

# A Self-Adapting Time-Optimal Control Algorithm for Second-Order Processes

A method for performing time-optimal control with only limited prior knowledge of specific process dynamics is described. The time constants of the process are identified during the transient period accompanying the desired set point change, and the valve switching times of the control algorithm are calculated based on these time constants. The adaptive features of this method make its use independent of process or operating variation. The effectiveness of the proposed control method was evaluated using digital simulation and experimental techniques. The experimental phase which involved random changes to the temperature set point of a batch reactor was carried out with the aid of an on-line digital computer.

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## SCOPE

Time-optimal control is a technique whereby a control valve is driven in such a way as to minimize the time required for the control variable to attain a new steady state. In a process where set point changes are frequent, such as a batch process involving a number of heating and cooling steps, a significant reduction in time could result from the use of time-optimal control. A large number of chemical processes are well represented by a second-order system with dead time. Thus, only such second-order systems are considered in this work. However, the technique can be extended to higher order systems.

One problem associated with the application of time-optimal control is that the process dynamics which determine the switching times, that is, the instants in time when the valve is moved, generally vary gradually with time. Thus, predetermined process dynamics are not always applicable. In this paper, a practical on-line technique which performs time constant identification in conjunction with

time-optimal control is presented. The on-line identification extends to the process time constants only; the steady state gain and system dead time are assumed to be predetermined and nonvariant. An assumption which eases the complexity of the problem, and which, in the real world, turns out to be reasonably valid.

The technique takes advantage of the information contained in the transient response to a set point change. A computer is used to obtain the response data and then to calculate the process time constants via time-domain regression. With the newly determined time constants, the computer is used to calculate the control valve switching times and complete the control adjustment. Since the time constants are updated each time prior to performing the time optimal control, the result is self-adjusting to process changes. The applicability of the method was verified experimentally with a production sized reactor interfaced to the digital computer.

## CONCLUSIONS AND SIGNIFICANCE

An adaptive time-optimal control algorithm which includes the time domain identification of process dynamics and on-line computation of valve switching time was developed. It was concluded from simulation and experimental results that the technique can be successfully implemented on a medium sized digital control computer and applied to processes whose dynamics can be represented by a second order system with dead time. When contrasted to conventional control techniques, time-optimal control was shown to respond significantly faster and to result in better control as measured by the degree of

overshoot. The method is especially valuable for batch reactors where set point changes are frequent and savings can be significant. From the experimental evidence, it can be further concluded that on-line time constant adaptation is necessary to achieve truly time-optimal performance. For processes with exceptionally long dead times (that is, of the order of the major process time constant), the technique may not be applicable since the transient response will not be sufficiently established prior to the time for the first valve switch.

The rapid growth in the use of on-line computers for process control has resulted in an increased interest in advanced control techniques such as adaptive and optimal control. One such application is time-optimal control of process set point changes. The principle of time-optimal

control is to drive the process in such a way as to minimize the time required for the controlled variable to attain a new operating level. Process operation in accordance with the minimum time criterion is a technique of considerable economic potential. In continuous processes

when a change in operating level is required, either for reasons of optimization, new product mix, etc., affecting the transition in minimum time has economic value. In batch processes, where set point changes are frequent, a significant reduction in the batch cycle with a concomitant increase in production capacity results from the employment of a time-optimal control strategy.

Time optimal control has been a subject treated by numerous investigators. The earliest work on general optimal control theory was that of Pontryagin (1962). From Pontryagin's maximum principle and phase plane analysis, Koppel and Latour (1965) developed a set of algebraic equations which solve for the two switching times of a second-order system with dead time. They demonstrated that time optimal control provided significant response time improvement over a well-tuned three-mode controller. Latour et al. (1967) applied time-optimal control to a class of high order processes for which the dynamics could be approximated by a second-order model with dead time. The technique was verified by analog simulation as well as experimental work. Mellichamp (1970) developed model predictive time optimal control for second-order processes. A high speed hybrid computer was utilized. Miller et al. (1969) presented a search technique to determine optimal switching time for processes that consistently underwent very nearly the same set point changes. Shinsky (1965) successfully applied time optimal control to an exothermic batch reactor using a dual-mode concept.

Although many different approaches were employed in these previous studies, one assumption common to all was that predetermined dynamics for the process were available. Of course, the assumption is valid if the dynamics can indeed be predetermined and will remain unchanged during long-term operation. Unfortunately, the dynamics of most processes, especially batch processes, are not easy to determine beforehand. In addition, the process time constants change as a result of changes in process variables and disturbances. Therefore, predetermined dynamics may not be applicable to a specific process all the time, and control based on these dynamics would be less than optimal.

