Application of Modern Control Theory to Distillation Columns

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Modern control theory for systems with load changes is applied to distillation column control. Both linear and nonlinear distillation models are developed and tested. Excellent control is achieved by using an optimal multivariable-proportional-integral (MPI) controller for systems with unmeasurable disturbances. When the disturbances are measurable an optimal multivariable proportional controller with error coordination (MPE) is desirable. Various structures for distillation control have also been investigated.

SCOPE

Since the early work of Kalman and Koepcke (1959) on the linear regulator problem, many interesting extensions have appeared in the literature. Of particular importance is the work of Anderson (1969) in which he derived optimal regulators for systems with constant measurable disturbances and Johnson (1968) who formulated an optimal control law for linear regulators with constant unmeasurable disturbances. The reasons for the wide interest in the linear regulator problem are the mathematical properties which allow optimal control solutions to be obtained in closed form and the fact that this problem provides a strong correlation between the classical methods of analytic feedback system design via frequency domain methods and the more recent variational approach favoring analysis in the time domain.

Most distillation control schemes (Hu, 1970) are synthesized by classical control theory based on single-loop stability analysis with the overall controlled system being a combination of individual controllers. With the advent of digital control computers it is now possible to monitor the entire multivariable process. Since modern control theory deals with multivariable systems and computing control policies based on the interrelations among all variables, a natural use is in direct digital computer control. The application of modern control theory to distillation column control is given in this work.

CONCLUSIONS AND SIGNIFICANCE

Since in digital computer control the control is applied at discrete time intervals, optimal control algorithms have been developed for discrete linear system models of distillation. Besides the standard Kalman-Koepcke (1959) formulation for pulse disturbances, algorithms are presented for both measurable and unmeasurable step disturbances. These algorithms based on a linear system model are used to control a binary five tray column with condensor and reboiler modeled via the nonlinear model of Franke, May, and Huckaba (1963).

The numerical magnitude of the control period (discrete time interval) used in the discrete system algorithms strongly influences the system performance. As the control period is decreased, the system performance approaches the performance of the system with continuous control. A control period of 0.25 min. was found adequate for distillation column control.

The results show that due to the nonlinear behavior of the system the MPE algorithm (measurable disturbances) drives the top and bottom compositions near the original steady state with some offset (0.06% maximum error). Its performance is not influenced by the discrete time control interval. On the other hand, the MIP algorithm (unmeasurable disturbances) drives the top and bottom compositions back to the steady state but with some overshoot. The overshoot is influenced by the discrete time control interval. Both of these optimal control algorithms give better control than does two well-tuned single loop proportional-integral controllers controlling the overheads and bottoms composition.

Since there are six disturbance variables for the binary distillation column system a variety of different control structures are possible besides the common reflux ratio, heat duty control structure. Three possible two control variable structures were investigated. All cases are feasible, but the case using the reflux ratio and feed flow rate as control variables gave the best performance.

The regulator problem as developed by Kalman and Koepcke (1959) is stated by considering a system which can be represented by a linear model

$$\underline{\dot{x}}(t) = \underline{\underline{A}}(t)\,\underline{x}(t) + \underline{\underline{B}}(t)\,\underline{u}(t) \tag{1}$$

We desire to bring the system from an initial state $\underline{x}_0$ to a terminal state $\underline{x}_f$ using acceptable levels of control $\underline{u}$ and not exceeding acceptable levels of the state. Kalman and Koepcke's original work minimized a performance index quadratic in the terminal state and quadratic in the time

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integral of the state and the control

$$J = \tfrac{1}{2}\, \underline{x}_f'\, \underline{\underline{S}}\, \underline{x}_f + \tfrac{1}{2} \int_{t_0}^{t_f} (\underline{x}'\underline{\underline{Q}}\underline{x} + \underline{u}'\underline{\underline{R}}\underline{u})\,dt \qquad (2)$$

The optimal control which minimizes this performance index is a proportional feedback controller

$$\underline{u}^* = -\underline{\underline{R}}^{-1}\underline{\underline{B}}'\underline{\underline{J}}\,\underline{x} \qquad (3)$$

where $\underline{J}$ is found from the solution of the Riccati equation

$$\dot{\underline{\underline{J}}} = -\underline{\underline{J}}\,\underline{\underline{A}} - \underline{\underline{A}}'\underline{\underline{J}} + \underline{\underline{J}}\,\underline{\underline{B}}\,\underline{\underline{R}}^{-1}\underline{\underline{B}}'\underline{\underline{J}} - \underline{\underline{Q}} \qquad (4)$$

Equation (3) is actually a multivariable proportional controller in which the controller constants can be computed from knowledge of the system parameters and performance index.

MATHEMATICAL MODELS

Mathematical models for distillation can be obtained via deterministic modeling (transport phenomena) or statistical modeling (indentification). We prefer the deterministic approach because the model can be used at the design stage to test potential optimal control laws before operation of the actual column.

Two types of models have been developed for use in this study. The first is a linear model used for control law computations. The second is a rigorous nonlinear model which considers the major factors affecting column performance. This model is used as a simulator to test the adequacy of the linear control laws. We have adopted the nonlinear model of Franke, May, and Huckaba (1963) as our nonlinear model. The linear model is obtained by linearizing the nonlinear model about the desired steady state. The system to be considered is the binary distillation of ethelene dichloride and toluene in a simple five tray column with condenser and reboiler. The system parameters and conditions are given in Table 1.

