



Empirical Model Identification

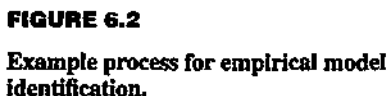
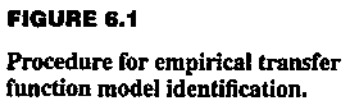
CHAPTER

6

6.1 ■ INTRODUCTION

To this point, we have been modelling processes using fundamental principles, and this approach has been very valuable in establishing relationships between parameters in physical systems and the transient behavior of the systems. Unfortunately, this approach has limitations, which generally result from the complexity of fundamental models. For example, a fundamental model of a distillation column with 10 components and 50 trays would have on the order of 500 differential equations. In addition, the model would contain many parameters to characterize the thermodynamic relationships (equilibrium K values), rate processes (heat transfer coefficients), and model nonidealities (tray efficiencies). Therefore, modelling most realistic processes requires a large engineering effort to formulate the equations, determine all parameter values, and solve the equations, usually through numerical methods. This effort is justified when very accurate predictions of dynamic responses over a wide range of process operating conditions are needed.

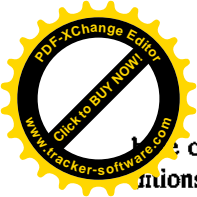
This chapter presents a very efficient alternative modelling method specifically designed for process control, termed *empirical identification*. The models developed using this method provide the dynamic relationship between selected input and output variables. For example, the empirical model for the distillation column discussed previously could relate the reflux flow rate to the distillate composition. In comparison to this simple empirical model, the fundamental model provides information on how all of the tray and product compositions and temperatures depend on variables such as reflux. Thus, the empirical models described in



The empirical methods involve designed experiments, during which the process is perturbed to generate dynamic data. The success of the methods requires close adherence to principles of experimental design and model fitting, which are presented in the next section. In subsequent sections, two identification methods are presented. The first method is termed the *process reaction curve* and employs simple, graphical procedures for model fitting. The second and more general method employs statistical principles for determining the parameters. Several examples are presented with each method. The final section reviews some advanced issues and other methods not presented in this chapter so that the reader will be able to select the most appropriate technology for model building.

Throughout this chapter several examples are presented. The first example is shown in Figure 6.2, which has two stirred tanks. The process model to be identified relates the valve opening in the heating oil line to the outlet temperature of the second tank.

An important and often underestimated aspect of empirical modelling is the need for proper experimental design. Since every method requires some type of input perturbation, the design determines its shape and duration. It also determines the



operating conditions for the process, which essentially determine the conditions about which the process model is accurate. Finally, the magnitude of the input perturbation is determined. This magnitude must be small enough to ensure that the key safety and product quality limitations are observed. It is important to begin with a perturbation that is on the safe (small) side rather than cause a severe process disturbance.

Clearly, the design requires a priori information about the process and its dynamic responses. This information is normally available from previous operating experience; if no prior information is available, some preliminary experiments must be performed. For the example in Figure 6.2, the time constants for each tank could be used to determine a first estimate for the response of the entire system.

The result of this step is a complete plan for the test which should include

1. A description of the base operating conditions
2. A definition of the perturbations
3. A definition of the variables to be measured, along with the measurement frequency
4. An estimate of the duration of the experiment

Naturally, the plan should be reviewed with all operating personnel to ensure that it does not interfere with other plant activities.

Plant Experiment

The experiment should be executed as close to the plan as possible. While variation in plant operation is inevitable, large disturbances during the experiment can invalidate the results; therefore, plant operation should be monitored during the experiment. Since the experiment is designed to establish the relationship between one input and output, changes in other inputs during the experiment could make the data unusable for identifying a dynamic model. This monitoring must be performed throughout the experiment, using measuring devices where available and using other sources of information, such as laboratory analysis, when process sensors are not available. For the example in Figure 6.2, variables such as the feed inlet temperature affect the outlet temperature of the second tank, and they should be monitored to ensure that they are approximately constant during the experiment.

Determining Model Structure

Currently, many methods are available to calculate the parameters in a model whose structure is set; however, few methods exist for determining the structure of a model (e.g., first- or second-order transfer function), based solely on the data. Typically, the engineer must assume a model structure and subsequently evaluate the assumption. The initial structure is selected based on prior knowledge of the unit operation, perhaps based on the structure of a fundamental model, and based on patterns in the experimental data just collected. The assumption is evaluated in the latter diagnostic step of this procedure.

The goal is *not* to develop a model that exactly matches the experimental data. Rather, the goal is to develop a model that describes the input-output behavior of the process adequately for use in process control.



Empirical methods typically use low-order linear models with dead time. Often (but not always) first-order-with-dead-time models are adequate for process control analysis and design.

At times, higher-order models are required, and advanced empirical methods are available for determining the model structure (Box and Jenkins, 1976).

Parameter Estimation

At this point a model structure has been selected and data has been collected. Two methods are presented in this chapter to determine values for the model parameters so that the model provides a good fit to the experimental data. One method uses a graphical technique; the other uses statistical principles. Both methods provide estimates for parameters in transfer function models, such as gain, time constant, and dead time in a first-order-with-dead-time model. The methods differ in the generality allowed in the model structure and experimental design.

Diagnostic Evaluation

Some evaluation is required before the model is used for control. The diagnostic level of evaluation determines how well the model fits the data used for parameter estimation. Generally, the diagnostic evaluation can use two approaches: (1) a comparison of the model prediction with the measured data and (2) a comparison of the results with any assumptions used in the estimation method.

Verification

The final check on the model is to verify it by comparison with *additional* data not used in the parameter estimation. Although this step is not always performed, it is worth comparing the model to data collected at another time to be sure that typical variation in plant operation does not significantly degrade model accuracy. The methods used in this step are the same as in the diagnostic evaluation step.

It is appropriate to emphasize once again that the model developed by this procedure relates the input perturbation to the output response. The process modelled includes all equipment between the input and output; thus, the typical model includes the dynamics of valves and sensors as well as the process equipment. As we will see later, this is not a limitation; in fact, the empirical model provides the proper information for control analysis, because it includes the elements in the control loop.

