C = constant
D = tube diameter, ft.
D_p = particle diameter, ft.
f = friction factor
f^* = modified friction factor
G_o = superficial mass velocity, lb./(sq.ft.)(sec.)
k = permeability, sq.ft.
K = consistency index, lb.(sec.^{n})/sq.ft.
L = depth of bed, ft.
L_c = length of capillary, ft.
n^1 = flow behavior index
$(N_{Re})_{mod}$ = modified Reynolds number
P_c = pressure drop in capillary, lb./sq.in.abs.
R = tube radius, ft.
R_H = hydraulic radius, ft.
V = average tube velocity, ft./sec.
V_o = superficial velocity, ft./sec.
ϵ = porosity
η_{mod} = modified viscosity, lb./(sec.)(ft.)
μ = viscosity, lb./(sec.)(ft.)

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Transient Response and Feed-Forward Control of a Distillation Tower Subject to a Sequence of Upsets

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A mathematical model of dynamic distillation was verified experimentally for transients resulting from a sequence of upsets in operating conditions, that is, for upsets occurring in the unsteady state before the effects of previous upsets died out.

The equations for feed-forward control of the top product composition by reflux ratio control action were derived and a computer program was written in FORTRAN for solution on a digital computer. This control model was employed in the feed-forward control of an experimental distillation column when subjected to an upset in feed composition.

Experimental data were obtained from a twelve-plate, 10-in. diameter distillation column with a methanol-tertiary butyl alcohol system. The numerical technique employed is a completely general divided difference method which can be utilized in the solution of any system of first-order differential equations.

The work described herein is an extension of that previously reported by Huckaba and co-workers (*1, 2*). These studies involved comparison of computed predictions with experimentally observed dynamic responses to upsets in reflux ratio, feed composition, thermal input to the reboiler, and simultaneous upsets in feed composition and reboiler heat duty. The model developed in these studies was based on assumptions of perfect mixing, constant mass of holdup, and plate efficiencies independent of time. This model, however, is not restricted by the frequently used assumption of constant molal overflow. Since the resulting differential equations are nonlinear, numerical integration on a digital computer was used to generate the predicted column dynamic response.

Distillation dynamics and control have attracted considerable attention in both academic and industrial circles. Complete reviews of the literature on distillation dynamics and control have been presented by Archer and Rothfus (*3*), Williams (*4*), and Buckley (*5*).

Rosenbrock (*6* to *8*) made considerable progress toward a general mathematical representation of transient distillation and the corresponding solution techniques associated with such complex systems of differential equations. Utilizing a model based on constant molal overflow, Rosenbrock presented a comparison of calculated and experimental results.

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Much work on dynamic distillation including feed-forward control techniques has been carried out at the University of Delaware by Gerster, Lamb, and others (*9* to *11*). This work is based on a linearized model which uses an analog computer for simulation in the feed-forward applications (*12, 13*). Experimental verification of computed results is included in all the above mentioned works.

Mah, Michaelson, and Sargent (*14*) studied the dynamics of multicomponent distillation. They applied a method (which is rigorous only for linear differential equations with constant coefficients) to nonlinear equations over a single interval, correcting the values of the coefficients at the end of each interval. They discussed the instabilities of forward-integration techniques and included discussions on relative interval size and error estimates of the recommended method.

Present developments in feed-forward control are typified by a paper by MacMullen and Shinskey (*15*), who applied feed-forward control to a commercial distillation tower. Although highly successful from a control standpoint (relative to feedback control), the authors reported no attempt at rigorous mathematical simulation of the process dynamics. The article does, however, illustrate the superiority of feed-forward control for a system with a slow response time.

It is believed that the work reported herein is an important step in the direction recommended by the Process Control Committee of the American Institute of Chemical Engineers (*16*) and discussed in some detail by Williams (*4*). The model is one of the most general that has been used in dynamic distillation studies, and for which direct experimental verification has been provided for all computed results, including an actual feed-forward control of the experimental distillation tower.

It is believed that the extra effort expended in development of a general nonlinear model is justified for two reasons, both of which are associated with the recent work with linearized models. First, the limitations of linearized models as to magnitude of disturbances do not apply to nonlinear models. In fact, a nonlinear model can be utilized to study the effects of large perturbations on a linearized version of the nonlinear model as compared with the effects on the nonlinear model. Second, once a general nonlinear model has been developed, the effects of linearization of certain variables can be studied, that is, one can test which variables are amenable to linearization for any particular application.

