J.*, **63**, No. 15, 95 (1965).
17. Smith, B. D., "Design of Equilibrium Stage Processes," McGraw-Hill, New York (1963).
18. Tetlow, N. J., Ph.D. dissertation, Texas A&M Univ., College Station (1966).
19. Tivy, V. V., St. L., *Hydrocarbon Process. Petrol. Refiner*, **27**, No. 11, 603 (1948).
20. Waggoner, R. C., and C. D. Holland, *A.I.Ch.E. J.*, **11**, 112 (1965).
21. Webber, W. O., *Proc. Texas A&M Symp. Instrumentation Process Ind.*, Texas A&M Univ., College Station (1958).
22. Wherry, T. C., and D. E. Berger, *ibid.*

Manuscript received February 14, 1966; revision received September 23, 1966; paper accepted September 23, 1966. Paper presented at A.I.Ch.E. Dallas meeting.

Model-Reference Adaptive Control System

ROBERT M. CASCIANO

Newark College of Engineering, Newark, New Jersey

H. KENNETH STAFFIN

Stevens Institute of Technology, Hoboken, New Jersey

An adaptive process control scheme—which uses a differential equation model, requires no differentiations in the adaptive circuitry, and no identification of the varying process parameter—was analyzed mathematically and studied on an analog computer. The adaptive loop is operative only during a transient and corrects only in the direction of mismatch between the process and model. Linear analysis of the system differential equations when the correction signal is not introduced into the controller provides a means of designing the adaptive circuitry and approximating the effect when the signal is introduced. The effects on system stability with a pure delay, measurement lag, or an additional pole in the process are presented. Computer results show that when large differences exist between the actual process time constant and the original controller setting, the adaptive feature reduces the overshoot to essentially zero.

Chemical engineers have been slow in applying quantitative principles of feedback control theory to the design of process control systems. The major factor limiting the application of this theory to processing systems is the lack of information about process dynamics. This situation has resulted in a serious curtailment of the full use of available process control capability. The majority of the installations utilize the field-adjustable, three-mode controllers in the control scheme that duplicates the control functions when the process is operated manually. Thus, prior experience is the primary design basis in the process industry rather than a quantitative application of control theory.

In recent years, there has been increasing interest and research in process dynamics as well as a major increase in the number of engineers with good background in control theory. This situation offers the possibility of applying more sophisticated control schemes to effect superior control performance in critical applications.

One such possibility is the use of adaptive control schemes. For the work presented here an adaptive process control system is defined as a system which can alter its response to changes in the process to be controlled and that this be accomplished by measurements of input and/or response and the corresponding automatic adjustment of one or more controller parameters. One of the most difficult problems when designing an adaptive control system is the determination of process parameters, that is, process identification. Determination of the gain and time constant of a first-order system is substantially complex and the difficulty increases with process order. A number of adaptive systems dependent primarily upon system identification have appeared in the recent literature (*1* to *5*).

One very important approach to the problem of system identification is the general model-reference [MR] scheme. Oppeldahl (*6*) devised and analyzed a MR system applicable to any order system, but this method requires first- and higher order derivatives. Marcus and Hougen (*7*) have applied the MR technique to the adaptive control of a heat exchanger with slowly varying time constant. The circuitry used requires taking the derivative of the model and process outputs. Nevertheless, the results obtained by analog simulation appear promising. There is no question that the identification problem can be solved when no restriction is placed on the number of derivatives taken. When the adaptive and compensation networks are analog computers, this approach is questionable from a practical standpoint. The MR technique nonetheless appears to offer many possibilities for a number of process control problems.

The method presented here uses a differential equation model, requires no differentiation and no identification of the varying parameter. The adaptive loop is operative only during a transient and corrects only in the direction of mismatch between the system and model. Adaptation is for a single varying parameter, although other param-

---

[*] Robert M. Casciano is with Avon Products, Inc., Suffern, New York.