A New Method for On-Line Controller Tuning

A new method for tuning controllers on-line has been developed based on a single experimental test, a step change in controller set point. The set-point response data and analytical formulae are used to calculate model parameters for a first-order plus time delay transfer function. Controller settings can then be calculated using the model parameters and standard controller tuning relations. Simulation results demonstrate that the new method provides good initial values for PID controller settings despite gross modeling errors and unanticipated load disturbances that may occur during the experimental test.

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SCOPE

Process control systems usually include adjustable controller settings which allow flexible operation over a wide range of conditions. In principle, these settings could be specified during control system design (Hougen, 1979); in practice, controller settings are typically tuned after the control system is installed. Commonly employed tuning procedures are quite time-consuming since they involve trial and error procedures and plant tests. Consequently, strong incentives exist for the development of practical tuning techniques which provide good initial controller settings for subsequent fine tuning.

Two on-line tuning methods have gained widespread industrial acceptance. In the "loop tuning" or "continuous cycling" method due to Ziegler and Nichols (1942), the controller gain is gradually increased until the controlled process undergoes a sustained oscillation. Recommended controller settings are then calculated using the Ziegler-Nichols rules. The major disadvantages of this approach are that it is quite time-consuming and the process must be forced into a condition of marginal stability. A second popular tuning technique is the process reaction curve method. Here a single experimental test is performed with the feedback controller placed in the manual mode. A major disadvantage is that the experimental step test must be performed during open-loop operation, i.e., without feedback control.

The objective of the present study is to develop a new on-line tuning method which avoids the serious disadvantages associated with the loop tuning and process reaction curve methods.

CONCLUSIONS AND SIGNIFICANCE

A new method for tuning controllers "on-line" has been developed based on a single experimental test performed during closed-loop operation. The experimental test, a small step change in the controller set point, is easily implemented and of relatively short duration. The response data are used to estimate parameters in a simple process model, a first-order plus time delay transfer function. Reasonable controller settings can then be calculated using the process model and standard tuning relations (e.g., Ziegler-Nichols, Cohen and Coon, etc.).

Simulation results for four numerical examples demonstrate that the new tuning method provides good initial values for PID controller settings. These values provide an excellent starting point for subsequent fine tuning of the controllers. The new method tends to provide controller settings which are more conservative than the standard continuous cycling (Ziegler-Nichols) method, a desirable feature since the continuous cycling method typically produces responses which are quite oscillatory. The simulation results indicate that the new tuning method is quite robust with regard to gross modeling errors, controller calibration errors, and unmeasured load disturbances that may occur during closed-loop identification. However, the new method is not recommended for processes with very large time delays due to the Padé approximation used in the theoretical development.

The new tuning method avoids significant disadvantages associated with the two most popular current methods: the time-consuming, trial and error tests associated with the continuous cycling method and the open-loop test requirement for the process reaction curve method. The new method should be attractive for practical applications since only a single, closed-loop test is required and since the recommended controller settings can be calculated analytically.

In this paper it is assumed that the set point response is oscillatory. A modification of the new method for overdamped (i.e., nonoscillatory) responses is reported elsewhere (Yuwana, 1980).

PREVIOUS WORK

Although a variety of on-line tuning techniques have been reported in the literature, the technique which has had the most widespread influence is the "loop tuning" or "continuous cycling" method of Ziegler and Nichols (1942). In this well-known approach, the integral and derivative modes of a *PID* controller are made inoperative and the controller gain is gradually increased until the controlled variable undergoes a sustained oscillation. The recommended controller settings are then calculated using the Ziegler-Nichols rules (Coughanowr and Koppel, 1965; Luyben, 1973). Despite widespread industrial application, the loop-tuning method has several significant disadvantages:

ISSN-0001-1541-82-5666-0434-$2.00

i) It forces the process into a condition of marginal stability which may lead to unstable operation, due to process changes or external disturbances.

ii) The loop-tuning method is quite time-consuming since a trial and error procedure is employed to obtain a sustained oscillation.

iii) The method is not suitable for control loops that are open-loop unstable since instability occurs at both very high and very low controller gains (Luyben, 1973).

Several modifications of the loop-tuning method have been proposed including damped oscillation methods (Harriott, 1964; Chidambara, 1970).

The process reaction curve method (Cohen and Coon, 1953) is a second on-line tuning technique which has received a great deal of attention. It involves placing the controller in the manual mode and making a small step change in the controller output. The resulting "process reaction curve" is approximated by a simple dynamic model, a first-order plus time delay transfer function, whose parameters are easily determined. The recommended controller settings are then calculated from the Cohen and Coon tuning relations (Coughanowr and Koppel, 1965).