In this paper, an adaptive time optimal control method is developed, which eliminates both the need to determine process dynamics a priori and problems caused by the changes in the dynamics. The method identifies the process dynamics first and then performs the control. It has been shown by Latour et al. (1967) that a second-order system with dead time can adequately represent the dynamics of most chemical processes in performing time-optimal control. Therefore, only the case of a second-order system with dead time is treated in this paper. Since a process model is assumed, the identification scheme is concerned simply with determining the time constants of a second-order process which can describe the real process with sufficient accuracy. Whenever a process variable is driven from one steady state to another, the initial process response is detected and compared with the calculated response of a second-order system in the time domain. The time constants are determined using a nonlinear regression technique and are then used to calculate the switching times. Since the identification of the time constants is an integral part of the control algorithm and is completed before the first switch in valve position is made, previous knowledge of the process dynamics is not required.

In a recent paper by Steadman and Koppel (1972), an adaptive bang-bang control technique similar to that treated in this work was developed. The major difference

is that the Steadman-Koppel time constant adaption is based on a previous set point change, and thus the updated model cannot be used until the next set point change. This is in contrast to the method described in this paper where, since the model is updated before the switching time, the adaptation is immediate.

The applicability of the adaptive time-optimal control strategy was evaluated experimentally and via digital simulation. The experimental work utilized a production sized stirrer tank reactor controlled by an on-line digital computer. Random changes in the set point of the reactor temperature were made and the time-optimally controlled temperature response was examined.

## METHOD

In general, the strategy of time-optimal control is to set the control valve at its extreme positions, that is, fully open or closed, throughout the transient period, and set the valve at a new steady state at the end of this period. The instants in time when the valve is switched between its extreme positions or between the extreme position and its final steady state are the so called switching times. These times can be related to the dynamics of the process, the bounds of the control valve, and the initial and the final set points. When a large step change is applied to a process of second order having large time constants (of the order of minutes or hours) and a relatively small dead time lag, the interval from the introduction of the step to the first switching time is relatively long. During this interval, a major portion of the controlled variable's response to the step forcing of the control valve has already been established. Since this portion of the response is closely related to the time constants of the system, the present method analyzes this response with the aid of an on-line computer to obtain the time constants. Based on these time constants, the switching times are calculated. Referring to Figure 1, the present control method can be considered to consist of the following five stages:

1. At time  $t_0$  the computer terminates the three-mode control and positions the control valve to one of its extremes so that the controlled variable is forced to move toward the new set point.
2. From time  $t_0$  to time  $t_1$  the computer collects data with regard to the response of the controlled variable.
3. From time  $t_1$  to time  $t_2$  the computer calculates the time constants and the switching times using the acquired data and periodically updates these based on new data

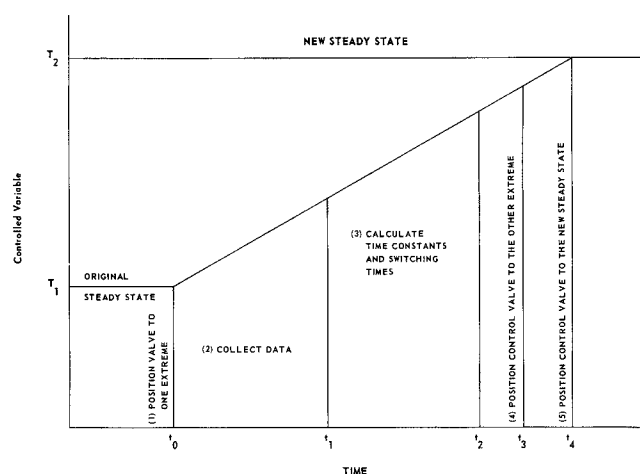


Fig. 1. The five steps of adaptive time-optimal control.

and proximity to the first switching time.

4. At time  $t_3$  the computer positions the control valve to the opposite extreme.

5. Finally at time  $t_4$  the computer moves the valve to the final steady state position and reactivates the conventional three-mode controller after one process dead time.