Finally, two conflicting objectives must always be balanced in performing this experimental procedure. The first objective is the maintenance of safe, smooth, and profitable plant operation, for which a small experimental input perturbation is desired. However, the second objective is the development of an accurate model for process control design that will be improved by a relatively large input perturbation. The proper experimental procedure must balance these two objectives by allowing a short-term disturbance so that the future plant operation is improved through good process control.

THE PROCESS REACTION CURVE

The process reaction curve is probably the most widely used method for identifying dynamic models. It is simple to perform, and although it is the least general method, it provides adequate models for many applications. First, the method is explained and demonstrated through an example. Then it is critically evaluated, with strong and weak points noted.

The process reaction curve method involves the following four actions:

1. Allow the process to reach steady state.
2. Introduce a single step change in the input variable.
3. Collect input and output response data until the process again reaches steady state.
4. Perform the graphical process reaction curve calculations.

The graphical calculations determine the parameters for a first-order-with-dead-time model: *the process reaction curve is restricted to this model*. The form of the model is as follows, with $X(s)$ denoting the input and $Y(s)$ denoting the output, both expressed in deviation variables:

$$\frac{Y(s)}{X(s)} = \frac{K_p e^{-\theta s}}{\tau s + 1} \quad (6.1)$$

There are two slightly different graphical techniques in common use, and both are explained in this section. The first technique, Method I, adapted from Ziegler and Nichols (1942), uses the graphical calculations shown in Figure 6.3 for the stirred-tank process in Figure 6.2. The intermediate values determined from the

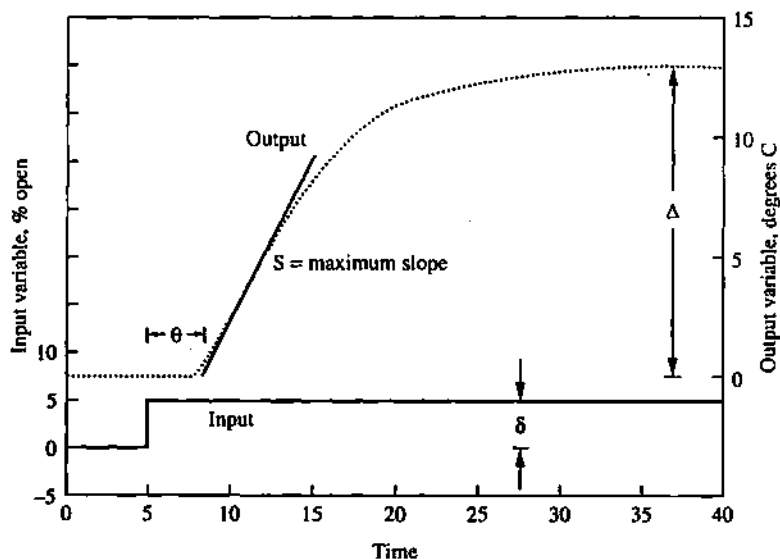


FIGURE 6.3
Process reaction curve, Method I.

graph are the magnitude of the input change, δ ; the magnitude of the steady-change in the output, Δ ; and the maximum slope of the output-versus-time plot. The values from the plot can be related to the model parameters according to the following relationships for a first-order-with-dead-time model. The general model for a step in the input with $t \geq \theta$ is

$$Y'(t) = K_p \delta [1 - e^{-(t-\theta)/\tau}] \quad (6.2)$$

The slope for this response at any time $t \geq \theta$ can be determined to be

$$\frac{dY'(t)}{dt} = \frac{d}{dt} \{ K_p \delta [1 - e^{-(t-\theta)/\tau}] \} = \frac{\Delta}{\tau} e^{-(t-\theta)/\tau} \quad (6.3)$$

The maximum slope occurs at $t = \theta$, so $S = \Delta/\tau$. Thus, the model parameters can be calculated as

$$\begin{aligned} K_p &= \Delta/\delta \\ \tau &= \Delta/S \\ \theta &= \text{intercept of maximum slope with initial value} \\ &\quad (\text{as shown in Figure 6.3}) \end{aligned} \quad (6.4)$$

A second technique, Method II, uses the graphical calculations shown in Figure 6.4. The intermediate values determined from the graph are the magnitude of the input change, δ ; the magnitude of the steady-state change in the output, Δ ; and the times at which the output reaches 28 and 63 percent of its final value. The values from the plot can be related to the model parameters using the general expression in equation (6.2). Any two values of time can be selected to determine the unknown parameters, θ and τ . The typical times are selected where the transient response is changing rapidly so that the model parameters can be accurately determined in spite of measurement noise (Smith, 1972). The expressions are

$$\begin{aligned} Y(\theta + \tau) &= \Delta(1 - e^{-1}) = 0.632\Delta \\ Y(\theta + \tau/3) &= \Delta(1 - e^{-1/3}) = 0.283\Delta \end{aligned} \quad (6.5)$$

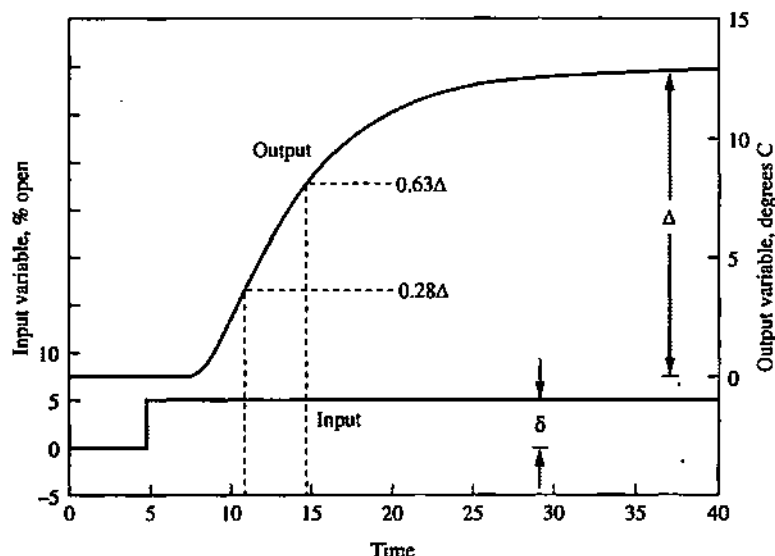


FIGURE 6.4
Process reaction curve, Method II.