THEORETICAL ANALYSIS

The basic differential equations describing the dynamics of distillation columns have been formulated and presented in numerous forms in the technical literature. All of the equations are based on material and energy balances around various sections of the column, but are different in final form because of differences in assumptions chosen by the various investigators. A completely realistic model would be virtually impossible to formulate.

For example, not enough is known about the physics of tray hydraulics, eddy currents, foaming, froth heights, etc., to describe completely tray mixing in mathematical form. The complexity of the differential equations representing a distillation tower is such as to require other assumptions, which may not be sound on physical grounds, in order to obtain solutions to the equations of the model. Although analytical solutions of the equations of realistic distillation models are not practical, high-speed digital and analog computers have aided in the solution of some highly useful simulation models. Because of the lack of analytical solutions, experimental comparison of computed results is often utilized to determine the validity of the model.

The Basic Mathematical Model

The basic mathematical model used in this work to describe the transient behavior of a stagewise distillation column for a binary mixture was formulated on the following assumptions: adiabatic operation, constant column pressure, negligible fluid dynamic lags, perfect mixing, negligible vapor holdup, linear enthalpy relationships, and plate efficiencies a function of liquid composition only.

The mathematical model is essentially that presented by Huckaba, May, and Franke (*1*). In the present study their basic model was modified for nonconstant weight holdup for the case where holdup is specified empirically as a function of flow rates. Since the vapor holdup was assumed negligible compared to liquid holdup, the rate of change of vapor holdup with time was of no concern in this work. Regarding liquid holdup, it was assumed that since the rate of change of plate holdup was small compared with the liquid flow rates, the plate holdup at the beginning of a time increment t could serve as the average holdup over a small time increment Δt. By using the empirical relationships for plate holdup as a function of flow rates, the plate holdup was corrected at the end of the increment (that is, at $t + \Delta t$) before proceeding to the next. Otherwise, the derivation is essentially the same as that given in reference *1* and therefore is presented below only in outline form. The empirical equations for equilibrium, plate efficiency, enthalpy, plate holdup, etc., are given by Distefano (*17*).

THE BASIC MATHEMATICAL MODEL

Compositions as a Function of Time

Condenser-accumulator system:

$$\frac{dx_0}{dt} = \frac{D}{H_0}(R+1)(y_1 - x_0) \tag{1}$$

Plates in rectifying section ($1 \leq n \leq N$):

$$\frac{dx_n}{dt} = \frac{1}{H_n}[L_n(y_{n+1} - x_n) - L_{n-1}(y_n - x_{n-1}) + D(y_{n+1} - y_n)] \tag{2}$$

Feed plate:

$$\frac{dx_{N+1}}{dt} = \frac{1}{H_{N+1}}[L_{N+1}(y_{N+2} - x_{N+1}) - L_N(y_{N+1} - x_N) + D(y_{N+2} - y_{N+1}) + F(x_F - y_{N+2})] \tag{3}$$

Plates in stripping section ($N + 2 \leq m \leq M$):

$$\frac{dx_m}{dt} = \frac{1}{H_m}[L_m(y_{m+1} - x_m) - L_{m-1}(y_m - x_{m-1}) - W(y_{m+1} - y_m)] \tag{4}$$

Reboiler system:

$$\frac{dx_{M+1}}{dt} = \frac{1}{H_{M+1}}[W(y_{M+1} - x_{M+1}) - L_M(y_{M+1} - x_M)] \tag{5}$$

Flow Rates

Top product rate:

$$D = \frac{Q_{M+1} - F\,C_p\Delta T_F}{(R+1)[(A-a) - B - b)\,y_1] + R\,C_p\Delta T_R} \tag{6}$$

$$L_0 = RD$$

Plates in rectifying section ($1 \leq n \leq N$):

$$L_n = \left[\frac{(R+1)[(A-a)-(B-b)\,y_1] + R\,C_p\Delta T_R}{(A-a)-(B-b)\,y_{n+1}} - 1\right] D \quad (7)$$

Plates in stripping section $(N+1 \leq m \leq M)$:

$$L_m = \frac{Q_{M+1}}{(A-a)-(B-b)\,y_{m+1}} + W \quad (8)$$

Vapor-Liquid Equilibrium

$$x_n^* = g_1(y_n) \quad (9)$$

Plate Efficiency

$$x_n = E_n\,x_n^* + (1-E_n)\,x_{n-1} \quad (10)$$

$$E_n = g_2(x_n) \quad (11)$$

Plate Holdups

$$H_0 = g_3(L_0) \quad (12)$$

$$H_n = g_4(L_n, V_n) \quad (13)$$

$$H_{M+1} = g_5(V_{M+1}) \quad (14)$$

Process Degrees of Freedom

Huckaba et al. (*1*) concluded that there are six process degrees of freedom from the process under investigation in this study. Therefore, six of the column operating conditions must be specified for the system to be determinate. The six process operating variables chosen in this study were: feed composition, feed enthalpy, feed rate, reflux ratio, reflux enthalpy, and reboiler heat duty (top product rate, or steam temperature could be used alternately).