The chief advantage of the process reaction curve method is that only a single experimental test is required rather than the lengthy trial and error procedure required for loop tuning. However, a significant disadvantage is that the experimental test is performed during open-loop operation and thus no control action is taken in response to unanticipated disturbances. A second disadvantage is that the controller settings obtained from the process reaction curve method tend to be more sensitive to controller calibration errors than the ones determined by loop tuning.

The objective of the present study is to develop a new on-line tuning method which avoids the serious disadvantages associated with the loop tuning and process reaction curve methods. Ideally, the new method should be practical, robust, and provide minimal disruption to normal process operation. Simplicity is also a desirable attribute since plant personnel will tend to be more receptive to a new tuning technique which does not require sophisticated mathematics or complex computer programs.

In this paper a new on-line tuning method is developed which requires only a single experimental test performed during closed-loop operation, namely, a small step change in set point. In analogy with the process reaction curve method, a simple process model (first order plus time delay) is back calculated from the response data and the recommended controller settings can then be determined from the wide variety of available tuning relations. In the following section, an approximate analysis is used to derive analytical expressions which allow the model parameters to be calculated in a straightforward fashion from experimental response data. An alternative approach would be to use more elegant methods for closed-loop identification (Eykhoff, 1974; Gustavsson et al., 1977) to determine a suitable dynamic model. However, this alternative was rejected for two reasons:

i) The desired degree of simplicity would be lost,

ii) An accurate process model is not necessary since the ultimate objective is controller tuning rather than model development.

The theoretical development of the new method is presented in the next section

THEORETICAL DEVELOPMENT

Consider the block diagram of the simple closed-loop system shown in Figure 1. It is assumed that the process transfer function, $G_p(s)$, and the load transfer function, $G_L(s)$, are unknown. For many applications, the first-order plus time delay transfer function in Eq. 1 is a suitable process model:

$$G_m(s) = \frac{K_m e^{-d_m s}}{\tau_m s + 1} \tag{1}$$

In Eq. 1 K_m is the steady-state gain, τ_m is the time constant, and d_m is the time delay. This transfer function has been used as an approximate model for a wide variety of processes (Coughanowr and Koppel, 1965; Luyben, 1973).

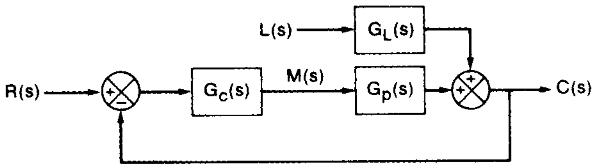

Figure 1. Block diagram of a simple feedback control system.

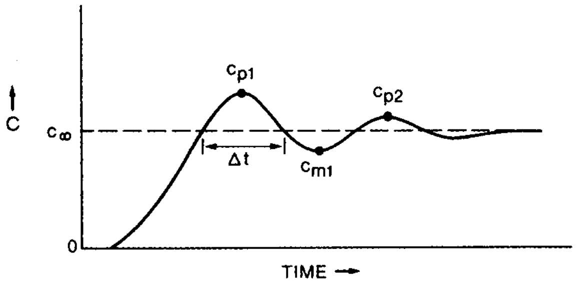

Figure 2. Response to a step change in set point.

Suppose that the feedback controller in Figure 1 is a proportional controller with transfer function, $G_c(s) = K_c$. Then the closed-loop transfer function for set point changes can be written as

$$\frac{C(s)}{R(s)} = \frac{Ke^{-d_m s}}{1 + \tau_m s + Ke^{-d_m s}} \tag{2}$$

where the open loop gain is $K = K_c K_m$. In order to develop a simple, analytical method for estimating model parameters, K_m, τ_m and d_m from closed-loop response data, we introduce a Padé approximation for the time delay term:

$$e^{-d_m s} \cong \frac{1 - 0.5\, d_m s}{1 + 0.5\, d_m s} \tag{3}$$

Substituting Eq. 3 into the denominator of Eq. 2 and rearranging gives

$$\frac{C(s)}{R(s)} = \frac{K'(1 + 0.5\, d_m s)e^{-d_m s}}{\tau^2 s^2 + 2\zeta\tau s + 1} \tag{4}$$

where

$$K' = \frac{K}{K + 1} \tag{5}$$

$$\tau = \left[\frac{d_m \tau_m}{2(K + 1)}\right]^{1/2} \tag{6}$$

$$\zeta = \frac{\tau_m + \frac{d_m}{2}(1 - K)}{[2 d_m \tau_m (K + 1)]^{1/2}} \tag{7}$$

If $0 < \zeta < 1$, then the closed-loop transfer function in Eq. 4 is underdamped and the response to a step change of magnitude A in set point R has the form shown in Figure 2. The analysis for an overdamped set-point response where $\zeta \geq 1$ is presented elsewhere (Yuwana, 1980).