Thus, the values of time at which the output reaches 28.3 and 63.2 percent of its final value are used to calculate the model parameters.

$$\begin{aligned} t_{28\%} &= \theta + \frac{\tau}{3} & t_{63\%} &= \theta + \tau \\ \tau &= 1.5(t_{63\%} - t_{28\%}) & \theta &= t_{63\%} - \tau \end{aligned} \quad (6.6)$$

Ideally, both techniques should give representative models; however, Method I requires the engineer to find a slope (i.e., a derivative) of a measured signal.

Because of the difficulty in evaluating the slope, especially when the signal has high-frequency noise, Method I typically has larger errors in the parameter estimates; thus, Method II is preferred.

EXAMPLE 6.1.

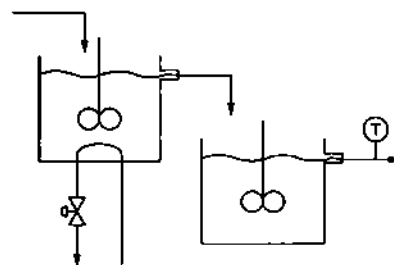
The process reaction experiments have been performed on the stirred-tank system in Figure 6.2 and the data is given in Figures 6.3 and 6.4 for Methods I and II, respectively. Determine the parameters for the first-order-with-dead-time model.

Solution. The graphical calculations are shown in Figure 6.3 for Method I, and the calculations are summarized as

$$\begin{aligned} \delta &= 5.0\% \text{ open} \\ \Delta &= 13.1^\circ\text{C} \\ K_P &= \Delta/\delta = (13.1^\circ\text{C})/(5\% \text{ open}) = 2.6^\circ\text{C}/\% \text{ open} \\ S &= 1.40^\circ\text{C}/\text{min} \\ \tau &= \Delta/S = (13.1^\circ\text{C})/(1.40^\circ\text{C}/\text{min}) = 9.36 \text{ min} \\ \theta &= 3.3 \text{ min} \end{aligned}$$

The graphical results are shown in Figure 6.4 for Method II, and the calculations are summarized below. Note that the calculations for K_P , Δ , and δ are the same and thus not repeated. Also, time is measured from the input step change.

$$\begin{aligned} 0.63\Delta &= 8.3^\circ\text{C} & t_{63\%} &= 9.7 \text{ min} \\ 0.28\Delta &= 3.7^\circ\text{C} & t_{28\%} &= 5.7 \text{ min} \\ \tau &= 1.5(t_{63\%} - t_{28\%}) = 1.5(9.7 - 5.7) \text{ min} = 6.0 \text{ min} \\ \theta &= t_{63\%} - \tau = (9.7 - 6.0) \text{ min} = 3.7 \text{ min} \end{aligned}$$



Further details for the process reaction curve method are summarized below with respect to the six-step empirical procedure.

Experimental Design

The calculation procedure is based on a perfect step change in the input as demonstrated in equation (6.2). The input can normally be changed in a step when it is a manipulated variable, such as valve percent open; however, some control designs will require models for inputs such as feed composition, which cannot be manipulated in a step, if at all. The sensitivity of the model results to deviations from a perfect input step are shown in Figure 6.5 for an example in which the true plant

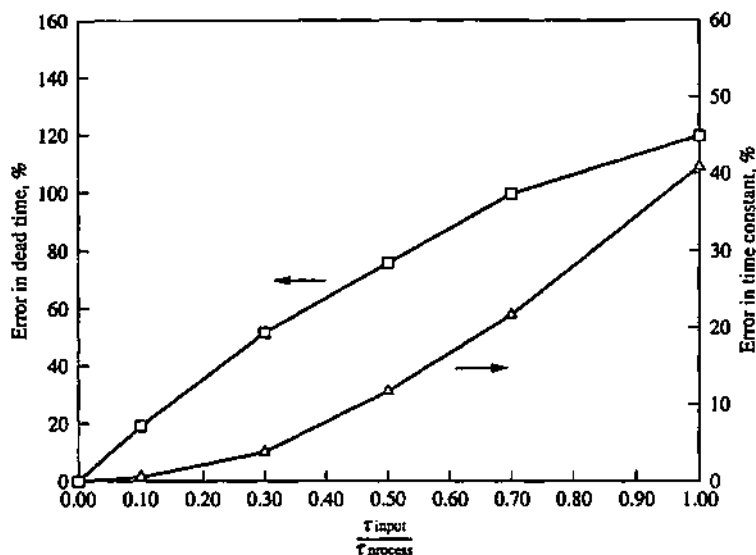


FIGURE 6.5

Sensitivity of process reaction curve to an imperfect step input, true process $\theta/(\theta + \tau) = 0.33$.

had a dead time of 0.5 and a process time constant ($\tau_{process}$) of 1.0. The step change was introduced through a first-order system with a time constant (τ_{input}) that varied from 0.0 (i.e., a perfect step) to 1.0. This case study demonstrates that very small deviations from a perfect step input are acceptable but that large deviations lead to significant model parameter errors, especially in the dead time.

In addition to the input shape, the input magnitude is also important. As previously noted, the accuracy of the model depends on the magnitude of the input step change. The output change cannot be too small, because of noise in the measured output, which is caused by many small process disturbances and sensor nonidealities. The output signal is the magnitude of the change in the output variable. Naturally, the larger the input step, the more accurate the modelling results but the larger the disturbance to the process.

A rough guideline for the process reaction curve is that the signal-to-noise ratio should be at least 5.

The noise level can be estimated as the variation experienced by the output variable when all measured inputs are constant. For example, if an output temperature varies $\pm 1^\circ\text{C}$ due to noise, the input magnitude should be large enough to cause an output change Δ of at least 5°C .