The data collection stage, step 2, obtains the response of the controlled variable to the step change. The value of the controlled variable is sampled by the computer at a fixed sampling rate and is then stored in memory as a single data point. The number of data points obtained is, of course, dependent on the total time allowed for collecting the data and on the sampling period. In general, a slow sampling rate is desirable since this lessens the work load on the computer. One means of relieving the computer burden while at the same time using as many data points as possible is to perform the time constant calculation just prior to that instant in time when the control valve is switched for the first time. However, since the first switching time is unknown prior to determining the time constants, one has to start the calculation much earlier. For example, the calculation can be started when the controlled variable reaches the halfway point between its initial and final set points. After that, the time constant and switching time calculation can be repeated after one or more data points are acquired until the time remaining for the first valve position switch is insufficient to perform further calculations.

The time constants are determined by fitting the data to the step response of a second-order system. Since the dead time lag is assumed to be small relative to the major process time constant, its variation is considered to be insignificant. In addition, for a specific process in the real world, dead time seldom varies. It may, therefore, be determined beforehand and excluded from the regression, thus simplifying this calculation considerably. In addition, small errors in determining the dead time are compensated for by the values obtained for the process time constants. A further assumption is that the process being modeled is linear. Thus, the process gains is a constant and is obtainable from steady state measurements. The time domain regression is based on a technique developed by Law and Bailey (1963). The mathematical development is briefly presented below. For a second-order process with a process gain  $G$ , and time constants,  $\tau_1$  and  $\tau_2$ , the process response to a step change  $L$  can be expressed as

$$Y = Y_0 + GL \left[ 1 - \frac{\tau_1}{\tau_1 - \tau_2} e^{-\frac{1}{\tau_1}t} - \frac{\tau_2}{\tau_1 - \tau_2} e^{-\frac{1}{\tau_2}t} \right]$$

where  $Y_0$  = steady state value of  $Y$ . If a set of  $N$  data points for the process response to a step change of set point are  $Z_i$  ( $i = 1, N$ ), the sum of the squares of the difference between the function  $Y$  and the data is

$$\sum S_i^2 = \sum (Z_i - Y_i)^2 \quad (2)$$

where  $\sum$  implies the sum of the terms from  $i$  equals 1 to  $i$  equals  $N$ . By the principle of least squares, the best set of time constants are obtained by minimizing the error square term. The minimum is obtained by differentiating Equation (2) with respect to  $\tau_1$  and  $\tau_2$  and letting the final expressions equal zero, that is

$$\frac{\partial \sum S_i^2}{\partial \tau_1} = 0 \quad (3)$$

$$\frac{\partial \sum S_i^2}{\partial \tau_2} = 0 \quad (4)$$

Solving the two algebraic equations with a linearized form of the function  $Y$ , obtained by expanding Equation (1) into a Taylor series around  $\tau_1$  and  $\tau_2$  and truncating all nonlinear terms, one can finally obtain the following expressions for the change of the two time constants from the  $n$ th to  $(n + 1)$ th iteration.

$$\Delta \tau_1 = (\tau_1)_{n+1} - (\tau_1)_n = \frac{C_1 \sum A_2 A_2 - C_2 \sum A_1 A_2}{\sum A_1 A_1 \sum A_2 A_2 - \sum A_1 A_2 \sum A_2 A_1} \quad (5)$$

$$\Delta \tau_2 = (\tau_2)_{n+1} - (\tau_2)_n = \frac{C_2 \sum A_1 A_1 - C_1 \sum A_2 A_1}{\sum A_1 A_1 \sum A_2 A_2 - \sum A_1 A_2 \sum A_2 A_1} \quad (6)$$

where

$$C_1 = \sum [(Z_i - Y_i)(A_1)_i] \quad (7)$$

$$C_2 = \sum [(Z_i - Y_i)(A_2)_i] \quad (8)$$

and

$$A_1 = \frac{\partial Y}{\partial \tau_1} \quad (9)$$

$$A_2 = \frac{\partial Y}{\partial \tau_2} \quad (10)$$

Given initial values for time constants,  $(\tau_1)_0$  and  $(\tau_2)_0$ , the values for  $C_1$ ,  $C_2$ ,  $A_1$ ,  $A_2$ , and finally  $\Delta \tau_1$ , and  $\Delta \tau_2$  can be calculated. Thus, a new set of time constants,  $(\tau_1)_1$  and  $(\tau_2)_1$  are obtained. The calculating process is then repeated again and again until the values of  $\Delta \tau_1$  and  $\Delta \tau_2$  become very small. As recommended by Law and Bailey (1963), a factor between zero and one is used to restrict the change in the time constants ( $f\Delta \tau_1$  and  $f\Delta \tau_2$  where  $0 < f < 1$ ) for each new iteration so that convergence is assured.