Since the first five of these inputs are considered as being known explicitly throughout the transient state, they are treated as measurable inputs to the unsteady state program. The sixth input, however, posed somewhat of a problem. In the experimental work described below, the observed operating variable was actually reboiler steam pressure (or steam temperature), which was controlled and recorded, and could be treated as a measurable input. Reboiler heat duty, however, could not be obtained directly from steam temperature. Knowledge of the heat transfer coefficient, variation of the heat transfer coefficient with liquid composition, and dependence of heat transfer on the temperature driving force were necessary before the reboiler heat duty could be calculated from steam temperature. A predictive relationship for reboiler heat duty as a function of liquid-side composition and steam-side temperature was developed (*17*) and steam temperature was used as a system input in lieu of reboiler heat duty. The equation for the predictive value of reboiler heat duty Q_{M+1} as a deviation from its initial steady state value is given by

$$Q_{M+1} = \overline{U}_0\; e^{0.8\,[x_{M+1}-(x_{M+1})_0]}\,(53.5\,x_{M+1} + T_s - 179.9)^2 \quad (15)$$

where

$$\overline{U}_0 = \frac{(Q_{M+1})_0}{[53.5\,(x_{M+1})_0 + (T_s)_0 - 179.9]^2} \quad (16)$$

Modification of the Basic Model for Feed-Forward Control

The usefulness of any mathematical model which describes a physical process lies in its ability to predict the response of the process under conditions of interest. A valid mathematical model, for instance, is the only reliable means of employing feed-forward control. If a model can accurately predict the response of the system to a given upset in operating conditions, then it can be modified to predict the conditions of another operating variable required to produce corrective action.

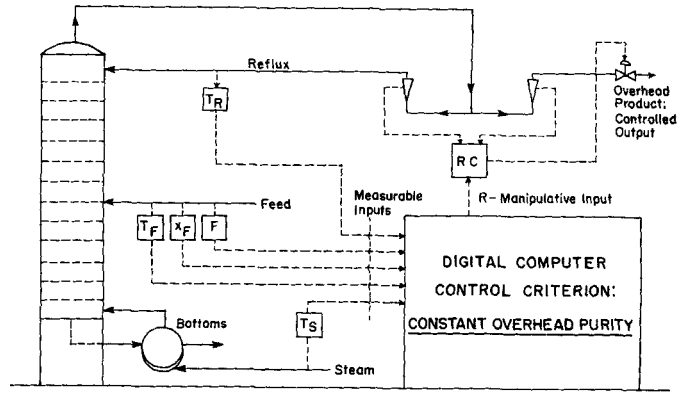

Fig. 1. Schematic diagram for feed-forward control system.

In feed-forward control it is conventional to classify inputs as manipulative, measurable, or unmeasurable. For simplicity, in this investigation the feed rate, composition, and temperature, the reflux temperature, and the steam temperature are considered as measurable inputs, and the reflux ratio as a manipulative input. The overhead composition is considered the controlled output, all other outputs being uncontrolled outputs. This feed-forward control scheme is illustrated in Figure 1.

The sole control criterion used in this work was constant overhead purity. In actual practice some economic criterion would be used, for example, maximum rate of overhead product with purity remaining above a minimum specification limit.

The modifications of the basic model required for feed-forward control with reflux ratio as the manipulative input and constant overhead purity as the controlled output are given by Franke (*18*). Affected are: (1) the derivation of the liquid composition in the condenser-accumulator system with respect to time, (2) the derivation of the liquid composition on the top plate with respect to time, (3) the overhead product rate, and (4) the liquid flow rates in the rectifying section of the column.