It is shown in the Appendix that the process parameters can be estimated from the following expressions:

$$\hat{K}_m = \frac{c_\infty}{K_c(A - c_\infty)} \tag{8}$$

$$\hat{\tau}_m = \frac{\Delta t}{\pi}[\hat{\zeta}\sqrt{\hat{K} + 1} + \sqrt{\hat{\zeta}^2(\hat{K} + 1) + \hat{K}}] \times [(1 - \hat{\zeta}^2)(\hat{K} + 1)]^{1/2} \tag{9}$$

$$\hat{d}_m = \frac{2\Delta t[(1 - \hat{\zeta}^2)(\hat{K} + 1)]^{1/2}}{\pi[\hat{\zeta}\sqrt{\hat{K} + 1} + \sqrt{\hat{\zeta}^2(\hat{K} + 1) + \hat{K}}]} \tag{10}$$

where $\hat{\zeta}$ can be evaluated from two different expressions:

$$\hat{\zeta} = \frac{-\ln\left[\frac{c_\infty - c_{m1}}{c_{p1} - c_\infty}\right]}{\left[\pi^2 + \left\{\ln\left(\frac{c_\infty - c_{m1}}{c_{p1} - c_\infty}\right)\right\}^2\right]^{1/2}} \tag{11}$$

and

$$\hat{\zeta} = \frac{-\ln\left(\frac{c_{p2} - c_\infty}{c_{p1} - c_\infty}\right)}{\left[4\pi^2 + \left\{\ln\left(\frac{c_{p2} - c_\infty}{c_{p1} - c_\infty}\right)\right\}^2\right]^{1/2}} \tag{12}$$

The parameter estimates in Eqs. 8–12 are functions of five measurable quantities, $\{c_{p1}, c_{p2}, c_{m1}, \Delta t \text{ and } c_\infty\}$, which are easily determined from the set-point response in Figure 2. Note that it is not necessary to wait for the process to reach a new steady state since c_∞ can be estimated from Eq. 13 which is derived in the Appendix.

$$\hat{c}_\infty = \frac{c_{p2}c_{p1} - c_{m1}^2}{c_{p1} + c_{p2} - 2c_{m1}} \tag{13}$$

The parameter estimates in Eqs. 8–12 can be used to determine initial controller settings for on-line tuning using tuning relations such as the Cohen and Coon or Ziegler-Nichols rules (Coughanowr and Koppel, 1965).

Next we consider the effect of controller calibration errors on the estimated parameters and the calculated controller settings. This is an important consideration since the indicated settings on conventional controllers are only nominal values which may differ significantly from the true values. Suppose that the calibration error in the controller gain has the form

$$K_c = \alpha K_n \tag{14}$$

where K_c is the actual gain, K_n is the nominal value indicated by the controller dial, and α is a constant. Yuwana (1980) has shown that the controller settings calculated from Eqs. 8–12 and the Ziegler-Nichols tuning relations are independent of the value of α even though the parameters estimates in Eqs. 8–12 do depend on α. Thus the proposed technique for tuning controllers is very robust with regard to this type of calibration error in the controller gain. By contrast, the standard process reaction curve method is very sensitive to calibration errors.

SIMULATION STUDY

In order to evaluate the new tuning method, a simulation study was performed using four numerical examples. An important objective of the simulation was to determine the robustness of the new method to the following conditions which arise in applications:

a) Incorrect model structure

b) Unmeasured load disturbances during the set-point change

c) Sensitivity to the choice of the controller gain that is used during closed-loop identification.

Example 1

The first example consisted of the third-order plus time delay transfer function in Eq. 15:

$$G_p(s) = \frac{e^{-s}}{(2s+1)(s+1)(0.5s+1)} \tag{15}$$

The closed-loop identification method described in the previous section was used to develop an approximate process model of the form of Eq. 1. Model parameters were estimated from Eqs. 8–13 with $\hat{\zeta}$ calculated as an average of the two values obtained from Eqs. 11 and 12. Table 1 compares parameter estimates obtained for two different values of K_c with the open-loop results obtained

TABLE 1. ESTIMATED MODEL PARAMETERS FOR EXAMPLE 1

Run No.	K_c	$\hat{K}_m$	$\hat{\tau}_m$	$\hat{d}_m$
1	2.00	1.00	3.50	2.46
2	1.00	1.00	3.18	2.25
3	OL	1.00	3.00	1.70

TABLE 2. ULTIMATE GAIN, ULTIMATE PERIOD AND ZIEGLER-NICHOLS CONTROLLER SETTINGS FOR EXAMPLE I

Run No.	K_u	P_u	*PID* Controller K_c	T_i	T_d
1	2.91	8.03	1.75	4.01	1.00
2	2.90	7.34	1.74	3.67	0.917
Z-N	3.08	6.91	1.85	3.45	0.863