The linear model can be expressed as

$$\dot{\underline{x}} = \underline{\underline{A}}\,\underline{x} + \underline{\underline{B}}\,\underline{u} + \underline{\underline{W}}\,\underline{d} \qquad (5)$$

where

$$\underline{x} = \begin{bmatrix} x_0 \\ x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_5 \\ x_6 \end{bmatrix} \qquad \underline{u} = \begin{bmatrix} R \\ Q_r \end{bmatrix} \qquad \underline{d} = \begin{bmatrix} F \\ x_F \\ T_f \\ T_d \end{bmatrix} \qquad (6)$$

In order to study the influence of the disturbance and control variables on the column composition profiles, a series of nonlinear steady state simulations were performed. Step changes in the six process variables of plus-minus 10% of the steady state values were applied. The sensitivity results are presented in Figure 1 for the top product. This figure indicates that these process variables can be divided into two groups. The first group x_F, F and R cause the column ethylene dichloride compositions to increase as the disturbances increase. The second group Q_r, T_r, and T_d cause the composition to decrease as they are increased. The first group is associated with the material balance equation while the second with the energy balances.

Step changes of plus-minus 10% in each of the six process variables have been applied to the nonlinear dynamic model in order to determine the uncontrolled response of the system. The response curves are not necessarily first-order, but it is convenient to use the "time constant" (time at which 63.2% of the new steady state is reached) to compare the response data. Calculated "time constants" for various step changes and trays are shown in Table 2.

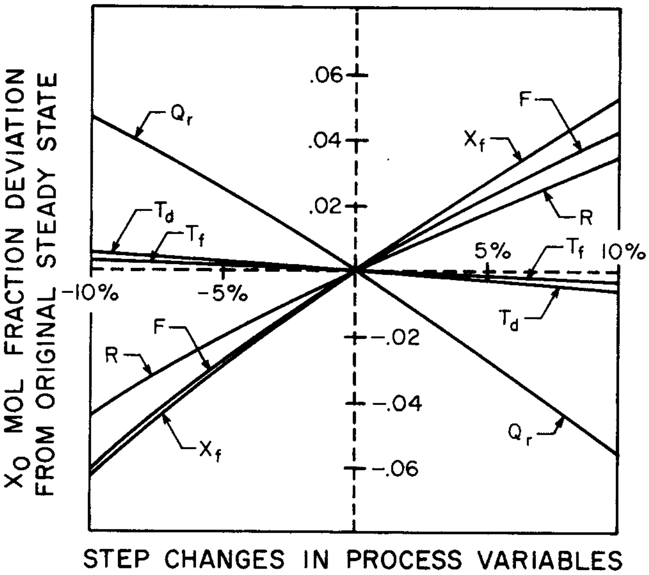

Fig. 1. New steady state after step changes overhead compositions deviation from original state.

TABLE 1. STEADY STATE PARAMETERS AND VARIABLES

Ethylene dichloride—Toluene System

F = Feed flow rate = 0.0338 lb.-mol./min.
R = Reflux ratio = 3.0
x_f = Feed composition = 0.5 mol fraction EDC
T_f = Feed temperature = 70°F.
T_d = Reflux temperature = 70°F.
Q_r = Reboiler heat duty = 1445 B.t.u./min.

Equilibrium data:

$$y_n = \frac{2.23x_n}{1 + 1.23x_n}$$

Liquid enthalpy: $I = 7702.4 - 3106.8x_n$

Vapor enthalpy: $J = 22178.0 - 3700y_n$

Liquid saturation temperature:

$$T = 229.26 - 63.84x_n + 18.41x_n^2$$

Supercooled Liquid heat capacity:

$$C_p = 35.829 + 0.03203\,T_{av} - (7.366 + 0.01712T_{av})x_n$$

Efficiency = E = 1.0

In order to compare the response of the linear and nonlinear models a rather severe disturbance of a 10% decrease in the feed rate and composition and a 10% increase in feed and reflux temperatures were applied simultaneously. Figure 2 shows the results. The ratio of linear to nonlinear model composition deviations vary from 0.825 to 1.38, giving a maximum discrepancy of 38% for the uncontrolled system.

CONTROL LAWS

The linear state regulator problem of Kalman and Koepcke was formulated for problems in which initial state

Table 2. "Time Constant" for Uncontrolled Nonlinear Responses to Step Changes

	Overhead θ, min.	Feed tray θ, min.	Bottom θ, min.
$+10\%$ R	10.2	10.2	20.0
-10% R	9.8	9.8	13.0
$+10\%$ Q_r	11.5	10.0	12.5
-10% Q_r	12.5	13.0	20.5
$+10\%$ x_f	10.5	11.0	23.0
-10% F	11.5	12.5	19.5
-10% F	12.5	10.8	14.0
$+10\%$ T_f	11.0	11.0	17.0
-10% T_f	11.0	11.0	17.0
$+10\%$ T_d	8.0	10.5	16.0
-10% T_d	8.0	10.5	16.0

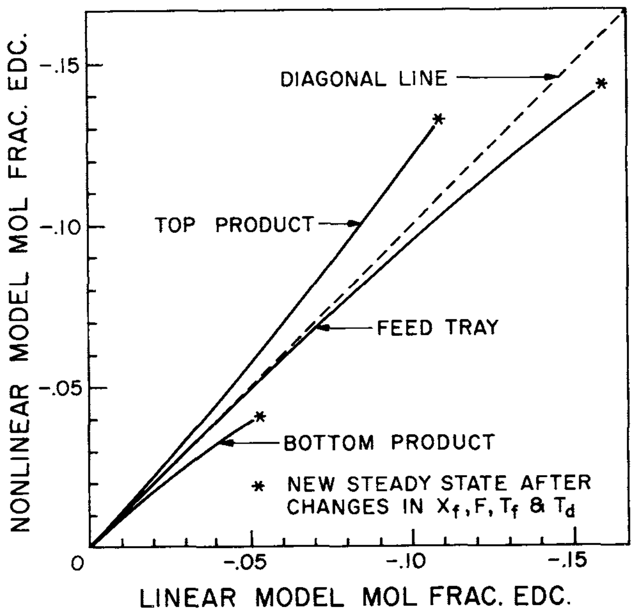

Fig. 2. Comparison of linear and nonlinear model compositions deviation from steady state subject to 10% decrease in X_f and F and 10% increase in T_f and T_d.

perturbations exist or equivalently, impulse load disturbances are applied to the system. However, when there are step disturbances or load changes, the optimal state regulator cannot attain and maintain the desired equilibrium condition.