Once the two time constants of the process are determined, the first switching time  $T_1$  for the control valve can be calculated according to the following implicit functions (Koppel and Latour, 1965):

$$\left[ \frac{P - Q - ((Y_0/G) - Q) \exp(-T_1/\tau_2)}{P - Y_f/G} \right]^{\tau_2/\tau_1} = \left[ \frac{P - Q - ((Y_0/G) - Q) \exp(-T_1/\tau_1)}{P - Y_f/G} \right] \quad (11)$$

if  $Y_f < Y_0$

$$\left[ \frac{Q - P - ((Y_0/G) - P) \exp(-T_1/\tau_2)}{Q - Y_f/G} \right]^{\tau_2/\tau_1} = \left[ \frac{Q - P - ((Y_0/G) - P) \exp(-T_1/\tau_1)}{Q - Y_f/G} \right] \quad (12)$$

if  $Y_f > Y_0$

The second switching time  $T_2$  can be calculated from the following two equations

$$T_2 = \tau_1 \ln \left[ \frac{Y_0/G - Q - (P - Q) \exp(T_1/\tau_1)}{Y_f/G - P} \right], \quad \text{if } Y_f < Y_0 \quad (13)$$

$$T_2 = \tau_1 \ln \left[ \frac{Y_0/G - P - (Q - P) \exp(T_1/\tau_1)}{Y_f/G - Q} \right], \quad \text{if } Y_f > Y_0 \quad (14)$$

Since Equations (11) and (12) are implicit functions, they cannot be used to solve for the first switching time analytically. The digital solutions can, however, be obtained via a variety of well known numerical methods. For the present work, the Newton-Raphson method was judged to be the most satisfactory.

Despite the extensive mathematical treatment, the computer programs which perform the regression analysis and the Newton-Raphson iteration do not require excessive amounts of core memory and are capable of being executed in less than a hundredth of a second when performed on a machine with a basic cycle time of 1  $\mu$  sec.

## SIMULATION STUDY

Digital simulation was used to establish the feasibility of adaptive time-optimal control. Its purpose was two-fold; first, to verify that the method used to obtain the time constants on-line was applicable, and second, to determine whether the on-line switching-time computation was sufficiently accurate.

The process studied was of second order and could be described by the following differential equations

$$\tau_2 \frac{dX}{dt} = -X + M \quad (15)$$

$$\tau_1 \frac{dY}{dt} = -Y + GX \quad (16)$$

Where  $M$  is the manipulated variable,  $X$  is the first-order process response,  $Y$  is the controlled variable, and  $G$  is the process gain. In accordance with the strategy of time-optimal control, the manipulated variable assumes the following values when the set point is changed.

$$M = P \quad \text{when} \quad 0 \leq t < T_1 \quad (17)$$

$$M = Q \quad \text{when} \quad T_1 \leq t < T_2 \quad (18)$$

$$M = M_f \quad \text{when} \quad t \geq T_2 \quad (19)$$

In the above relationships  $P$  is the upper bound,  $Q$  is the lower bound,  $M_f$  is the final value of the manipulated variable which will maintain the controlled variable at the new set point, and  $T_1$  and  $T_2$  are the first and second switching times respectively. Equations (15) to (19) were used to simulate the process response and the control algorithm. The response of the controlled variable  $Y$  to a change in the manipulated variable  $M$  can be obtained from Equations (15) and (16) by treating the differential term  $dY$  as a difference term  $\Delta Y$  and using a small time increment  $\Delta t$ . However, the calculated values of  $Y$  are only the theoretical response and cannot be used to represent the actual data points simply because all real data have associated noise. The actual data points were simulated by superimposing 60 cycle noise, in the form of sine waves, on the ideal response. The values of  $Y$  thus produced then used in the regression analysis described previously.