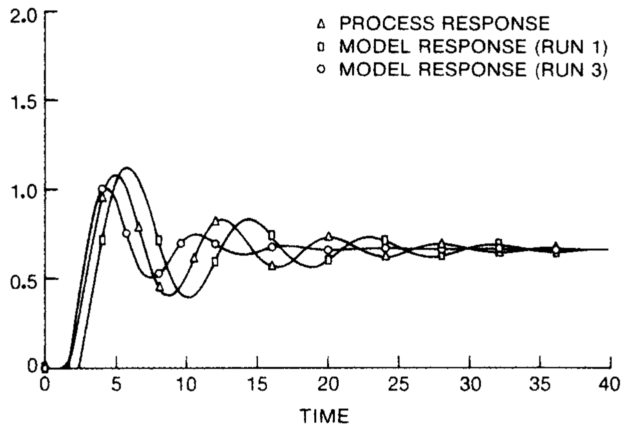

Figure 3. Closed-loop responses for Example 1 (proportional control, K_c = 2).

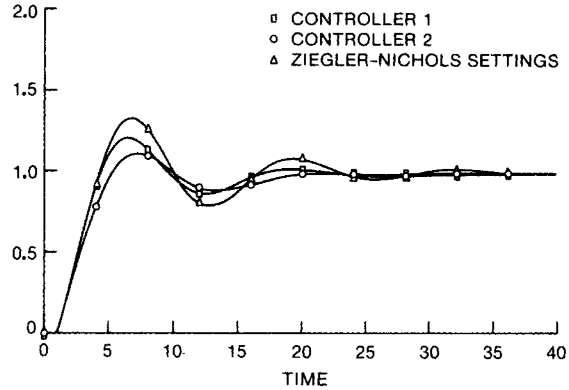

Figure 4. Comparison of *PID controllers for Example 1.*

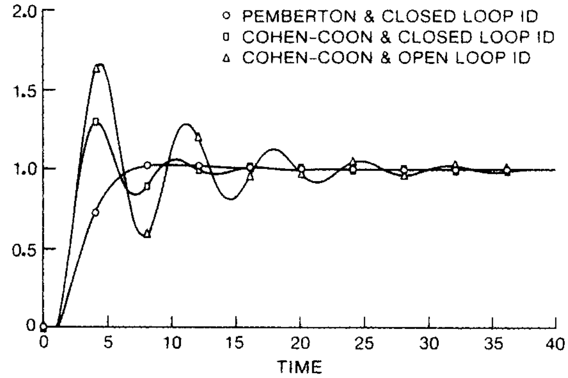

Figure 5. Comparison of tuning methods for Example 1.

from the standard process reaction curve method (i.e., the latter parameter estimates were determined under open-loop conditions from the response to a step change in the manipulated variable). The parameter estimates for Runs 1 and 2 were then used to calculate the ultimate gain, K_u, the ultimate period, P_u, and the Ziegler-Nichols settings shown in Table 2. For purposes of comparison, the corresponding values for the actual process transfer function in Eq. 15 are included as the bottom line of Table 2.

Figure 3 compares the process response with a model identified from closed-loop data (Run 1) and a model obtained from open-loop data (Run 3). For Example 1, closed-loop and open-loop identification produce dynamic models of comparable accuracy but provide only an approximation of the actual third-order plus time delay process.

The performance of the three PID controllers in Table 2 is compared in Figure 4. Controllers 1 and 2, which were based on the identified process models from Runs 1 and 2, provide an improvement over the Ziegler-Nichols settings. Throughout the simulation study, the ideal PID Controller in Eq. 16 was employed:

$$G_c(s) = K_c\left(1 + \frac{1}{\tau_I s} + \tau_D s\right) \tag{16}$$

Simulation results were also obtained for other controller tuning relations (Yuwana 1980), with typical results for Example 1 shown in Figure 5. Closed-loop identification resulted in satisfactory *PID* controllers when either the Cohen and Coon or Pemberton (1972a,b) tuning relations were used, but open-loop identification and the Cohen and Coon Relations resulted in a poorly tuned controller. [See Hang et al. (1979) or Miller et al. (1967) for more detailed comparisons of controller tuning techniques.]

A practical difficulty in on-line identification is that unknown disturbances can occur during the experimental test. In order to investigate the sensitivity of the proposed method to unknown disturbances, closed-loop identification was repeated for the situation where a 20% load disturbance occurred simultaneously with the set-point change. (The load transfer function was assumed to be identical to the process transfer function for the sake of simplicity.) Figure 6 illustrates that satisfactory PID controller settings could be obtained even though unmeasured step disturbances of ±20% occurred in the load variable during the process identification.