These considerations lead to the following restrictions on the model:

$$y_1 = x_0 = \text{constant} \quad (17)$$

$$x_1 = \text{constant, and} \quad (18)$$

$$\frac{dx_0}{dt} = \frac{dx_1}{dt} = 0 \quad (19)$$

Equation (19) satisfies the first two modifications of the basic model. Further modifications are given below in outline form. Equation (7) of the basic model is replaced by the relations

$$L_1 = \frac{(x_0 - y_2)D}{(y_2 - x_1)} \quad (20)$$

$$L_n = \left[\frac{(A-a+By_2-bx_1)\left(\dfrac{x_0-y_2}{y_2-x_1}\right) + (A-a+By_2-bx_0)}{(A-a)+(B-b)y_{n+1}} D\right] - D \quad (21)$$

for $(2 \leq n \leq N)$.

Equation (6) of the basic model is replaced by

$$D = \frac{Q_{M+1} - FC_p\,\Delta T_F}{(A - a + By_2 - bx_1)\left(\frac{x_0 - y_2}{y_2 - x_1}\right) + (A - a + By_2 - bx_0)} \quad (22)$$

With the above modifications, the expression for reflux ratio is given by

$$R = \left[\frac{(A - a + By_2 - bx_1)\left(\frac{x_0 - y_2}{y_2 - x_1}\right) + (A - a + By_2 - bx_0) + C_p\,\Delta T_R}{(A - a + By_1 - bx_0) + C_p\,\Delta T_R}\right] - 1 \quad (23)$$

The basic model was altered to include the above modifications and was used in the actual control of an experimental distillation column to an upset in feed composition. The computer program gave values of reflux ratio as a function of time which were necessary to compensate for an upset in operating conditions to maintain top product composition constant at its initial steady state value.

CALCULATION PROCEDURE

The mathematical model which describes transient stagewise distillation includes a system of $M + 2$ first-order, differential difference equations, where M is the number of plates. Although analytical techniques such as perturbation theory, operational calculus, and matrix methods have been employed successfully in the solution of linear differential equations, the present trend is toward high-speed digital, analog, and hybrid computers as aids in the solution of the complex systems of differential equations which result from simulation of intricate physical processes. Analog computers have proven adequate for the solution of systems of linear differential equations. For large systems of equations, or for nonlinear systems of equations, digital computers have been shown to be more practical. Employing numerical methods with a digital computer, one need not differentiate between linear and nonlinear differential equations. Also, one can use the same technique independent of the size of the system of differential equations, the time of solution being the main limitation. The advent of large-scale hybrid computers, which make optimum use of the best features of both the analog and digital computers, should make studies of this nature economically feasible even for large, multicomponent commercial distillation columns.

The mathematical model was programmed in FORTRAN II for solution on an IBM 709 computer. The steady state solution technique is unavoidably one of trial and error, employing a modification of the Newton-Raphson root finding method to expedite the convergence. The unsteady state solution technique, on the other hand, is one of numerical integration of a system of differential equations starting from steady state with an upset. The results of the steady state program are used as initial conditions for the unsteady state program. The transient response is then calculated from these steady state operating conditions and the imposed upsets. The only inputs required are the steady state operating conditions and the disturbed conditions.

Numerical Methods

After considerable research it was decided that Shell (*19*) presented the most satisfactory numerical technique in the literature for the solution of ordinary differential equations. In Part II of his paper, Shell (*19*) extended the Adams-Moulton finite-difference technique to a versatile divided difference technique, thus eliminating the requirement of constant interval size on history points. This technique was utilized in this work and will hereinafter be referred to as the AMOS (Adams-Moulton-Shell) technique. Also described is a self-starting procedure. A FORTRAN II program which uses this technique for the numerical solution of ordinary differential equations is described in detail in a bulletin published by the Chemical Engineering Department of the University of Florida (*20*).

For a step change in any operating variable in the transient state, there is an abrupt change in the slope of the computed output curves at the instant of the step. The numerical routine used in this work, as in the case with all predictor-corrector methods of order greater than one, is an extrapolation technique which uses the information of the so-called history points. After a step change in the transient, however, the trend bears no relation to the trend preceding the change. One must, therefore, provide a means of generating new history points for the extrapolation procedure after each step change. This was accomplished by recalling the starting points subroutine, which proceeded to provide four new history points for the AMOS routine.

The average calculation time on the IBM 709 digital computer for the transient runs presented in this work was approximately 12 min. For a large, multicomponent distillation column (either unsteady state continuous or a batch distillation column of, say, fifty plates and twenty components), it is possible that the time required to carry out a complete transient solution might be measured in hours even on the largest of the present generation of digital computers. For this reason, it is believed that analog/digital/hybrid computers (which for problems of this nature are capable of speed-ups in excess of 100 over the largest present-day digital computers) will dominate future work in this area.