Finally, the duration of the experiment is set by the requirement of achieving a final steady state after the input step. Thus, the experiment would be expected to last at least a time equal to the dead time plus four time constants, $\theta + 4\tau$. In the stirred-tank example, the duration of the experiment could be estimated from the time constants of the two tanks, plus some time for the heat exchanger

sensor dynamics. If the data is not recorded continuously, it should be collected frequently enough for the graphical analysis; 40 or more points would be preferable, depending on the amount of high-frequency noise.

Plant Experiment

Since model errors can be large if another, perhaps unmeasured, input variable changes, experiments should be designed to identify whether disturbances have occurred. One way to do this is to ensure that the final condition of the manipulated input variable is the same as the initial condition, which naturally requires more than one step change. Then, if the output variable also returns to its initial condition, one can reasonably assume that no long-term disturbance has occurred, although a transient disturbance could take place and not be identified by this checking method. If the final value of the output variable is significantly different from its initial value, the entire experiment is questionable and should be repeated. This situation is discussed further in Example 6.3.

Diagnostic Evaluation

The basic technique for evaluating results of the process reaction curve is to plot the data and the model predictions on the same graph. Visual comparison can be used to determine whether the model provides a good fit to the data used in calculating its parameters. This procedure has been applied to Example 6.1 using the results from Method II, and the comparison is shown in Figure 6.6. Since the data and model do not differ by more than about 0.5°C throughout the transient, the model would normally be accepted for most control analyses.

Most of the control analysis methods presented in later parts of the book require linear models, and information on strong nonlinearities would be a valuable result

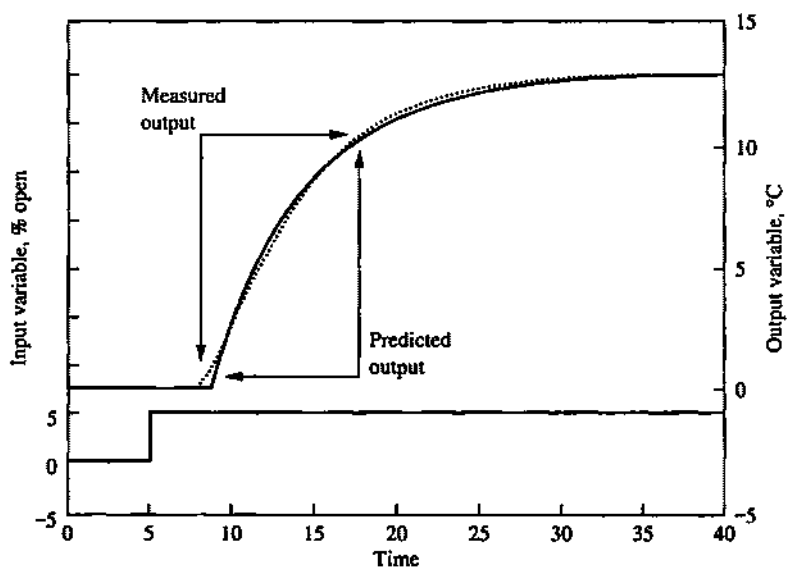


FIGURE 6.6

Comparison of measured and predicted outputs.

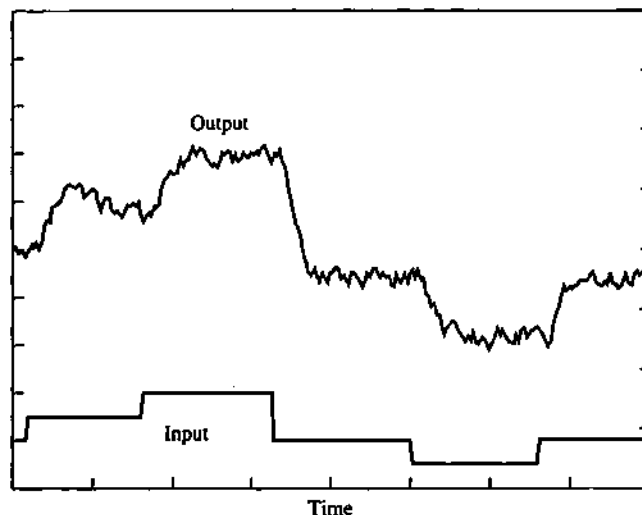


FIGURE 6.7

Example of experimental design to evaluate the linearity of a process.

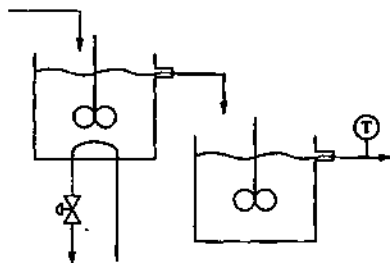
of empirical model identification. The linearity can be evaluated by comparing the model parameters determined from experiments of various magnitudes and directions, as shown in Figure 6.7. If the model parameters are similar, the process is nearly linear over the range investigated. If the parameters are very different, the process is highly nonlinear, and control methods described in Chapter 16 may have to be applied.

Verification

If additional data is collected that is not used to calculate the model parameters, it can be compared with the model using the same techniques as in the diagnostic step.

EXAMPLE 6.2.

A more realistic set of data for the two stirred-tank heating process is given in Figure 6.8. This data has noise, which could be due to imperfect mixing, sensor noise, and variation in other input variables. The application of the process reaction curve requires some judgment. The reader should perform both methods on the data and note the difficulty in Method I. Typical results for the methods are given in the following table, but the reader can expect to obtain slightly different values due to the noise.