A very reasonable approach to the linear regulator problem with step disturbances is to use an algorithm in which the optimal control vector is a function of both the state vector and the disturbance vector. For this type of algorithm the disturbances need to be measurable. Salukadze (1962) dealt with this problem by using a combination of dynamic programming and Liapunov stability theory. Anderson (1969) developed two algorithms which effectively handle measurable disturbances. His algorithms are in discrete form which is ideal for computer control usage and will be used for distillation control with measurable step disturbances.

Unfortunately, in practical applications most of the disturbances are not measurable. Since disturbances often encountered vary randomly, some have suggested that the theory of optimal stochastic control (Kushner, 1966) be applied. However, a priori information about disturbance probability distributions is usually not available.

In classical control theory for a single loop the concept of proportional-plus-integral feedback is used to counter the effects of constant input disturbance and proportional-plus-multiple-integral feedback is used to compensate the effects of load disturbances that can be expressed as a polynomial. Johnson (1968) has extended these concepts to optimal multivariable control systems. He suggested that instead of the $\underline{u}$ vector the $\dot{\underline{u}}$ vector be included in the quadratic performance index. The resulting optimal-control law with this modified quadratic performance index is not an explicit function of the external disturbances and can therefore be used for systems with step disturbances which are not accessible for measurement. Denn (1967) and Kalman (1964) discussed the inverse problem, which can also be used to obtain Johnson's result. For the inverse problem the control law is given and performance index for which the control law is optimal is computed. Johnson's derivation is in phase-variable form using only one control variable. Smith and Murrill (1969) used partition matrices to extend Johnson's derivation to two control variables, and presented the results in state-variable form. Both Johnson and Smith and Murrill's work are for continuous systems with continuous control.

CONTROL ALGORITHM FOR PULSE DISTURBANCES—CONTINUOUS SYSTEM

The continuous stationary linear system model is given by

$$\dot{\underline{x}}(t) = \underline{\underline{A}}\,\underline{x}(t) + \underline{\underline{B}}\,\underline{u}(t) \tag{7}$$

and the optimal regulator of Kalman and Koepcke is

$$\underline{u}^*(t) = -\underline{\underline{K}}(t)\,\underline{x}(t) \tag{8}$$

where

$$\underline{\underline{K}}(t) = \underline{\underline{R}}^{-1}(t)\,\underline{\underline{B}}'\underline{\underline{J}}(t) \tag{9}$$

CONTROL ALGORITHM FOR PULSE DISTURBANCES—DISCRETE SYSTEM

Since in direct digital computer control the control will be applied at discrete time intervals a discrete-time system model is needed (Tou, 1964).

$$\underline{x}(k+1) = \underline{\underline{\phi}}\,\underline{x}(k) + \underline{\underline{\Delta}}\,\underline{u}(k) \quad k = 0, 1, \ldots P \tag{10}$$

where the state transition matrix for the discrete system is

$$\underline{\underline{\phi}} = \sum_{i=0}^{\infty} \frac{(\underline{\underline{A}}\,T)^i}{i!} \tag{11}$$

and the control transition matrix for the discrete system is

$$\underline{\underline{\Delta}} = \sum_{i=0}^{\infty} \frac{\underline{\underline{A}}^i\,T^{i+1}}{(i+1)!}\,\underline{\underline{B}} \tag{12}$$

The optimal control which minimizes the quadratic performance

$$I[\underline{x}(0), P] = \sum_{k=1}^{P} \underline{x}'(k)\,\underline{\underline{Q}}\,\underline{x}(k) + \underline{u}'(k-1)\,\underline{\underline{R}}\,\underline{u}(k-1) \tag{13}$$

is

$$\underline{u}^*(k) = -\underline{\underline{K}}_{P-k}\,\underline{x}(k) \tag{14}$$

where the recurrence relations are

$$\underline{\underline{J}}_{P-k} = \underline{\underline{\phi}}'(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})(\underline{\underline{\phi}} - \underline{\underline{\Delta}}\,\underline{\underline{K}}_{P-k}) \tag{15}$$

$$\underline{\underline{K}}_{P-k} = [\underline{\underline{\Delta}}'(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})\,\underline{\underline{\Delta}} + \underline{\underline{R}}\,]^{-1}$$

$$\underline{\underline{\Delta}}\,(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})\,\underline{\underline{\phi}} \quad (16)$$

$$\underline{\underline{J}}_P = \underline{\underline{0}} \quad (17)$$

We see that for both the continuous and discrete case the optimal control which minimizes the quadratic performance index of Equation (2) and (13) for systems with pulse disturbances is a multivariable feedback proportional controller (MP controller).

CONTROL ALGORITHMS FOR MEASUREABLE STEP DISTURBANCES—DISCRETE SYSTEM

For systems with measurable disturbances, the disturbance terms should appear in the system equations. For discrete linear system models we have

$$\underline{x}\,(k+1) = \underline{\underline{\phi}}\,\underline{x}\,(k) + \underline{\underline{\Delta}}_1\,\underline{u}\,(k) + \underline{\underline{\Delta}}_2\,\underline{d}\,(k) \quad (18)$$

where $\underline{d}\,(k)$ is the disturbance vector.