The proposed control method was evaluated with processes assumed to have the following four sets of time constants: (1)  $\tau_1 = 3000$ ,  $\tau_2 = 400$ ; (2)  $\tau_1 = 2000$ ,  $\tau_2 = 400$ ; (3)  $\tau_1 = 1600$ ,  $\tau_2 = 400$ ; and (4)  $\tau_1 = 1000$ ,  $\tau_2 = 400$ . In each case, the process gain  $G$  was assumed to be unity and the control valve was assumed to operate between the limit of 80 ( $P$ ) and 25 ( $Q$ ). Under the time-optimal control strategy, the set point of the controlled variable was changed from 40-50, and was then changed from 50-40. Two different magnitudes of noise (0.25 and 0.5%) were assumed in the simulation of the data. The results of these investigations are shown in Tables 1 and 2 respectively. From these results it can be seen that all the calculated values generally agree with the actual values. The accuracy of the identified time constants is closely related to the total number of data points available. For the present study, the data was sampled once every 30 seconds, and the total time for which the data was obtained was ( $T_1 - 120$ ) sec where  $T_1$  was the first switching time. Thus, the

TABLE 1. ACTUAL AND CALCULATED TIME CONSTANTS AND SWITCHING TIMES  
(Measurement noise magnitude 0.25%)

Actual time constants $\tau_1^\circ$ $\tau_2^\circ$		Actual switching time $T_1^\circ$ $T_2^\circ$		Step change	Number of data points	Identified time constants $\tau_1$ $\tau_2$		Calculated switching time $T_1$ $T_2$	
$\tau_1^\circ$	$\tau_2^\circ$	$T_1^\circ$	$T_2^\circ$			$\tau_1$	$\tau_2$	$T_1$	$T_2$
3000	400	1136.2	1434.2	40-50	33	2842.0	446.9	1120.1	1445.2
2000	400	840.9	1119.1	40-50	23	1805.1	472.6	823.8	1132.1
1600	400	719.5	983.5	40-50	19	1310.7	526.2	695.0	996.33
1000	400	529.5	758.8	40-50	11	712.4	449.2	454.5	670.8
3000	400	1896.0	2021.7	50-40	59	3012.6	389.9	1893.1	2015.8
2000	400	1387.8	1509.4	50-40	42	2035.6	382.9	1390.3	1507.6
1600	400	1181.7	1299.5	50-40	35	1653.7	375.4	1187.6	1299.8
1000	400	864.3	970.2	50-40	24	1061.8	365.5	869.6	970.2

TABLE 2. ACTUAL AND CALCULATED TIME CONSTANTS AND SWITCHING TIMES  
(Measurement noise magnitude 0.5%)

Actual time constants $\tau_1^\circ$ $\tau_2^\circ$		Actual switching time $T_1^\circ$ $T_2^\circ$		Step change	Number of data points	Identified time constants $\tau_1$ $\tau_2$		Calculated switching time $T_1$ $T_2$	
$\tau_1^\circ$	$\tau_2^\circ$	$T_1^\circ$	$T_2^\circ$			$\tau_1$	$\tau_2$	$T_1$	$T_2$
3000	400	1136.2	1434.2	40-50	32	2655.7	498.9	1097.1	1448.5
2000	400	840.9	1119.1	40-50	23	1630.4	544.7	807.8	1138.9
1600	400	719.5	983.5	40-50	19	1123.1	636.7	684.3	1004.6
1000	400	529.5	758.8	40-50	8	742.4	259.6	374.0	529.6
3000	400	1896.0	2021.7	50-40	59	3042.5	379.5	1898.5	2018.2
2000	400	1387.8	1509.4	50-40	42	2084.3	364.3	1398.0	1510.5
1600	400	1181.7	1299.5	50-40	35	1714.8	350.5	1196.7	1303.0
1000	400	864.3	970.2	50-40	25	1128.0	331.6	876.2	970.9

number of data points used for the calculation increases with an increase in the total time required for the controlled variable to reach the new set point, and also with an increase in the ratio of the two time constants ( $\tau_1/\tau_2$ ). The deviation of the calculated time constants from their actual values ( $(\tau_1 - \tau_1^0)/\tau_1^0$ ,  $(\tau_2 - \tau_2^0)/\tau_2^0$ ), which can be used to express the quality of the control, are plotted against the ratio of the two process time constants for the cases where the step change is made from 50 to 40 (Figure 2 and Figure 3). Despite the point scatter, it can be seen that the deviation decreases with decreasing noise and decreasing ratio of the two time constants ( $\tau_2/\tau_1$ ). For the case where a step change from 40 to 50 was made, the same type of behavior could be observed except that the magnitude of the deviation was relatively larger.