EXPERIMENTAL WORK

The object of this phase of the work was to determine how well the mathematical model would predict the dynamic response of an experimental distillation column under extreme transient conditions, and to demonstrate the usefulness of the model in feed-forward control of the experimental column. The data from the experimental column were compared with calculated results. The comparison served as a test of the mathematical model and its computer program.

The experimental column was a twelve-plate, 10-in. diameter, bubble cap distillation column with a tray spacing of 1 ft. The capacity of the column allowed liquid rates up to 80 gal./hr. at a boil-up rate of 65 gal./hr. for the system methanol-tertiary butyl alcohol. The reader is referred to Huckaba et al. (*2*) for a detailed description and a schematic diagram of the column.

Experimental Data

The objective of the experimental work was to obtain the dynamic response of the experimental distillation column resulting from upsets in operating conditions both at steady state and during transient operation. After steady state was attained in the column, upsets in operating conditions were introduced successively, thus creating a sequence of upsets at various

TABLE 1. INITIAL STEADY STATE OPERATING CONDITIONS

Quantity	Run No. 1	2	3	4	5	6	7
Feed rate, lb./hr.	245.0	267.7	235.5	151.4	189.2	161.2	264.0
Feed composition, wt. % MeOH	49.7	50.2	50.2	48.4	53.1	44.7	50.2
Feed temperature, °F.	76.5	68.5	75.5	71.0	68.7	79.0	70.0
Reflux ratio, dimensionless	2.065	2.050	2.560	2.503	2.644	2.500	2.160
Reflux temp., °F.	118.5	119.5	125.0	122.5	115.0	123.0	120.0
Steam temp.,† °F.	247.6	247.6	248.5	244.7	247.5	248.5	249.8
Reboiler duty,† B.t.u./hr.	196,719	220,407	212,795	171,182	199,968	174,224	214,760
Top product rate,† lb./hr.	130.3	147.0	120.2	114.1	113.3	118.6	135.0
Feed plate	7	7	6	6	7	6	6

† Any one of these variables can serve as the sixth input.

times in the transient state. Samples were taken from every third plate on the column at regular intervals.

A sequence of upsets in the six process operating variables at various times affords the possibility of infinite number of combinations of upsets. It was the purpose of this work to use combinations of upsets that were realistic from a practical viewpoint as well as interesting from an academic point of view.

The first of these runs had a disturbance which was simply a square pulse in feed composition. The second run was composed of a sequence of steps in feed rate which were chosen at random, that is, random steps in feed rates at random times, and introduced systematically to the experimental operating unit. The third experimental run was similar in all respects to the second, except that upsets in reflux ratio were used instead of feed rate upsets. The fourth and fifth experimental runs were made up of random upsets in different operating variables at random times. For example, the fourth run used a sequence of steps in feed composition, feed rate, and reflux ratio at times $t = 0$, $t = 21$, and $t = 41$ min., respectively. The sixth experimental run consisted of a rapid succession of random upsets in operating conditions (seven upsets in 16 min.) performed to test the ability of the model to follow the rapid sequence and to continue on the correct path after the last upset toward a final steady state. No attempt was made to follow the dynamic response experimentally during the rapid sequence, although spot samples were taken at random to check the position of the experimental points in relation to the calculated curves during the rapid sequence of disturbances.

In the seventh experimental run the reflux ratio was varied continuously as a function of time in order to compensate for a step change in feed composition in an effort to maintain constant overhead purity. This run actually served two purposes. First, it illustrated the usefulness of the model in feedforward control; second, it tested the ability of the model to handle continuous time dependent variables as well as step disturbances.

Summary of Runs

Note: The initial steady state operating conditions for all runs are given in Table 1.

Run No. 1. Square pulse in feed composition (*17*):

In this run the feed composition was pulsed from an initial steady state value of 49.7 to 29.7 (wt. % MeOH) for 5 min.

Run No. 2. Sequence of upsets in feed rate (Figure 2):

In this run the feed rate was changed from an initial steady-rate value of 267.69 to 316.12, 222.53, 165.59, 370.45, and 291.00 (lb./hr.) at time, $t = 0$, 11, 32, 44, and 58 min., respectively. These steps represented changes in feed rate in excess of 100% and resulted in plate composition changes of up to 30% MeOH on a single plate.