Method I	Method II	
K_p	2.6	2.6 °C/%open
θ	2.4	3.7 min
τ	10.8	5.9 min

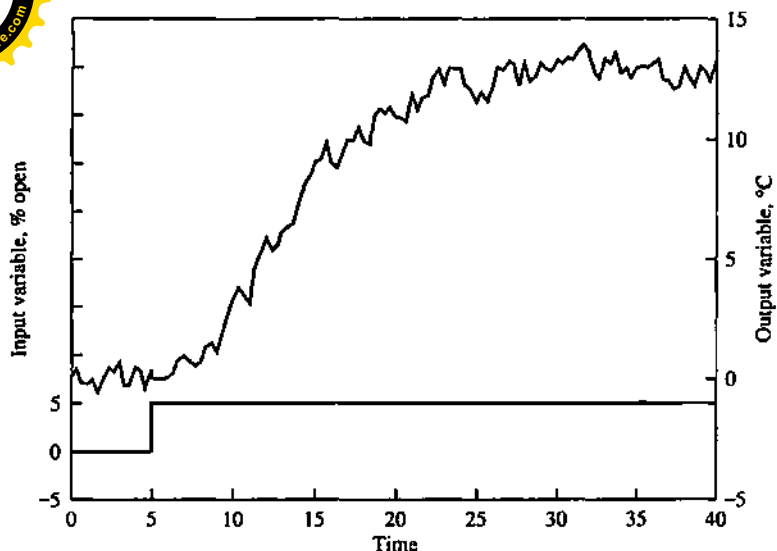


FIGURE 6.8

Process reaction curve for Example 6.2.

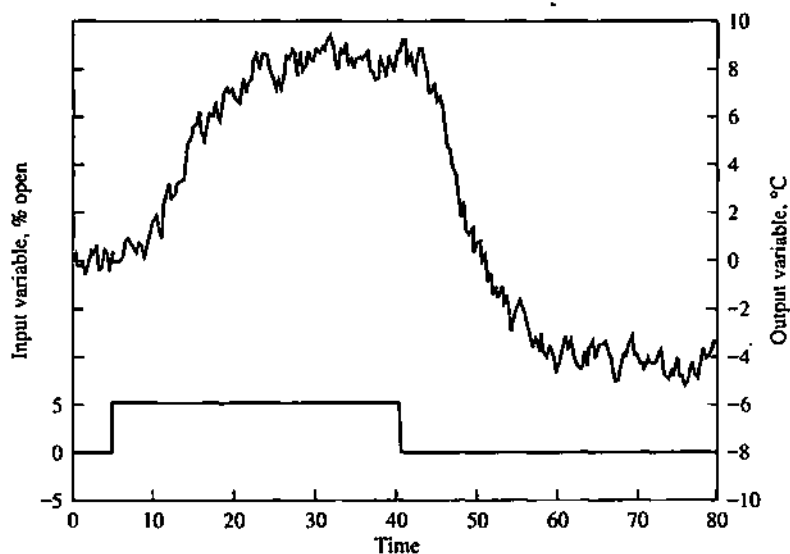


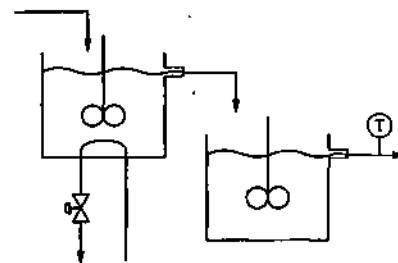
FIGURE 6.9

Experiment data for process reaction curve when input is returned to its initial condition.

EXAMPLE 6.3.

Data for two step changes is given in Figure 6.9. Determine a dynamic model using the process reaction curve method.

Note that there is no difference between the initial and final values of the input valve opening. However, the output temperature does not return to its initial value. This is due to some nonideality in the experiment, such as an unmeasured



disturbance or a sticky valve that did not move as expected. Naturally, the output variable will not return to exactly the same value, but the difference between the initial and final values in this example seems suspiciously large, because 4°C is 50 percent of the temperature change occurring during the experiment. Therefore, this data should not be used, and the experiment should be repeated.

EXAMPLE 6.4.

A fundamental model for a tank mixing process similar to Figure 6.10a will be developed in Chapter 7, where the time constant of each tank is shown to be volume/volumetric flow rate (V/F). Determine approximate models for this process at three flow rates of stream B given below when each tank volume is 35 m^3 .

This example demonstrates the usefulness of the insight provided from fundamental modelling, even though a simplified model is determined empirically. The process reaction curve experiment was performed for this process at the three flow

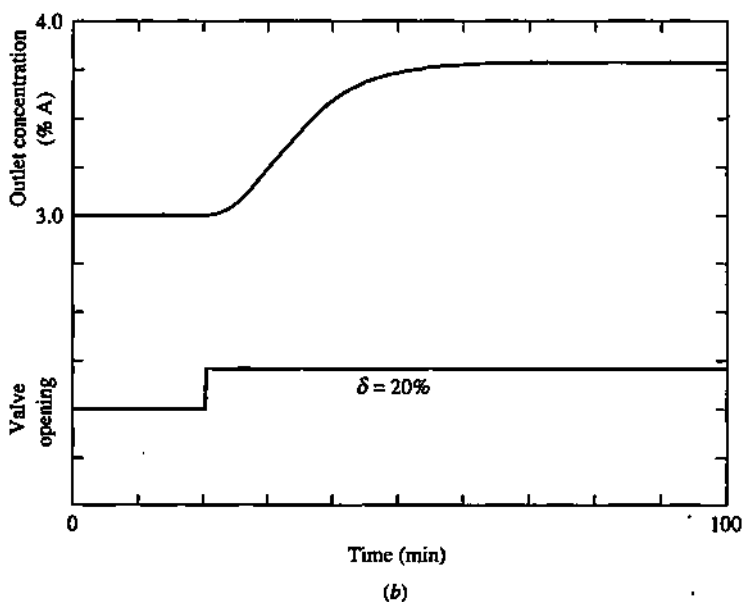
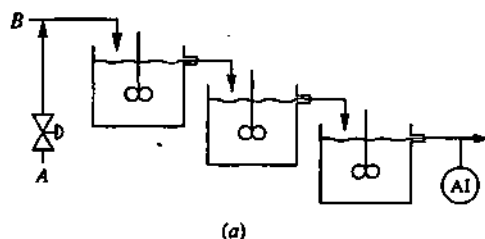


FIGURE 6.10

For Example 6.4: (a) Three-tank mixing process; (b) process reaction curve for base case.

es, all at a base exit concentration of 3 percent A, and the results at the base case flow are shown in Figure 6.10b. The results are summarized in the following table.