Two optimal control algorithms have been proposed by Anderson (1969) for systems with measurable step disturbances. His first algorithm is a multivariable proportional control with disturbance compensation (MPD algorithm). The optimal control law for systems described by Equation (18) which minimize the quadratic performance index of Equation (13) is

$$\underline{u}^*(k) = \underline{\underline{K}}_r\,(P-k)\,\underline{x}\,(k) + \underline{\underline{K}}_s\,(P-k)\underline{d}\,(k) \quad (19)$$

with the recurrence relations

$$\underline{\underline{K}}_r\,(P-k) = -\,[\underline{\underline{R}} + \underline{\underline{\Delta}}_1'\underline{\underline{J}}_a\,(P-k-1)\,\underline{\underline{\Delta}}_1]^{-1}$$

$$\underline{\underline{\Delta}}_1'\underline{\underline{J}}_a(P-k-1)\,\underline{\underline{\phi}} \quad (20)$$

$$\underline{\underline{K}}_s\,(P-s) = -\,[\underline{\underline{R}} + \underline{\underline{\Delta}}_1'\underline{\underline{J}}_a\,(P-k-1)\,\underline{\underline{\Delta}}_1]^{-1}$$

$$\underline{\underline{\Delta}}_1'\,[\underline{\underline{J}}_b\,(P-k-1) + \underline{\underline{J}}_a\,(P-k-1)\,\underline{\underline{\Delta}}_2] \quad (21)$$

$$\underline{\underline{J}}_a\,(P-k) = \underline{\underline{Q}} + [\underline{\underline{\phi}} + \underline{\underline{\Delta}}_1\underline{\underline{K}}_r\,(P-k)]'$$

$$\underline{\underline{J}}_a(P-k-1)\,[\underline{\underline{\phi}} + \underline{\underline{\Delta}}_1\,\underline{\underline{K}}_r\,(P-k)]$$

$$+\,\underline{\underline{K}}_r'\,(P-k)\,\underline{\underline{R}}\,\underline{\underline{K}}_r\,(P-k) \quad (22)$$

$$\underline{\underline{J}}_b\,(P-k) = [\underline{\underline{\phi}} + \underline{\underline{\Delta}}_1\underline{\underline{K}}_r(P-k)]'[\underline{\underline{J}}_b\,(P-k-1)$$

$$+\,\underline{\underline{J}}_a\,(P-k-1)\,(\underline{\underline{\Delta}}_2 + \underline{\underline{\Delta}}_1\underline{\underline{K}}_s(P-k))]$$

$$+\,\underline{\underline{K}}_r'\,(P-k)\,\underline{\underline{R}}\,\underline{\underline{K}}_r\,(P-k) \quad (23)$$

The recurrence relations can be programmed for digital computation. As P becomes large, the control matrices become constant, and $\underline{\underline{K}}_r$ and $\underline{\underline{K}}_s$ tend to the optimal control matrices associated with an infinite-stage decision process. When the weighting matrix $\underline{\underline{R}}$ is null, the optimal control is bang-bang and if $\underline{\underline{\Delta}}_2$ is null, the recurrence relation reduces to the MP algorithm.

Anderson's second algorithm, the so-called error coordinated form of control (MPE algorithm) is actually the modification of tracking or servo-regulation. For a system with step disturbances there will exist a new steady state equilibrium state $\underline{x}_e$ and equilibrium control vector $\underline{u}_e$. It is possible to partition the new equilibrium state $\underline{x}_e$ into the state variables $\underline{x}_{1e}$ to be brought to a desired equilibrium state, and those $\underline{x}_{2e}$ free to obtain any equilibrium value. Assuming the number of state variables which are to be brought to a desired state is equal to the number of control variables, then $\left[\underline{\underline{A}} \,\vdots\, \underline{\underline{B}}\right]$ is a square matrix and its inverse is defined so that the equilibrium state $\underline{x}_{2e}$ and control $\underline{u}_e$ is given by

$$\begin{bmatrix} x_{2e} \\ \cdots \\ \underline{u}_e \end{bmatrix} = -\left[\underline{\underline{A}}_2 \,\vdots\, \underline{\underline{B}}\right]^{-1} (\underline{\underline{A}}_1\,\underline{x}_{1e} + \underline{\underline{W}}\,\underline{d}) \quad (24)$$

Anderson also showed that

$$\underline{x}_e = \begin{bmatrix} \underline{x}_{1e} \\ \cdots \\ \underline{x}_{2e} \end{bmatrix} = \underline{\underline{M}}_1\,\underline{x}_{1e} + \underline{\underline{N}}_1\,\underline{d} \quad (25)$$

and

$$\underline{u}_e = \underline{\underline{M}}_2\,\underline{x}_{1e} + \underline{\underline{N}}_2\,\underline{d} \quad (26)$$

Defining

$$\hat{\underline{x}} = \underline{x} - \underline{x}_e \quad \text{and} \quad \hat{\underline{u}} = \underline{u} - \underline{u}_e \quad (27)$$

the optimal control for the system

$$\hat{\underline{x}}\,(k+1) = \underline{\underline{\phi}}\,\hat{\underline{x}}\,(k) + \underline{\underline{\Delta}}_1\,\hat{\underline{u}}\,(k) \quad (28)$$

which minimizes the quadratic performance index

$$I\,[\hat{\underline{x}}(0), P] = \sum_{k=1}^{P} [\hat{\underline{x}}'\,(k)\,\underline{\underline{Q}}\,\hat{\underline{x}}\,(k) + \hat{\underline{u}}'\,(k-1)\,\underline{\underline{R}}\,\hat{\underline{u}}\,(k-1)] \quad (29)$$

is

$$\hat{\underline{u}}^*\,(k) = -\,\underline{\underline{K}}_{P-k}\,\hat{\underline{x}}\,(k) \quad (30)$$

where

$$\underline{\underline{J}}_{P-k} = \underline{\underline{\phi}}'\,(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})\,(\underline{\underline{Q}} - \underline{\underline{\Delta}}_1\,\underline{\underline{K}}_{P-k}) \quad (31)$$

$$\underline{\underline{K}}_{P-k} = [\,\underline{\underline{\Delta}}'_1\,(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})\,\underline{\underline{\Delta}}_1 + \underline{\underline{R}}\,]^{-1}$$

$$\underline{\underline{\Delta}}'_1\,(\underline{\underline{Q}} + \underline{\underline{J}}_{P-k-1})\,\underline{\underline{Q}} \quad (32)$$