Run No. 3. Sequence of upsets in reflux ratio (*17*):

Reflux ratio was stepped from an initial steady state value of 2.560 to 0.970, 1.427, 2.455, and 1.702 at times, $t = 0$, 21, 37, and 47 min., respectively. The maximum change in operating conditions was approximately 160%, resulting in composition changes in excess of 40% MeOH on a single plate.

Run No. 4. Sequential upsets in feed composition, feed rate, and reflux ratio (Figure 3):

The feed composition was stepped from a steady state value of 48.4 to 61.5 (wt. % MeOH, a change of 13.1% MeOH) at time, $t = 0$, the feed rate from 151.37 to 273.09 (lb./hr., an 80% change) at time, $t = 21$ min., and the reflux ratio from 2.053 to 0.994 (a change of 110%) at time, $t = 41$ min. These changes produced a maximum change of 45% MeOH in composition on the plates in the center portion of the column.

Run No. 5. Sequential upsets in feed rate, reflux ratio, and steam temperature (*17*):

The feed rate was changed from an initial steady state value of 189.15 to 264.75 (lb./hr., a 50% change) at time, $t = 0$, the reflux ratio from 2.644 to 1.060 (a change of 150%) at time, $t = 21$ min., and the steam temperature from 247.45° to 243.60°F. at time, $t = 41$ min. The maximum composition change on a single plate was 35% MeOH.

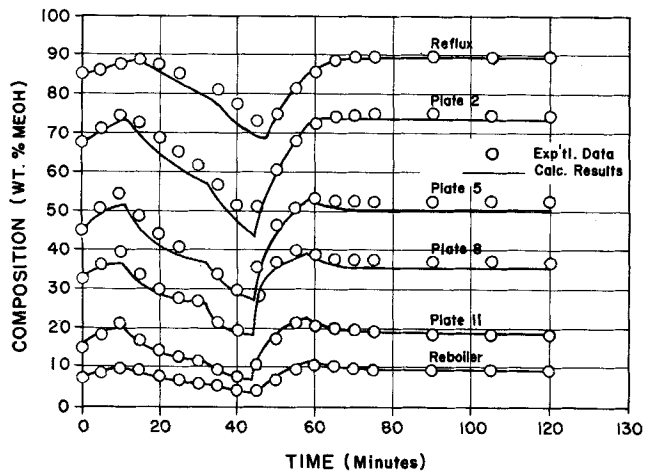

Fig. 2. Transient response for run No. 2. Sequence of upsets in feed rate.

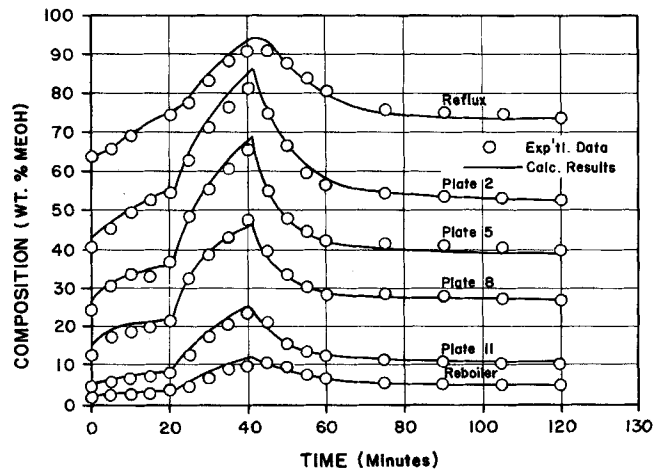

Fig. 3. Transient response for run No. 4. Sequence of upsets in feed composition, feed rate, and reflux ratio.

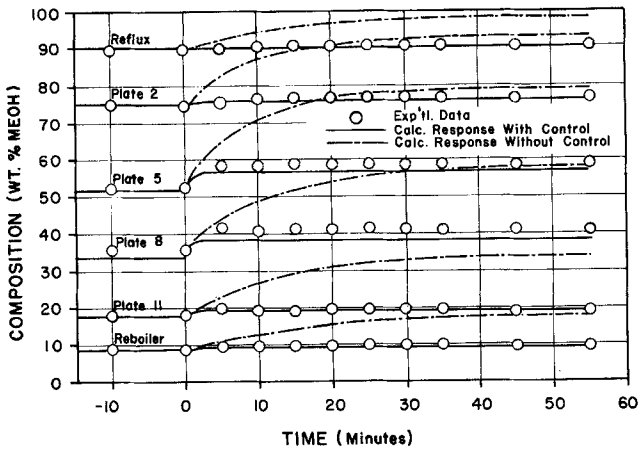

Fig. 4. Transient response for run No. 7. Feed-forward control of overhead purity.