Flow (m ³ /min)	Simplified		Fundamental		
	K_p (% A/% open)	θ (min)	τ (min)	$\theta + \tau$ (min)	$\approx \sum \tau_i$ (min)
5.1	0.055	7.6	14.5	22.1	20.7
7.0	0.04	5.5	10.5	16.0	15.0 ← base case
8.1	0.036	4.7	9.1	13.8	12.9

The fundamental model demonstrates that the time constants ($\tau = V/F$) depend on the flow rate, decreasing as the flow increases. This trend is confirmed in the simplified model as well. Also, the approximate relationship for systems of noninteracting time constants in series, equation (5.41b), that the sum of the dead times plus time constants is unchanged by model simplification, is rather good for this process.

The most important characteristics of the process reaction curve method are summarized in Table 6.1. The major advantages of the process reaction curve method are its simplicity and short experimental duration, which result in its frequent application for simple control models.

TABLE 6.1
Summary of the process reaction curve

Characteristic	Process reaction curve
Input magnitude	Large enough to give an output signal-to-noise ratio greater than 5
Experiment duration	The process should reach steady state; thus the duration is at least $\theta + 4\tau$
Input change	A nearly perfect step change is required
Model structure	The model is restricted to first-order with dead time; this model structure is adequate for processes having overdamped, monotonic step responses
Accuracy with unmeasured disturbances	Accuracy can be strongly affected (degraded) by significant disturbances
Diagnostics	Plot model versus data; return input to initial value
Calculations	Simple hand and graphical calculations

6.4 ■ STATISTICAL MODEL IDENTIFICATION

The previously described graphical method had two major limitations: a first-order-with-dead-time model and a perfect step input. Statistical model identification methods provide more flexible approaches to identification that relax these limits to model structure and experimental design. In addition, the statistical method uses all data and not just a few points from the response, which should provide better parameter estimates from noisy process data. A simple version of statistical model fitting is presented here to introduce the concept and provide another useful identification method. The same six-step procedure described in Section 6.2 is used with this method.

The statistical method introduced here involves the following three actions:

1. Introduce a perturbation (or sequence of perturbations) in the input variable. There is no restriction on the shape of the perturbation, but the effect on the output must be large enough to enable a model to be identified.
2. Collect input and output response data. It is not necessary that the process regain steady state at the end of the experiment.
3. Calculate the model parameters as described in the subsequent paragraphs.

The statistical method described in this section uses a regression method to fit the experimental data, and the closed-form solution method requires an algebraic equation with unknown parameters. Thus, the transfer function model must be converted into an algebraic model that relates the current value of the output to past values of the input and output. There are several methods for performing this transform; the most accurate and general for linear systems involves z-transforms, which serve a similar purpose for discrete systems as Laplace transforms serve for continuous systems (see Appendix L). The method used here is much simpler and is adequate for demonstrating the statistical identification method and fitting models of simple structure, such as first-order with dead time (see Appendix F).

The first-order-with-dead-time model can be written in the time domain according to the equation

$$\tau \frac{dY'(t)}{dt} + Y'(t) = K_p X'(t - \theta) \quad (6.7)$$

Again, the prime denotes deviation from the initial steady-state value. This differential equation can be integrated from time t_i to $t_i + \Delta t$ assuming that the input $X'(t)$ is constant over this period. Note that the dead time is represented by an integer number of sample delays (i.e., $\Gamma = \theta/\Delta t$). The resulting equation is

$$Y'_{i+1} = e^{-\Delta t/\tau} Y'_i + K_p (1 - e^{-\Delta t/\tau}) X'_{i-\Gamma} \quad (6.8)$$

In further equations the notation is simplified according to the equation

$$Y'_{i+1} = aY'_i + bX'_{i-\Gamma} \quad (6.9)$$

The challenge is to determine the parameters a , b , and Γ that provide the best model for the data. Then the model parameters K_p , τ , and θ can be calculated.

The procedure used involves linear regression, which is briefly explained here and is thoroughly presented in many references (e.g., Box et al., 1978). Assume



from the moment that we know the value of Γ , the dead time (this assumption will be addressed later in the method). Typical data from the process experiment is given in Table 6.2; note that the measurements are provided at equispaced intervals. Since we want to fit an algebraic equation of the form in equation (6.9), the data must be arranged to conform to the equation. This is done in Table 6.2, where for every measured value of $(Y'_{i+1})_m$ the corresponding measured values of $(Y'_i)_m$ and $(X'_{i-\Gamma})_m$ are provided on the same line. Using the model it is also possible to predict the output variable at any time, with $(Y_{i+1})_p$ representing the predicted value, using the appropriate measured variables.

$$(Y'_{i+1})_p = a(Y'_i)_m + b(X'_{i-\Gamma})_m \quad (6.10)$$

Note that the subscript m indicates a measured value, and the subscript p indicates a predicted output value. The “best” model parameters a and b would provide an accurate prediction of the output at each time; thus, the goal is to calculate the values of the parameters a and b so that $(Y'_{i+1})_m$ and $(Y'_{i+1})_p$ are as nearly equal as possible. The common technique for determining the parameters is to apply the *least squares* method, which minimizes the sum of error squared between the measured and predicted values over all samples, $i = \Gamma + 1$ to n . The error can be expressed as follows:

$$\sum_{i=\Gamma+1}^n E_i^2 = \sum_{i=\Gamma+1}^n [(Y'_{i+1})_m - (Y'_{i+1})_p]^2 = \sum_{i=\Gamma+1}^n [(Y'_{i+1})_m - (a(Y'_i)_m + b(X'_{i-\Gamma})_m)]^2 \quad (6.11)$$

The minimization of this term requires that the derivatives of the sum of error

TABLE 6.2
Data for statistical model identification

Data in original format as collected in experiment			Data in restructured format for regression model fitting, first-order-with-dead-time model with dead time of two sample periods			
			z vector in equation (6.16)		U matrix in equation (6.16) $X' = X - X_s$ with $X_s = 50$ $Y' = Y - Y_s$ with $Y_s = 75$	
Time t	Input, X	Output, Y	Sample no. i	Output, Y'_{i+1}	Output, Y'_i	Delayed input, X'_{i-2}
0	50	75	1			
0.2	50	75	2			
0.4	52	75	3	0	0	0
0.6	52	75	4	0.05	0	0
0.8	52	75.05	5	0.1	0.05	2
1.0	52	75.1	6	0.3	0.1	2
1.2	52	75.3	7	0.6	0.3	2
1.4	52	75.6	8	0.7	0.6	2
1.6	52	75.7