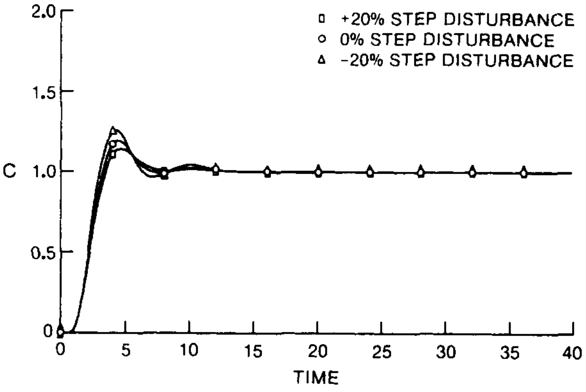

Figure 6. Effect of unmeasured load disturbances during process identification for Example 1.

TABLE 3. ESTIMATED MODEL PARAMETERS FOR EXAMPLE 2

Run No.	K_c	$\hat{K}_m$	$\hat{\tau}_m$	$\hat{\theta}_m$
1	2.00	1.00	4.10	3.18
2	1.00	1.00	3.50	3.00
3	OL	1.00	3.50	2.00

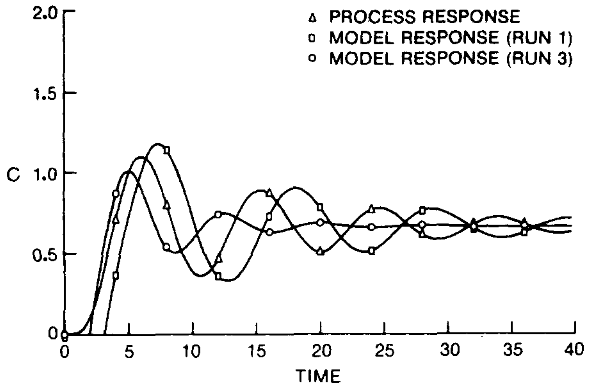

Figure 7. Closed-loop responses for Example 2 (proportional control, K_c = 2).

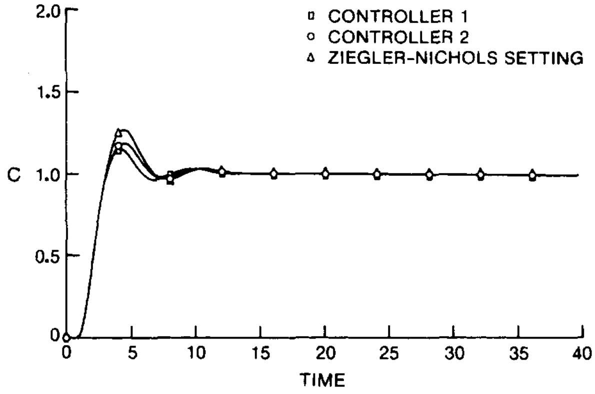

Figure 8. Comparison of *PID* controllers for Example 2.

Example 2

In order to evaluate the effectiveness of the proposed technique for high-order systems, the fifth-order transfer function in Eq. 17 was selected as Example 2:

$$G_p(s) = \frac{1}{(s+1)^5} \tag{17}$$

Application of the closed-loop identification method produced the process models in Table 3 and the controller settings in Table 4.

Figure 7 compares the process and model responses for the conditions used in closed-loop identification, namely, a set-point change and proportional control. The approximate nature of the identified models is readily apparent. Figure 8 indicates that the resulting PID controllers perform somewhat better than the Ziegler-Nichols settings.

Example 3

Since the theoretical development of the proposed tuning method employs a Padé approximation for a time delay term, one would intuitively expect the new method to be inappropriate for processes which contain relatively large time delays. Consequently, the process model in Eq. 18 was selected to provide a severe test of the new method:

$$G_p(s) = \frac{e^{-3s}}{(s+1)^2(2s+1)} \tag{18}$$

TABLE 4. ULTIMATE GAIN, ULTIMATE PERIOD AND ZIEGLER-NICHOLS CONTROLLER SETTINGS FOR EXAMPLE 2

Run			*PID* Controller		
No.	K_u	P_u	K_c	T_i	T_d
1	2.71	10.2	1.62	5.13	1.28
2	2.52	9.51	1.57	4.76	1.19
Z-N	2.89	8.65	1.73	4.32	1.08

TABLE 5. ESTIMATED MODEL PARAMETERS FOR EXAMPLE 3

Run No.	K_c	$\hat{K}_m$	$\hat{\tau}_m$	$\hat{d}_m$
1	1.00	1.00	3.92	4.69
2	0.25	1.00	3.57	3.19
3	OL	1.00	3.25	4.00

TABLE 6. ULTIMATE GAIN, ULTIMATE PERIOD AND ZIEGLER-NICHOLS CONTROLLER SETTINGS FOR EXAMPLE 3

Run			PID Controller		
No.	K_u	P_u	K_c	T_i	T_d
1	2.01	14.1	1.21	7.04	1.76
2	2.45	10.1	1.47	5.03	1.26
Z-N	1.73	12.9	1.04	6.45	1.61