$$\underline{\underline{J}}_P = \underline{\underline{0}} \quad (33)$$

CONTROL ALGORITHM FOR UNMEASUREABLE STEP DISTURBANCES—DISCRETE SYSTEM

Optimal controllers can be designed for continuous systems with unmeasurable step disturbances if a performance index is chosen quadratic in the state and the time derivative of the control vector (Johnson, 1968). The resulting controllers are generalized proportional integral controllers (MPI control). Hu (1970) has extended Johnson's work to discrete time systems. The optimal control law for the system

$$\tilde{\underline{x}}\,(k+1) = \tilde{\underline{\underline{\phi}}}\,\tilde{\underline{x}}\,(k) + \tilde{\underline{\underline{\Delta}}}\,\tilde{\underline{u}}\,(k) \quad (34)$$

where

$$\tilde{\underline{x}} = \begin{bmatrix} \underline{x} \\ \cdots \\ \underline{y} \end{bmatrix} \quad \tilde{\underline{u}} = [\,\dot{\underline{u}}\,] \quad \tilde{\underline{\underline{A}}} = \begin{bmatrix} \underline{\underline{A}} & \vdots & \underline{\underline{I}} \\ \cdots & & \cdots \\ \underline{\underline{O}} & \vdots & \underline{\underline{O}} \end{bmatrix}$$

$$\underline{y} = \underline{\underline{B}}\,\underline{u} + \underline{\underline{W}}\,\underline{d} \quad \tilde{\underline{\underline{B}}} = \begin{bmatrix} \underline{\underline{O}} \\ \cdots \\ \underline{\underline{B}} \end{bmatrix} \quad (35)$$

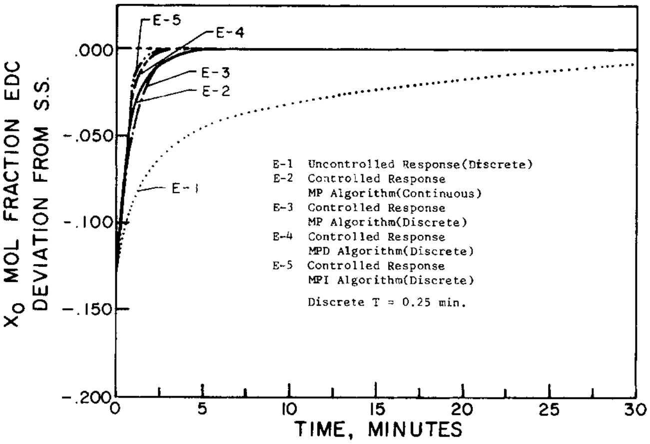

Fig. 3. Linear responses with impulse disturbances for top support.

and

$$\underset{\approx}{\tilde{\phi}} = \sum_{k=1}^{\infty} \frac{(\underset{=}{A}\, T)^i}{i!} \quad \underset{=}{\tilde{\Delta}} = \sum_{i=0}^{\infty} \frac{\underset{=}{\tilde{A}}^{\,i}\, T^{i+1}}{(i+1)!} \; \underset{=}{\tilde{B}} \tag{36}$$

which minimizes the performance index

$$I[\underset{-}{\tilde{x}}(0), P] = \sum_{k=1}^{P} \underset{-}{\tilde{x}}'(k)\, \underset{=}{\tilde{Q}}\, \underset{-}{\tilde{x}}(k) + \underset{-}{\tilde{u}}'(k-1)\, \underset{=}{R}\, \underset{-}{\tilde{u}}(k-1) \tag{37}$$

is

$$\underset{-}{u}^*(k) = \underset{-}{u}^*(k-1) - \underset{=}{K_1}\, \underset{-}{x}(k)\, T - \underset{=}{K_2}[\underset{-}{x}(k) - \underset{-}{x}(k-1)] + \underset{=}{K_2}\, \underset{=}{A}\, \underset{-}{x}(k)\, T \tag{38}$$

where

$$\underset{=}{\tilde{K}}_{P-k} = \left[\underset{=}{K_1} \vdots \underset{=}{K_2} \right]$$

$$\underset{=}{\tilde{J}}_{P-k} = \underset{=}{\tilde{\phi}}'[\underset{=}{\tilde{Q}} + \underset{=}{\tilde{J}}_{P-k-1}][\underset{=}{\tilde{\phi}} - \underset{=}{\tilde{\Delta}}\, \underset{=}{K}_{P-k}] \tag{39}$$

$$\underset{=}{\tilde{K}}_{P-k} = [\underset{=}{\tilde{\Delta}}'(\underset{=}{\tilde{Q}} + \underset{=}{\tilde{J}}_{P-k-1})\underset{=}{\tilde{\Delta}} + \underset{=}{\tilde{R}}]^{-1} \underset{=}{\tilde{\Delta}}'(\underset{=}{\tilde{Q}} + \underset{=}{\tilde{J}}_{P-k-1})\underset{=}{\tilde{\phi}}$$

As stated by Johnson (1968) this control policy is capable of returning the entire state to the original steady state as long as the system is completely controllable and the disturbance and control matrices $\underset{=}{W}$ and $\underset{=}{B}$ are colinear. If the disturbance and control matrices are not colinear, the number of state variables which can be returned to the original steady state is equal to the number of control variables (similar to the result of the MPE algorithm). The rest of the state variables are driven to new steady state values. We can dictate the state variables which are desired to return to the origin by assigning large values to the corresponding $\underset{=}{Q}$ weighting matrix elements.

EVALUATION OF CONTROL ALGORITHMS

In order to achieve a "best performance" the weighting matrices $\underset{=}{Q}$ (for state variables) and $\underset{=}{R}$ (for control variables) must be tuned. Our criterion of the "best performance" is to minimize the overshoot and steady state deviations of the top product x_0 and the bottom product x_6 from their desired steady state values.