Run No. 6. Rapid sequence of steps change in operating conditions (*17*):

This run involved steps in feed composition from 44.7 to 52.6, 61.6, and 52.6 (wt. % MeOH) at times, $t = 0$, 4, and 16 min., respectively, feed rate from 161.20 to 241.50 and 200.00 (lb./hr.) at times, $t = 2$ and 9 min., respectively, and reflux ratio from 2.500 to 0.980 and 1.410 at times, $t = 6$ and 12 min., respectively. These changes represented changes in operating conditions in excess of 150%. The maximum change on any one plate was 15% MeOH.

Run No. 7. Feed-forward control of experimental column (Figure 4):

With constant overhead purity as the control criterion, reflux ratio was used as the manipulative input in feed-forward control of the experimental distillation column to disturbances in the measurable inputs. For purposes of illustration, the feed composition was stepped from an initial steady state value of 50.2 to 66.3 (wt. % MeOH) at time, $t = 0$. The reflux ratio was manipulated as dictated by the digital computer solution. The dynamic response with and without feed-forward control is given in Figure 4.

DISCUSSION OF RESULTS

Deviations between calculated and experimental results for the dynamic response of runs 1 to 7 (for example, see Figures 2, 3, and 4) are slightly larger than the deviations observed in the steady state ($t = 0$), and generally occur at different locations in the column than do the largest of the steady state discrepancies. As opposed to the steady state findings, the largest differences in transient comparisons usually occur in the top section of the column.

An investigation of this effect showed that the largest discrepancies in the transient results occurred where the predicted reboiler heat duty differed greatly from the reboiler heat duty calculated from experimental values of D, using an approximate form of Equation (6). It was found from a steady state analysis that errors in Q_{M+1} of $\pm$ 5% caused errors in upper column compositions of $\pm$ (5-7)% (high Q_{M+1} producing low composition and vice versa). Furthermore, it is known that the predictive relation for Q_{M+1} as a function of steam-side temperature and liquid-side composition is accurate to only $\pm$ 5%. A check of the sign and magnitude of the errors in Q_{M+1} revealed that the sign and magnitude of these errors were correlated with errors in the calculated transient response curves (*17*).

From the above considerations it was concluded that the discrepancies in computed and experimental observations result largely from an inability to predict Q_{M+1} accurately. This problem arose because the steam temperature and not reboiler heat input was the measurable input, so that Q_{M+1} had to be calculated from the temperature driving force and the overall heat transfer coefficient. Had heat input to the reboiler been measurable (such as with electric immersion heaters), this problem would not have arisen.

The problem discussed above was by no means a limitation of the mathematical model or the calculation procedure, but was simply an experimental difficulty. It has been stated that the major discrepancies arose because of the inability to determine the correct input value of one of the column operating variables. Certainly no model can be expected to produce the exact process dynamics unless correct values of the system inputs are available.

Run 7 shown in Figure 4 can be considered as closed-loop, feed-forward control of an operating distillation unit. As discussed previously a control criterion of constant overhead purity was used, with reflux ratio as the manipulative input, and feed rate, composition and temperature, reflux temperature, and steam temperature as measurable inputs. Any or all of the measurable inputs could have been considered as variable for the proposed feed-forward control system. For the purpose of experimental simplicity, however, only the feed composition was allowed to vary, a simple step change in feed composition occurring at time zero. In effect, a high-speed digital computer detected the change in feed composition and calculated reflux ratio as a function of time necessary to satisfy the control criterion. In feed-forward control it is necessary that the speed of computer calculation exceed the response time of the physical process by some reasonable value (by enough, for instance, to allow disturbances to be detected, transduced, if necessary, and relayed to computer, and the computer outputs sent back to the process for corrective action).

The digital computer was not actually tied in on-line to the experimental column, but it can be considered to have been so in a meaningful sense. Actually, the operating conditions and upsets were set in advance and the calculations performed. The experimental column was then set to duplicate the initial operating conditions, the upset in feed composition imposed, and the reflux ratio manipulated manually as dictated by computer calculation. The resulting response was observed experimentally and is shown in Figure 4. Also shown is the calculated dynamic response to the upset in feed composition with and without reflux ratio corrective action. For a rather severe change in feed composition (16% MeOH) the overhead purity was maintained within 0.5% of the initial steady state value. With feedback control these limits could hardly have been realized throughout the entire transient.