## EXPERIMENTAL PROCEDURE

The experimental studies involved the use of a jacketed stirred tank reactor, which was operated and controlled by an on-line computer. The reactor was a 200-gal. glass-lined internally baffled unit. As shown in Figure 4, cold water and steam were mixed to give hot water, which was applied to the jacket. The temperature of the fluid in the reactor was controlled by manipulating the temperature of the hot water to the jacket, while the temperature and the flow of the hot water were automatically controlled by valves on the steam and cold water lines. The temperature of the hot water was varied be-

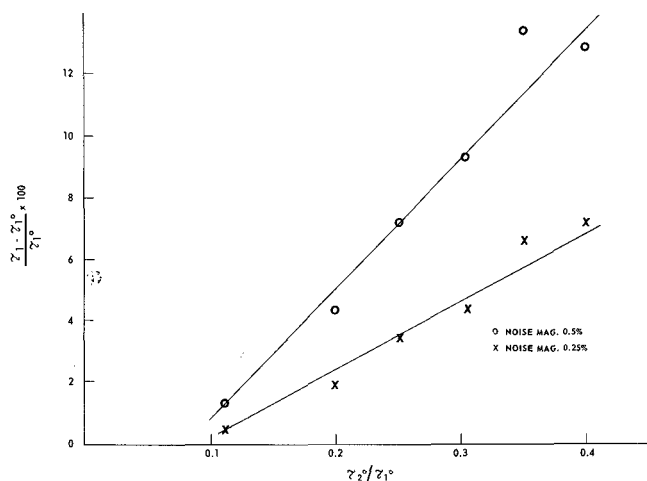


Fig. 2. Calculated deviation for  $\tau_1$ .

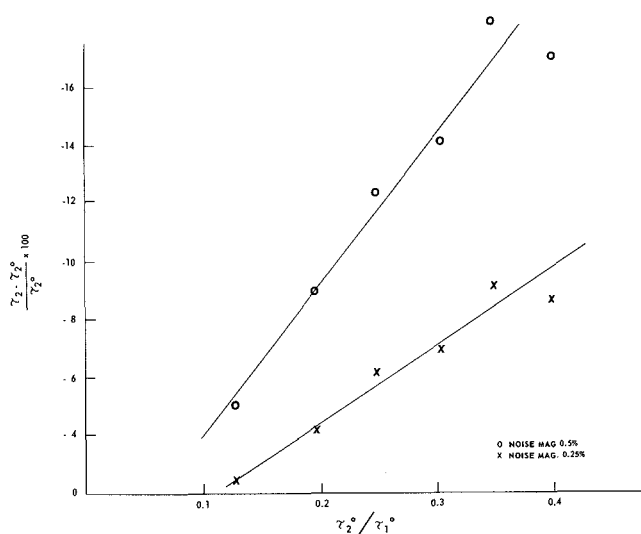


Fig. 3. Calculated deviation for  $\tau_2$ .

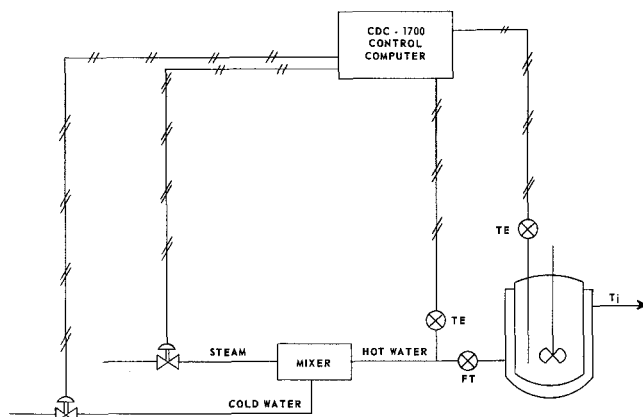


Fig. 4. Schematic diagram of the experimental setup.

tween 25° and 80°C, and the flow was arbitrarily controlled at 10 GPM.

Both the reactor and the jacket were assumed to be well mixed. Therefore, the response of the reactor temperature to a temperature change in the hot water to the jacket was second order. The dynamics of the mixer was neglected because the mixer holdup was negligible compared with the reactor. The dead time of the system was experimentally measured and was found to be one minute.

A series of experiments, involving heating up and cooling down the contents of the reactor by varying the temperature of the water in the jacket, was performed. Water or benzene was used in the reactor, and the absence of chemical reaction was assumed. The procedure followed for each of the experiments is summarized below:

1. Charge to the reactor a prespecified amount of water or benzene.
2. Start the agitator.
3. Start water flow to the jacket and control it at a fixed rate.
4. Start steamflow to mixer and control hot water temperature.
5. Start the control loop for the reactor temperature and bring the temperature to a desired steady state.
6. Introduce the desired change to the set point of the reactor temperature.
7. Allow the adaptive time-optimal control algorithm to bring the reactor temperature to the new set point.