The numerical magnitude of the control period (discrete time interval) used in the discrete system algorithms strongly influences the control matrix and the resulting control performance. As the control period is decreased, the system performance approaches the performance of the continuous system with continuous control. It takes significantly longer computation time to compute optimal continuous control policies as compared to discrete control policies. Also, as the control period is decreased the computing time is increased. After several runs a control period of 0.25 min. was found to be adequate for discrete distillation column control. Figure 3 shows that for this control period the optimal continuous and discrete MP responses are nearly identical. For the continuous case, it took about 50 sec. of CDC 6400 central processor time to compute the feedback coefficients and a 30-min. linear transient response. For the discrete case (with 0.25 min. sampling time) 7 sec. were needed. Thirty steps of the backward iteration sequence of the recurrence relations gave essentially the constant control coefficients of the infinite stage process.

Figure 3 shows the linear responses for the "best" tuned control algorithms to an initial impulse disturbance of:

$$\underset{-}{x} = \begin{bmatrix} -0.1333 \\ -0.1712 \\ -0.1766 \\ -0.1445 \\ -0.1448 \\ -0.0747 \\ -0.0415 \end{bmatrix}$$

All state variables will eventually return to the steady state since the system is stable. The figure also shows that the MPI and MPD algorithms efficiently control the process with impulse disturbances. For impulse disturbances the MPD and MPE algorithms are identical.

Figure 4 presents the linear response of the system to a step load disturbance of minus 10% in the feed rate and feed composition and plus 10% in the feed temperature and reflux temperature acting simultaneously. This represents the most severe 10% disturbance possible since all tend to drive the system in the same direction from the steady state. The results show that the uncontrolled response gives steady state errors of $x_0 = 0.1$ and $x_6 = 0.5$ mole fraction deviations. The MP algorithm does give some control but the steady state offsets for the top and bottom compositions are significant, 0.024 and 0.017 mole

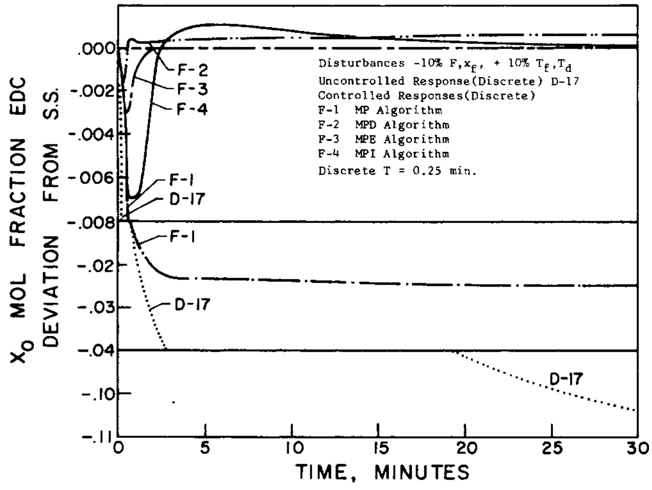

Fig. 4. Linear responses with step disturbances for top product.

Table 3. Time Required to Compute Two Major Algorithms on CDC 6400 Computer

	Total computing time for 120 time interval transient responses ($T = 0.25$ min.)	Time required to calculate $\underline{\underline{\phi}}$, $\underline{\underline{\Delta}}$ and feedback constants	Time required to calculate $\underline{u}^*$ and transient responses for each time interval
MPE Algorithm	8.4 sec.	4.5 sec.	0.032 sec.
MPI Algorithm	18.2 sec.	14.6 sec.	0.03 sec.

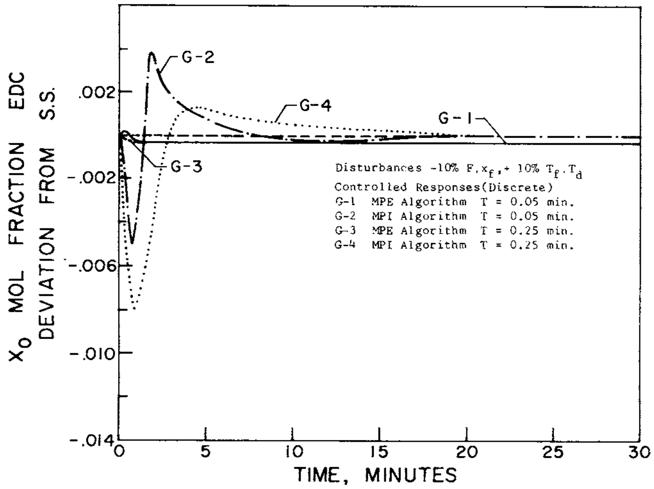

Fig. 5. Nonlinear responses with step disturbances for top product.

fractions respectively. The MPD algorithm also gives steady state error although not as severe. The MPI and MPE algorithms perform well as expected.

Figures 5 and 6 show the results of testing the applicability of the MPE and MPI algorithms to the nonlinear distillation model system. The figures give results for discrete time control intervals of 0.05 and 0.25 min. The results show that due to the nonlinear behavior of the system the MPE algorithm drives the top and bottom compositions near the original steady state with some offset. Its performance is not influenced by the discrete time control interval. On the other hand, the MPI algorithm drives the top and bottom compositions back to the steady state but with some overshoot. The overshoot is influenced by the discrete time control interval. Our conclusion from these simulation results is that both the MPE and MPI algorithm can be applied successfully to the nonlinear distillation column system. When the disturbances are measurable it is better to use the MPE algorithm because it does not give overshoot in the state variables and it drives the critical state variables to the original steady state with tolerable offset values. If the disturbances are not measurable, we can use the MPI algorithm. The overshoot can be reduced by properly tuning the weighting matrices and selecting the proper discrete time control interval. The results also indicate that the MPI algorithm not only handles unmeasurable disturbances, but can also compensate for inaccuracies in the linear mathematical control model.

Table 3 gives the time required to compute the two major algorithms on the CDC 6400 computer. If we use a discrete time control interval of 0.05 min. (3 sec.) we can compute $\underline{u}^*$ with off-line computed control constants (infinite-stage case). For a discrete time control interval of 0.25 min. (15 sec.) the control constants can be computed continually under digital control.