CONCLUSIONS

The objectives of this work were to provide experimental data for comparison with the results of the mathematical model for a sequence of upsets and to apply the mathematical model in feed-forward control of the experimental column. It is concluded that the experimental data provided confirmation of the calculated transient response and proved the usefulness of the model in feed-forward control. The computed results predicted the experimental response to within 5%. Considering the relatively large magnitude of the disturbances in operating conditions, this seems to represent impressive accuracy. In addition, a corresponding error of up to 5% in reboiler heat duty, which is an input to the program, is believed to have contributed greatly to the above-mentioned error in the dynamic response.

The numerical integration routine used in this work (as well as many other popular predictor-corrector methods

investigated) is known to be restricted to very small interval sizes from a stability standpoint when integrating distillation equations, even as steady state is approached. Use of a truncation error control so vital to the accuracy of predictor-corrector methods further reduces the tolerable increment size. Perhaps other methods of solution, particularly the piecewise linearization of Mah, Sargent, and Michaelson (*14*), would lead to greater efficiency in computing. Although the method requires more labor per increment than do numerical integration techniques, especially for nonlinear systems, in many cases the interval size can be increased greatly due to greater inherent stability. Large increments, of course, result in less increments per solution, thereby possibly reducing the overall labor.

The feed-forward control application of the dynamic model presented here is simple in form to illustrate the technique. Further work should consider situations of practical interest such as disturbances in unmeasurable inputs known only on a statistical basis, high-frequency random upsets in a measurable input, and upsets in more than one process operating variable. The control criterion could also be modified to include more than one process output. Finally, more sophisticated control schemes, such as the feedback–feed-forward system, should be evaluated in experimental runs which utilize the relative advantages of each type of control.

The dynamic mathematical model has been shown to be a useful tool in process systems studies and should find wide utility in control system design. An illustration of the ability of the model to predict the experimental response to relatively severe operating condition changes has been shown, and one of the first known applications of a rigorous dynamic model employing a digital computer in feed-forward control of an experimental distillation column has been included (see also reference *13*).

Because of the relatively large changes in operating conditions and the correspondingly large deviations of plate compositions from the steady state values, the experimental data presented in this work should be of value to workers who desire to test linearized models.

NOTATION

A = intercept in the vapor enthalpy equation, $J = A + B\,y$, B.t.u./lb.
a = intercept in the liquid enthalpy equation, $I = a + bx$, B.t.u./lb.
B = slope in the vapor enthalpy equation, $J = A + B\,y$, B.t.u./lb.
b = slope in the liquid enthalpy equation, $I = a + bx$, B.t.u./lb.
C_p = heat capacity of liquid at average temperature, B.t.u./(lb.)(F.°)
D = overhead product rate, lb./hr.
E = Murphree liquid plate efficiency
F = feed rate, lb./hr.
g_i = representation of any arbitrary functional notation
H_i = liquid holdup on plate i, lb.
I = saturated liquid enthalpy, B.t.u./lb.
J = saturated vapor enthalpy, B.t.u./lb.
L = liquid flow rate down the column, lb./hr.
L_0 = reflux rate, lb./hr.
M = total number of plates in column
$M + 1$ = still or reboiler
m = arbitrary plate in stripping section of the column
N = number of plates in the rectifying section of the column
$N + 1$ = feed plate
n = arbitrary plate in rectifying section of the column
Q_{M+1} = heat input to the reboiler, B.t.u./hr
R = reflux ratio
S = heat transfer area in reboiler
T = temperature, °F.
t = time, hr.
U = overall heat transfer coefficient in reboiler, $\overline{U} = (US)$
V = vapor rate up the column, lb./hr.
W = bottoms product rate, lb./hr.
x = liquid composition, weight fraction more volatile component
x^* = composition of liquid in equilibrium with vapor of composition y, weight fraction more volatile component
y = vapor composition, weight fraction more volatile component
y^* = composition of vapor in equilibrium with liquid of composition x, weight fraction more volatile component

Subscripts

F = feed to the column
m = plate in the stripping section of the column
M = last plate in the stripping section of the column
$M + 1$ = reboiler
n = plate in the rectifying section of the column
N = last plate in the rectifying section of the column
$N + 1$ = feed plate
O = initial condition
S = steam side of reboiler

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