The experiments were completely computer controlled. All the above steps including the necessary calculations and valve movements were programmed into the CDC-1700 computer using FORTRAN and AUTRAN (Gaspar et al., 1968). The details of the computer system and instrumentation have been described previously (Bacher and Kaufman, 1970).

In all experiments, the temperature of the reactor was sampled every 30 seconds. Calculation of the time constants and switching times was started when the reactor temperature reached 60% of the applied step change, and then continued every two minutes until two minutes before the first switching time was reached.

## EXPERIMENTAL RESULTS

Experiments with varying operating conditions have been carried out, and the results of these are tabulated (Table 3). Runs 1 through 12 were all cases where the reactor volume was held constant, but the vessel was subjected to step changes of different magnitude starting from various original steady states. Runs 13 through 15 were cases where the reactor volume was varied and the vessel subjected to the same step change (30° to 50°C). Run 16 and 17 were cases where benzene was used. In all these runs, the resulting response showed that the temperature of the reactor attained the new set point in minimum time. The amount of overshoot (or undershoot),

TABLE 3. EXPERIMENTAL RESULTS

No.	Liquid used	Batch volume, gal	Step, °C	Identified time constant		Calculated switching time		Overshoot (+) or undershoot (-), °C
				$\tau_1$ (sec)	$\tau_2$ (sec)	$T_1$ (sec)	$T_2$ (sec)	
1	Water	100	30.2-40	5491	252	1220	1253	+0.4
2	Water	100	29.9-50	4664	128	2482	2583	+0.2
3	Water	100	30.4-60	4557	136	4252	4313	-0.3
4	Water	100	39.6-50	4639	216	1523	1693	+0.0
5	Water	100	39.6-60	4607	165	3373	3448	+0.1
6	Water	100	40.1-70	4794	182	6736	6772	-0.2
7	Water	100	59.4-40	4381	115	3737	3774	-0.5
8	Water	100	60.1-50	4687	84	1652	1702	+0.4
9	Water	100	59.8-70	6371	65	4538	4551	+0.3
10	Water	100	69.9-60	4467	75	1157	1233	-0.1
11	Water	100	69.8-50	4345	41	2564	2589	-0.6
12	Water	100	71.8-40	3930	77	4537	4562	-0.4
13	Water	75	29.7-50	4553	47	2388	2425	+0.3
14	Water	125	31.6-50	4612	201	2347	2505	-0.5
15	Water	200	30.4-50	5122	117	2658	2751	+0.2
16	Benzene	100	50.7-40	1831	126	1099	1139	-0.3
17	Benzene	100	39.6-60	1438	221	1203	1302	-0.8

which is shown in the last column of Table 3, was generally small for all cases studied. The maximum value, which occurred in run 17, was only 0.8°C.

Since the temperature response curves are all similar in shape, only the temperature response to the 30° to 50° step change (Run 2) is shown in Figure 5. To give a comparison between time optimal control and conventional control, the temperature response of a well-tuned three-mode controller is also shown in Figure 5. It can be observed that, with the three-mode controller, the response is slower and shows noticeable overshoot. In this specific case, the time saved by time-optimal control is approximately 25%.

The satisfactory response obtained in all the cases studied indicated that the time constants of the process were correctly identified and the switching times were determined with good accuracy. The set of data collected in run 4 and the calculated response with the regression results are shown in Figure 6. It can be seen that the calculation matches the data perfectly.

Due to the fact that the heat transfer area increases proportionally as the hold up volume of the reactor is increased, the major time constant ( $\tau_1$ ) showed only a slight increase when the volume was increased. However, the major time constant changed markedly when benzene was

used primarily because benzene has a very low heat capacity and also a low viscosity which provides for better heat transfer.

The time constants identified in runs 1 through 12 display some variance, especially the minor time constant. The variation of the time constants from one run to another is only partially due to errors made in the identification process. The measurement noise, the disturbances in the water flow to the jacket, and many unpredictable changes, such as the change of the agitator power or the change of the valve hysteresis, are all important factors which can contribute to the change in the process time constants. For example, a relatively large deviation was detected in the major time constant in run 9. Yet, the response in this case did not show any large overshoot. This implies that the increase of the time constant is real and due to reasons other than an error made in the identification process. Therefore, we can conclude that the time constants of a process change from time to time and that time constant adaptation is necessary to achieve time-optimal performance.