Figures 7 and 8 give the comparison of the MPE and MPI optimal control responses with that obtained via two well tuned single loop proportional-integral controllers controlling the overhead and bottoms composition. All three control systems use reflux ratio and heat duty as control variables. The results show that the optimal algorithms control the overhead composition better than the standard single loop control scheme. All three control schemes control the bottoms composition well.

CONTROL STRUCTURE STUDIES

Since there are six disturbance variables for the binary distillation column system a variety of different control structures are possible besides the common reflux ratio, heat duty control structure. Three possible two control variable structures are R and F, Q_r and F, and Q_r and R. Generally speaking, the compositions x_0, x_1, and x_6 can be brought back to their steady states. The other compositions are driven to new steady states. Based on the concept of degrees of freedom, we should only be able to bring two state variables back to the origin if we use two control variables. The reason we can effectively bring three states to the origin with two controls is that we have assumed a total condenser in our mathematical model so that

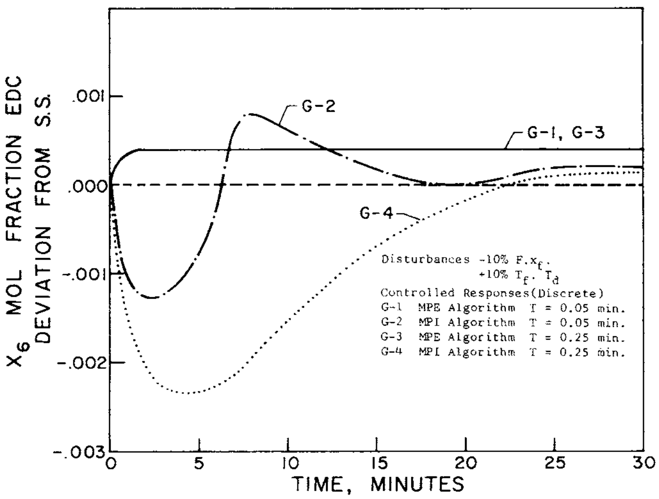

Fig. 6. Nonlinear reponses with step disturbances for bottom product.

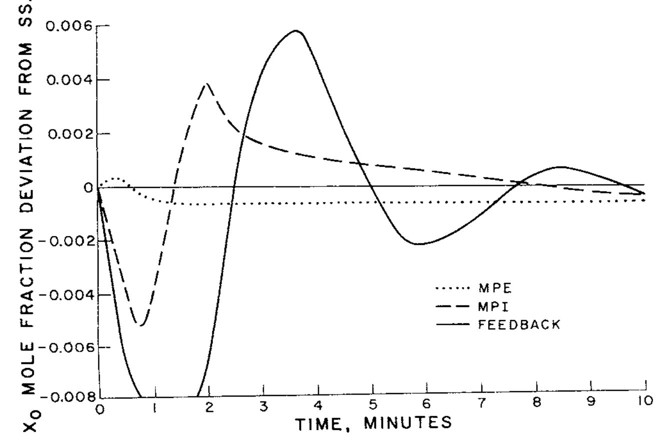

Fig. 7. Nonlinear responses for top product.

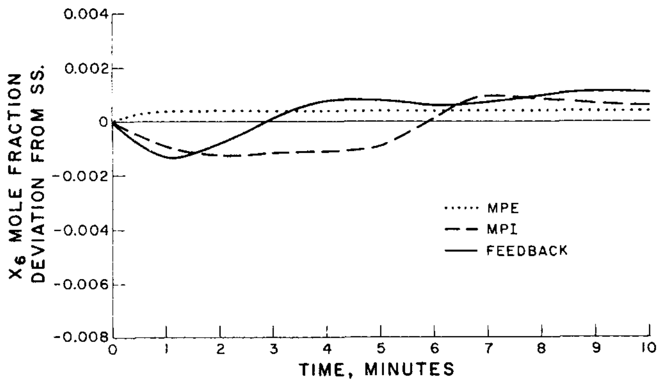

Fig. 8. Nonlinear responses for bottom product.

once x_0 is driven to the origin, x_1 is also driven very near to the origin.

All cases studied gave good controlled responses with the case using R and F as control variables giving slightly better performance. Since most industrial columns operate at maximum throughput, the use of the feed flow as a control variable cannot usually be used but should be considered when practically feasible.

For most distillation columns interaction among the process variables is serious; therefore, a single loop scheme does not control efficiently for both top and bottom compositions (Rosenbrock, 1962, and Rijnsdrop, 1965). Noninteracting control has been proposed as a means of countering the interaction (Rijnsdrop, 1965) but the calculation of the controller transfer functions is quite complicated. In fact, it is by no means certain that the elimination or minimization of interaction within the system is desirable, except that it may enable classical design procedures to be adopted for multivariable systems. Modern control theory recognizes the existence of interactions within the system and seeks to optimize the overall plant performance with respect to a prescribed objective function, without necessarily aiming to achieve a noninteracting system. The results of this study show that the optimal algorithms of the MPI and MPE form led to excellent distillation control in the face of load disturbances.

NOTATION

$\underline{\underline{A}}$ = state coefficient matrix $(n \times n)$

$\tilde{\underline{\underline{A}}}$ = pseudo state coefficient matrix $(2n \times 2n)$

$\tilde{\underline{\underline{B}}}$ = pseudo control coefficient matrix $(2n \times m)$

$\underline{\underline{B}}$ = control coefficient matrix $(n \times m)$

B = bottom flowrate, lb.-mol./min.

D = overhead product rate, lb.-mol./min.

$\underline{d}$ = disturbance vector (1×1)

E = Murphree liquid plate efficiency

EDC = ethylene dichloride

F = feed rate, lb.-mol./min.

H_i = liquid holdup on plate i, lb.-mol.

I = saturated liquid enthalpy, B.t.u./lb.-mol.

J = saturated vapor enthalpy, B.t.u./lb.-mol.