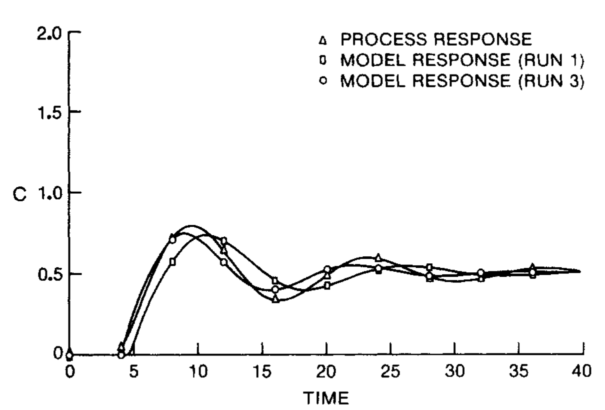

Figure 9. Closed-loop responses for Example 3 (proportional control, K_c = 1).

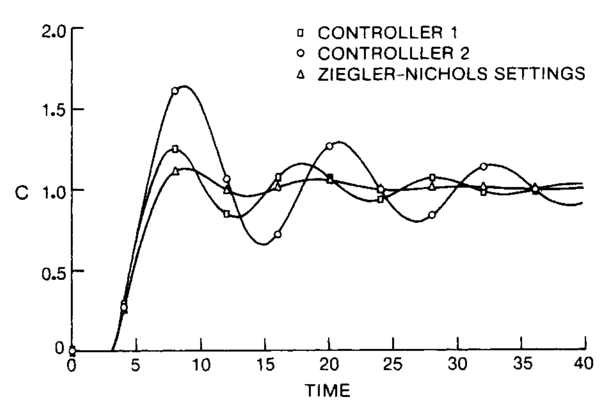

Figure 10. Comparison of *PID* controllers for Example 3.

The results of the closed-loop identification are summarized in Tables 5 and 6 while the process and model responses are shown in Figure 9. Figure 10 illustrates that Controllers 1 and 2 produce very oscillatory responses due to the large controller gains shown in Table 6. Consequently, the new method is not recommended for processes with dominant time delays.

Example 4

The theoretical development of the new method was based on the first-order plus time delay model in Eq. 1. This dynamic model is appropriate for processes whose open-loop responses are overdamped rather than underdamped. The question arises as to whether the new method would provide satisfactory controller settings for the latter case where the open-loop response is oscillatory. As the fourth numerical example, consider the following process transfer function:

$$G_p(s) = \frac{e^{-s}}{9s^2 + 2.4s + 1} \tag{19}$$

Note that the damping coefficient for this underdamped process is $\zeta = 0.4$. Closed-loop identification produced the dynamic models in Table 7 and the controller settings in Table 8. Figure 11 illustrates that the process and model responses are quite oscillatory for proportional control when $K_c = 2$.

Despite the gross modeling error provided by the first-order plus time delay model (for this example), the new method produces satisfactory PID controllers which are an improvement over the Ziegler-Nichols settings (cf. Figure 12). These results for Example

TABLE 7. ESTIMATED MODEL PARAMETERS FOR EXAMPLE 4

Run No.	K_c	$\hat{K}_m$	$\hat{\tau}_m$	$\hat{d}_m$
1	2.0	1.00	4.69	4.20
2	1.0	1.00	3.89	4.90

TABLE 8. ULTIMATE GAIN, ULTIMATE PERIOD AND ZIEGLER-NICHOLS CONTROLLER SETTINGS FOR EXAMPLE 4

Run			PID Controller		
No.	K_u	P_u	K_c	T_i	T_d
1	2.45	13.2	1.47	6.62	1.65
2	1.95	14.6	1.17	7.30	1.82
3	2.54	10.7	1.53	5.34	1.34

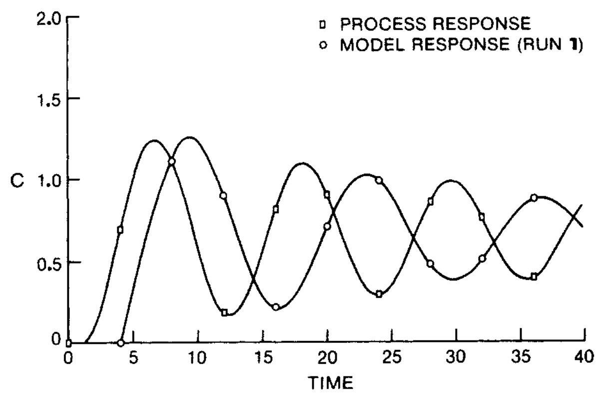

Figure 11. Closed-loop responses for Example 4 (proportional control, K_c = 2).