Table continued for duration of experiment

squares with respect to the parameters are zero.

$$\frac{\partial}{\partial a} \left[\sum_{i=\Gamma+1}^n E_i^2 \right] = -2 \sum_{i=\Gamma+1}^n (Y'_i)_m [(Y'_{i+1})_m - a(Y'_i)_m - b(X'_{i-\Gamma})_m] = 0 \quad (6.12)$$

$$\frac{\partial}{\partial b} \left[\sum_{i=\Gamma+1}^n E_i^2 \right] = -2 \sum_{i=\Gamma+1}^n (X'_{i-\Gamma})_m [(Y'_{i+1})_m - a(Y'_i)_m - b(X'_{i-\Gamma})_m] = 0 \quad (6.13)$$

Equations (6.12) and (6.13) are linear in the two unknowns a and b , as is perhaps more easily recognized when the equations are rearranged as follows:

$$a \sum_{i=\Gamma+1}^n (Y'_i)_m^2 + b \sum_{i=\Gamma+1}^n (Y'_i)_m (X'_{i-\Gamma})_m = \sum_{i=\Gamma+1}^n (Y'_i)_m (Y'_{i+1})_m \quad (6.14)$$

$$a \sum_{i=\Gamma+1}^n (Y'_i)_m (X'_{i-\Gamma})_m + b \sum_{i=\Gamma+1}^n (X'_{i-\Gamma})_m^2 = \sum_{i=\Gamma+1}^n (X'_{i-\Gamma})_m (Y'_{i+1})_m \quad (6.15)$$

The values of the unknowns can be determined using various methods for solving linear equations (Anton, 1987); however, a more convenient approach is to use a computer program that is designed to solve the least squares problem. With these programs, the engineer simply enters the data in the form of Table 6.2, and the program automatically sets up and solves equations (6.14) and (6.15) for a and b .

These programs are designed to solve the least squares method by matrix methods. The measured values for this problem can be entered into the following matrices:

$$U = \begin{bmatrix} Y'_3 & X'_{3-\Gamma} \\ Y'_4 & X'_{4-\Gamma} \\ \vdots & \vdots \\ Y'_{n-1} & X'_{n-1-\Gamma} \end{bmatrix} \quad z = \begin{bmatrix} Y'_4 \\ Y'_5 \\ \vdots \\ Y'_n \end{bmatrix} \quad (6.16)$$

The least squares solution for the parameters can be shown to be (Graupe, 1972)

$$\begin{bmatrix} a \\ b \end{bmatrix} = (U^T U)^{-1} U^T z \quad (6.17)$$

Many computer programs exist for solving linear least squares, and simple problems can be solved easily using a spreadsheet program with a linear regression option.

Given this method for determining the coefficients a and b , it is necessary to return to the assumption that the dead time, $\Gamma = \theta/\Delta t$, is known. To determine the dead time accurately, it is necessary to solve the least squares problem in equations (6.14) and (6.15) for several values of Γ , with the value of Γ giving the lowest sum of error squared (more properly, the sum of error squared divided by the number of degrees of freedom, which is equal to the number of data points minus the number of parameters fitted) being the best estimate of the dead time. This approach, which is essentially a search in one direction, is required because the variable Γ is discrete (i.e., it takes only integer values), so that it is not possible



to determine the analytical derivative of the sum of errors squared with respect to dead time. Caution should be used, because the relationship between the dead time and sum of errors squared may not be monotonic; if more than one minimum exists, the dead time resulting in the smallest sum of errors squared should be selected.

The statistical method presented in this section, minimizing the sum of errors squared, is an intuitively appealing approach to finding the best values of the parameters. However, it depends on assumptions that, if violated significantly, could lead to erroneous estimates of the parameters. These assumptions are completely described in statistics textbooks (Box et al., 1978). The most important assumptions are the following:

1. The error E_i is an independent random variable with zero mean.
2. The model structure reasonably represents the true process dynamics.
3. The parameters a and b do not change significantly during the experiment.

The following assumptions are also made in the least squares method; however, the model accuracy is not as strongly affected when they are slightly violated:

4. The variance of the error is constant.
5. The input variable is known without error.

When all assumptions are valid, the least squares assumption will yield good estimates of the parameters. Note that the experimental and diagnostic methods are designed to ensure that the assumptions are satisfied.

EXAMPLE 6.5.

Determine the parameters for a first-order-with-dead-time model for the stirred-tank example data in Figure 6.3.

The data must be sampled at equispaced periods, which were chosen to be 0.333 minutes for this example. Since the data arrays are very long, they are not reported. The data was organized as shown in Table 6.2. Several different values of the dead time were assumed, and the regression was performed for each. The results are summarized in the following table.

Dead time, Γ	a	b	$\sum E^2$
7	0.964	0.101	7.52
8	0.9605	0.108	6.33
9	0.9578	0.1143	5.86 ← (minimum)
10	0.9555	0.1196	6.21

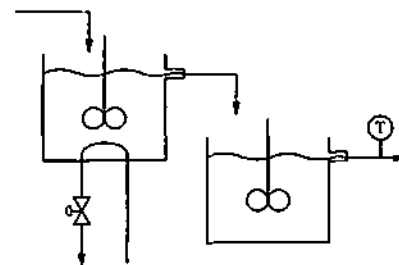
The dead time is selected to be the value that gives the smallest sum of errors squared; thus, the estimated dead time is 3 minutes, $\theta = (\Gamma)(\Delta t) = 9(0.333)$. The other model parameters can be calculated from the regression results.

$$\tau = -\Delta t / (\ln a) = -0.333 / (-0.0431) = 7.7 \text{ min}$$

$$K_p = b / (1 - a) = 0.1143 / (1 - 0.9578) = 2.7^\circ\text{C}/\% \text{open}$$



Statistical Model Identification



The comments in Section 6.3 regarding the process reaction curve and six-step procedure are also relevant for this statistical method. Some additional comments specific to the statistical method are given here.