$\underline{\underline{J}}$ = Riccati matrix $n \times n$

$\underline{\underline{K}}$ = feedback coefficient MP algorithm

$\underline{\underline{K_r}}$ = feedback coefficient MPD algorithm

$\underline{\underline{K_s}}$ = feedforward coefficient MPD algorithm

$\tilde{\underline{\underline{K}}}$ = pseudo feedback coefficient MPI algorithm

k = discrete sampling stage

L = liquid flowrate down the column, lb.-mol./min.

L_0 = reflux rate, lb.-mol./min.

$\underline{\underline{M_1}}$ = state constant for new equilibrium state vector in MPE algorithm

$\underline{\underline{M_2}}$ = state constant for new equilibrium control vector in MPE algorithm

$\underline{m}$ = control and disturbance vector $(n + 1) \times 1$

$\underline{m_d}$ = control deviations from steady state

$\underline{\underline{N_1}}$ = disturbance constant for new equilibrium state vector in MPE algorithm

$\underline{\underline{N_2}}$ = disturbance constant for new equilibrium control vector in MPE algorithm

$\underline{p}$ = costate variable

Q_c = heat removed from the condensor, B.t.u./min.

Q_r = heat supplied to the reboiler, B.t.u./min.

$\underline{\underline{Q}}$ = weighting matrix for state vector $(n \times n)$

$\tilde{\underline{\underline{Q}}}$ = pseudo weighting matrix for state vector $(2n \times 2n)$

R = reflux ratio, refractive index

$\underline{\underline{R}}$ = weighting matrix for control vector $(m \times m)$

$\tilde{\underline{\underline{R}}}$ = pseudo weighting

$\underline{\underline{S}}$ = weighting matrix

$s.s.$ = steady state

T = temperature °F., time interval

T_f = feed temperature

T_d = reflux temperature

t = time, minutes

$\underline{u}$ = control vector $(m \times 1)$

$\tilde{\underline{u}}$ = pseudo control vector $(m \times 1)$

$\underline{u}^*$ = optimal control vector $(m \times 1)$

V = vapor rate up the column, lb.-mol./min.

$\underline{\underline{W}}$ = disturbance coefficient matrix $(m \times 1)$

x = liquid composition, mol. fraction ethylene dichloride

$\underline{x}$ = state vector $(n \times 1)$

$\tilde{\underline{x}}$ = pseudo state vector $(n \times 1)$

$\underline{x_d}$ = state deviation from steady state

x_d = desired composition

$\underline{x}^*$ = state vector at $\underline{u}^*$

y = vapor composition, mol. fraction ethylene dichloride

α = relative volatility

$\underline{\underline{\phi}}$ = state coefficient matrix for discrete system $(n \times n)$ or transition matrix

$\underline{\underline{\Delta}}$ = control (and disturbance) coefficient matrix with discrete system $(n \times n)$ or $n \times (m + 1)$

$\underline{\underline{\Delta_1}}$ = control coefficient matrix $n \times m$

$\underline{\underline{\Delta_2}}$ = disturbance coefficient $n \times 1$

θ = time constant

Subscripts

b = bottom product

d = overhead product

f = feed to the column, or final condition

r = reflux

0 = condenser, or initial condition

1, 2, 3, 4, 5 = number of trays

6 = reboiler

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Mass Transfer of Water from Single Thoria Sol Droplets Fluidized in 2-Ethyl-1-hexanol

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The rate at which water is extracted from thoria sols was investigated by fluidizing single thoria sol droplets in 2-ethyl-1-hexanol (2EH) and measuring the diameter of a droplet over a period of time until shrinkage no longer occurred. Diameter data from both water and sol drops were obtained at 25°C. The experimental variables were initial drop diameter (0.1 to 0.2 cm), sol molarity (0 to 2.5 $\underline{M}$ ThO_2), and water concentration in the 2EH (2-12 mg./cc.). The water and sol droplet data were correlated by Equation (5). The single relationship for the fluidized water and sol drops verified that an organic-phase film surrounding the drop is the rate-controlling resistance. The sphere Reynolds number was based on the approach velocity and varied from 0.4 to 14. The Schmidt number for the system was fixed at 35,700. During the extraction of water, the mass transfer coefficients for fluidized sol drops were found to depend only on the molarity of the sol. By expressing the mass transfer coefficients as a function of the density difference between the aqueous sol and the organic phase, an equation was derived to predict the gelation time required for any initial sol molarity and drop diameter fluidized in 2 EH at 25°C.

The sol-gel process which was developed at the Oak Ridge National Laboratory is a method for preparing a wide variety of ceramic fuel materials for use in nuclear reactors. As compared with conventional preparation procedures, the sol-gel process has at least three distinct advantages: simplicity, flexibility, and a low calcination temperature for obtaining particles of near theoretical density (*4*).

The original objective of the sol-gel process was to produce thoria-urania fragments suitable for vibratory compaction in metal tubes; however, during the past five years emphasis has been shifted toward the preparation of spherical particles, or microspheres. Microspheres are prepared by dispersing uniformly sized drops of the appropriate sol into a partially miscible alcohol such as 2-ethyl-1-hexanol (2EH). The sol droplets must be fluidized in the organic phase until enough water is extracted from the aqueous sol to cause gelation. After drying, the gelled spheres are calcined at 1,150°C. to yield an oxide product having a density within 1% of theoretical (*10*).

In this study, various sizes of thoria sol droplets of different initial molarities were fluidized, and the diameter of a particular droplet was measured as a function of time until shrinkage no longer occurred (*3*). Mass transfer coefficients were determined from the decrease in drop diameter over a period of time for different water concentrations in the 2EH. Diameter data from droplets of both water and sol were obtained in order to test the validity of a mass transfer model based on an organic-phase film as the controlling resistance. In most of the runs, either 0.01 or 0.1 vol. % Ethomeen S/15 was added to the 2EH to produce a rigid sol droplet having no induced circulation. The mass transfer results obtained when this surfactant was present in the organic phase are representative of the conditions that are proposed for a production microsphere column.

LITERATURE REVIEW

The processes by which mass may be transferred through a fluid film surrounding a sphere are radial diffusion and natural and forced convection. For any given problem, these three transport processes may act independently or