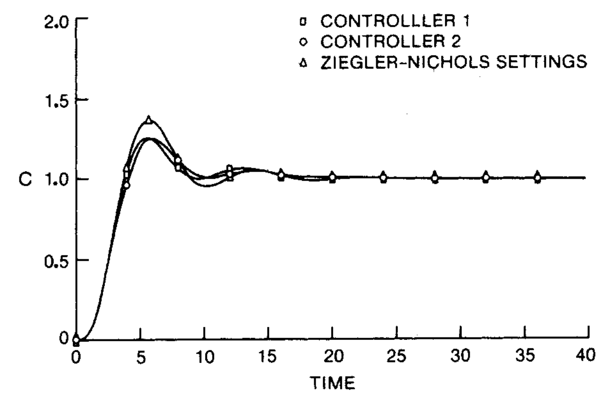

Figure 12. Comparison of *PID* controllers for Example 4.

4 provide further evidence of the robustness of the new tuning method.

ACKNOWLEDGMENT

Financial support for M. Yuwana from the Government of Indonesia is gratefully acknowledged. The authors are also grateful to R. E. Zumwalt of Exxon Research and Engineering for suggesting this controller tuning problem.

APPENDIX

In this appendix Eqs. 8–13 are derived using the closed-loop transfer function in Eq. 4 as the starting point. For a step change in set point of magnitude A, the transient response is given by:

$$c(t') = AK'[1 - D\exp(-\zeta t'/\tau)\sin(Et' + \phi)] \quad \text{(A-1)}$$

where $t' \equiv t - d_m$ and,

$$D = \frac{\left[1 - \frac{\zeta d_m}{\tau} + \frac{1}{4}\left(\frac{d_m}{\tau}\right)^2\right]^{1/2}}{\sqrt{1-\zeta^2}} \quad \text{(A-2)}$$

$$E = \frac{\sqrt{1-\zeta^2}}{\tau} \quad \text{(A-3)}$$

$$\phi = \tan^{-1}\left[\frac{\tau\sqrt{1-\zeta^2}}{\zeta\tau - 0.5d_m}\right] \quad \text{(A-4)}$$

By differentiating Eq. A-1 with respect to t and setting the derivative equal to zero, one can determine the critical points of the response and the times at which they occur. The corresponding values of t' can be written as

$$t_k' = \frac{\tan^{-1}\left(\frac{1-\zeta^2}{\zeta}\right) + k\pi - \phi}{\sqrt{1-\zeta^2}/\tau} \quad \text{(A-5)}$$

where k is a non-negative integer. Thus the first peak of the response occurs at t_1', the first minimum at t_2', the second peak at t_3', etc.

For Figure 2, ratio δ_p is defined as

$$\delta_p \equiv \frac{c_\infty - c_{m1}}{c_{p1} - c_\infty} \quad \text{(A-6)}$$

By combining Eqs. A-1, A-5 and A-6, we can derive

$$\delta_p = \exp[\zeta(t_1' - t_2')/\tau] \quad \text{(A-7)}$$

From Eq. A-5, it follows that

$$t_1' - t_2' = -\pi\tau/\sqrt{1-\zeta^2} \quad \text{(A-8)}$$

Substituting into Eq. A-7 gives

$$\delta_p = \exp[-\pi\zeta/\sqrt{1-\zeta^2}] \quad \text{(A-9)}$$

In a similar fashion, we can show that the decay ratio, δ_r, is given by:

$$\delta_r = \frac{c_{p2} - c_\infty}{c_{p1} - c_\infty} = \exp(-2\pi\zeta/\sqrt{1-\zeta})^2 \quad \text{(A-10)}$$

From Eq. A-8 it follows that the half-period of the response, Δt, is:

$$\Delta t = t_2' - t_1' = \pi\tau/\sqrt{1-\zeta^2} \quad \text{(A-11)}$$

Solving Eq. A-10 for the damping coefficient, ζ, and denoting the calculated value as $\hat{\zeta}$ gives the expression in Eq. 12. Similarly, Eqs. A-6 and A-9 can be combined to yield Eq. 11.

From Eqs. A-1 and 5 the new steady-state value of c_∞ is given by

$$c_\infty = AK' = \frac{AK}{K+1} \quad \text{(A-12)}$$

Since $K \equiv K_cK_m$, Eq. A-12 can be rearranged to provide the expression for $\hat{K}_m$ in Eq. 8. Letting $\hat{K} = K_c\hat{K}_m$, the expressions for $\hat{\tau}_m$ and $\hat{d}_m$ in Eqs. 9 and 10 are obtained by combining Eqs. 6, 7 and A-11 with the average of the values of $\hat{\zeta}$ calculated from Eqs. 11 and 12.

In order to estimate c_∞ without waiting for the set-point response to reach the new steady state, Eqs. A-9 and A-10 can be combined to eliminate ζ. Rearrangement then gives the expresssion for $\hat{c}_\infty$ in Eq. 13.