#### NOTATION

$A_i$	= parameter defined by Equations (9) and (10)
$C_i$	= quantity defined by Equations (7) and (8)
$f$	= convergence parameter used in nonlinear regression technique
$G$	= process gain ( $Y_0/X_0$ )
$L$	= step function
$M$	= manipulated variable
$M_f$	= value of $M$ at final steady state
$n$	= number of iterations
$N$	= number of data points
$P$	= upper bound of control valve
$Q$	= lower bound of control valve
$S$	= error between data and calculated response
$t$	= time
$T_1$	= calculated first switching time
$T_1^0$	= actual first switching time
$T_2$	= calculated second switching time
$T_2^0$	= actual second switching time
$X$	= variable defined by Equation (15)
$Y$	= controlled variable

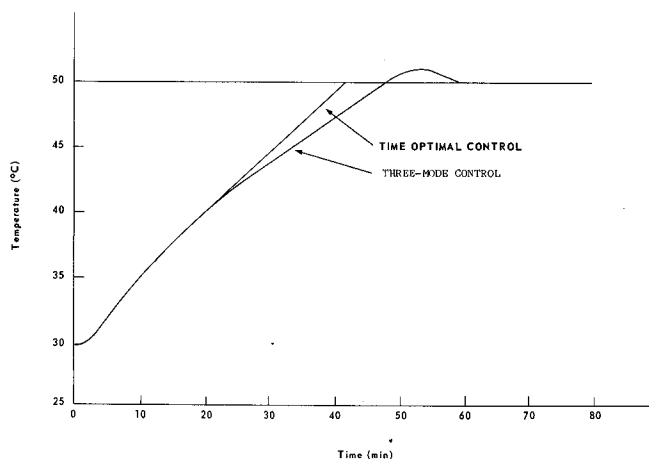


Fig. 5. Temperature response to 20°C step change.

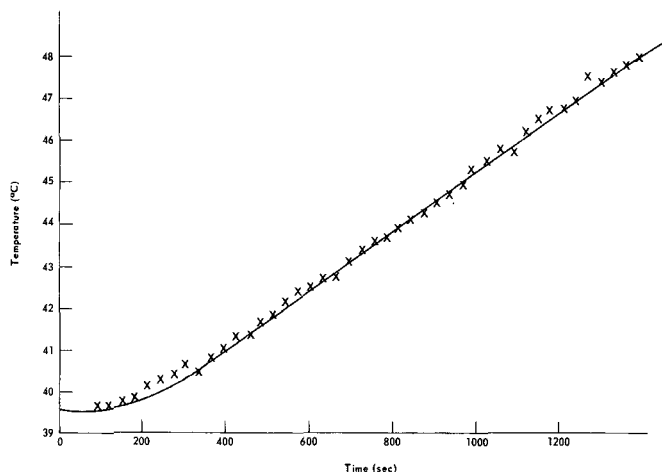


Fig. 6. Temperature data and least square fit.

- $Y_0$  = value of  $Y$  at original steady state  
 $Y_f$  = value of  $Y$  at final steady state  
 $Z_i$  = data point  
 $\tau_1$  = calculated major time constant  
 $\tau_1^0$  = actual major time constant  
 $\tau_2$  = calculated minor time constant  
 $\tau_2^0$  = actual minor time constant

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# Fixed Bed Desorption Behavior of Gases With Non-Linear Equilibria:

## Part I. Dilute, One Component, Isothermal Systems

Generalized depletion curves for desorption (and breakthrough curves for adsorption) were calculated for a system characterized by the Langmuir-type equilibria and controlled by a film type rate model. The depletion points generally appear sooner than the corresponding breakthrough points, and the desorption profiles are significantly broader than the corresponding adsorption curves. These phenomena may be best explained in terms of the prevailing driving forces. The effects of adsorbate properties and operating variables (inlet composition and flow rate) were established and experimentally substantiated.

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### SCOPE

If both the adsorption and desorption operations in fixed beds could be described as first-order linear processes, the desorption profiles, or depletion curves, would be mirror images of the adsorption breakthrough curves. However, experiments have shown that even when the desorption step was carried out as an identical opposite of the adsorption, that is, same flow rate, same temperature,

etc., a longer time was needed on desorption to return the bed to its initial starting condition than was allowed for the previous adsorption step.

To accommodate these differences, processes have been designed with pressure swing cycling, with elevated temperature regeneration, or even with chemical displacement