NOTATION

c	= controlled variable
C	= Laplace transform of c
c_{m1}	= first minimum of the output response
c_{m2}	= second minimum of the output response
c_{p1}	= first peak of the output response
c_{p2}	= second peak of the output response
c_∞	= steady state value
D	= constant defined in Eq. A-2
d_m	= model time delay
E	= constant defined in Eq. A-3
G_m	= model transfer function
G_p	= process transfer function
K	= open loop gain (= K_cK_m)
K'	= closed-loop gain (= $K/K + 1$)
K_c	= controller gain
K_m	= steady-state gain of the model
K_n	= nominal or indicated value of the controller gain
K_u	= ultimate gain
PI	= proportional and integral
PID	= proportional, integral and derivative
P_u	= ultimate period
R	= set point
s	= Laplace transform variable
t	= time
t'	= $t - d_m$
Δt	= half-period of oscillation
T_d	= derivative time
T_i	= integral time

Greek Letters

α	= constant
δ_r	= decay ratio
δ_p	= peak to minimum ratio
ζ	= damping coefficient for second-order model
τ	= model parameter for second-order model
τ_m	= model time constant
ϕ	= phase lag

Superscript

$\hat{}$ = estimated value

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Manuscript received October 7, 1980; revision received July 21, and accepted August 7, 1981.

Multiple-Phase Equilibria in Hydrates from Methane, Ethane, Propane and Water Mixtures

Phase-equilibrium conditions for multicomponent hydrocarbon-water mixtures were experimentally determined, demonstrating that both structure I and structure II hydrates can form from a single mixture. Model parameters were optimized to allow prediction of the hydrate structure, and prediction of the pressure and temperature of hydrate formation for the experimental mixtures.

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SCOPE

In the past five years, the existence of natural gas hydrates in the earth has become a subject of increasing concern since hydrates may impede the production of petroleum and natural gas from reservoirs where these crystalline structures can be formed (Holder et. al., 1976). This interest has been fueled by studies which suggest that hydrates may exist under the ocean (Stoll et. al., 1971), an occurrence which supports the possibility of vast reserves of natural gas existing in hydrate form.

In efforts to develop a generalized procedure for predicting hydrate formation in the earth, the lack of compositionally quantitative, experimental hydrate data for multicomponent mixtures is evident. In particular, no data has been presented showing that an equilibrium locus exists for structure I and structure II hydrate phases. In this paper, the ethane-propane-water and methane-ethane-propane water systems are studied to provide a better data base for theoretically calculating hydrate dissociation pressures, and to provide experimental evidence for the existence of hydrate I-hydrate II equilibria.

For prediction of hydrate-hydrate equilibria, Parrish and Prausnitz's (1972) widely used algorithm for determining hydrate equilibrium conditions is modified by using the data obtained in this and previous studies to obtain model parameters. By optimizing the experimentally undetermined zero-point properties (the enthalpy and chemical potential differences between the unoccupied hydrate lattice and ice at 273 K and zero pressure) a more accurate predictive scheme is developed. This method enables the prediction of hydrate formation from hydrocarbon-rich liquids and vapors whenever a water-rich liquid phase co-exists.

CONCLUSIONS AND SIGNIFICANCE

Hydrates formed from certain mixtures of ethane-propane and of methane-ethane-propane may form structure I crystals under certain *P-T-x* conditions and structure II crystals under other *P-T-x* conditions. Consequently, the methane-ethane-propane-water system exhibits several quadruple and one quintuple point loci where two liquids, two solids and a vapor are all in equilibrium. Because two different hydrate structures can form in this system, hydrate formers such as ethane may exhibit unusual anti-freeze behavior.

In predicting hydrate-forming conditions for all systems consisting entirely of methane and/or ethane and/or propane, the optimal values for the zero-point thermodynamic properties are in relatively good agreement with those expected from theoretical considerations although the zero-point enthalpic differences between the empty hydrate and ice are markedly different from those used by Parrish and Prausnitz (1972). In addition to prediction of three-phase (water rich liquid-hydrate-vapor) equilibria, this work predicts the quintuple and quadruple point loci displayed by this system. A generalization of the method used could be applied to predicting hydrate formation from multicomponent mixtures containing both hydrate-formers (butanes and lighter) and non-hydrate-formers (pentane-plus) and could be used for predicting hydrate formation in the earth.

INTRODUCTION

Gas hydrates, which are crystalline compounds composed of water and dissolved gas, have been studied extensively since Hammerschmidt (1934) discovered that they were the cause of plugged natural gas pipelines. These studies, while primarily focused on determining the pressure and temperature conditions at which hydrates formed, also revealed that hydrates were non-stoichiometric compounds and that the number of gas molecules per water molecule in the equilibrium hydrate phase depends upon the temperature and pressure at which the hydrates are formed.

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ISSN-0001-1541-82-9122-0440-$2.20