Experimental Design

The input change can have a general shape (i.e., a step is *not required*), although Example 6.5 demonstrates that the statistical method works for step inputs. This generality is very important, because it is sometimes necessary to build models for inputs that are not directly manipulated, such as measured disturbance variables.

Sufficient input changes are required to provide enough information to overcome random noise in the measurement. Also, the data selected from the transient for use in the least squares determines which aspects of the dynamic response are fitted best. For example, if the duration of the experiment is too short, the method will provide a good fit for the initial part of the transient, but not necessarily for the steady-state gain. For this method with one or a few input changes, the input changes should be large enough and of long enough duration that the output variable reaches *at least* 63 percent of its final value. Note that more sophisticated experimental design methods (beyond the treatment in this book) are available that require much smaller output variation at the expense of longer experiment duration (Box and Jenkins, 1976).

Finally, the dead time cannot be determined with accuracy greater than the data collection sample period Δt . Thus, this period must be small enough to satisfy control system design requirements explained in later parts of the book. For now, a rough guideline can be used that Δt should be less than 5 percent of the sum of the dead time plus time constant.

Plant Experimentation

The input variable must be measured without significant noise. If this is not the case, more sophisticated statistical methods must be used.

Model Structure

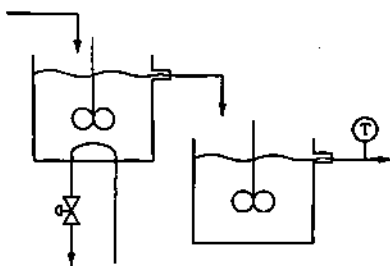
Equations have been derived for a first-order model in this chapter. Other models could be derived in the same manner. The simplest model structure that provides an adequate fit should be selected.

Diagnostic Procedure

One of the assumptions was that the error—the deviation between the model prediction and the measurement—is a random variable. The errors, sometimes referred to as the *residuals*, can be plotted against time to determine whether any unexpected, large correlation in time exists. This is done for the results of the following example.

EXAMPLE 6.6.

Data has been collected for the same stirred-tank system analyzed in Example 6.2; however, the data in this example contains noise, as shown in Figure 6.8. Determine the model parameters using the statistical identification method.



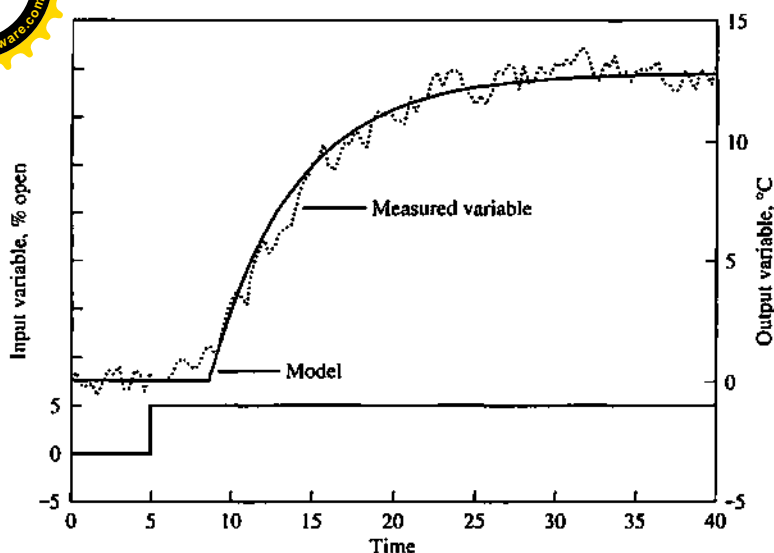


FIGURE 6.11

Comparison of measured and predicted output values from Example 6.6.

The procedure for this data set is the same as used in Example 6.5. No judgment is required in fitting slopes or smoothing curves as was required with the process reaction curve method. The results are as follows, plotted in Figure 6.11:

$$\begin{aligned} \Delta t &= 0.33 \text{ min} & \Gamma &= 11 & a &= 0.9384 & b &= 0.2578 \\ \theta &= 3.66 \text{ min} & \tau &= 5.2 \text{ min} & K_p &= 2.56^\circ\text{C}/\% \text{ open} \end{aligned}$$

Note that the model parameters are similar to the Method II results without noise, but that a slightly different value is determined for the dead time. The graphical comparison indicates a good fit to the experimental data.

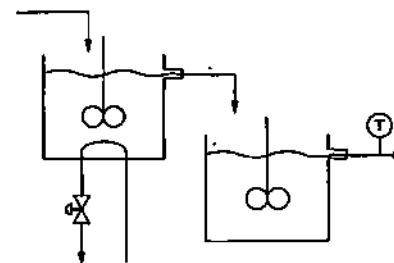
Further diagnostic analysis is possible by plotting the residuals to determine whether they are nearly random. This is done on Figure 6.12. The plot shows little correlation; note that some correlation is expected, because the simple model structure selected will not often provide the best possible fit to a set of data. Since the errors are only slightly correlated and small, the model structure and dead time are judged to be valid.

EXAMPLE 6.7.

The dynamic data in Figure 6.13 was collected, showing the relationship between the inlet and outlet temperatures of the stirred tanks in Figure 6.2. Naturally, this data would require an additional sensor for the inlet temperature to the first tank. When this data was collected, the heating valve position and all other input variables were constant. Note that the input change was not even approximately a step, because the temperature depends on the operation of upstream units. Determine the parameters for a first-order-with-dead-time model.

Again, the statistical procedure was used. The results are as follows:

$$\begin{aligned} \Gamma &= 11 & a &= 0.9228 & b &= 0.0760 \\ \theta &= 3.66 \text{ min} & \tau &= 4.2 \text{ min} & K_p &= 0.98^\circ\text{C}/^\circ\text{C} \end{aligned}$$



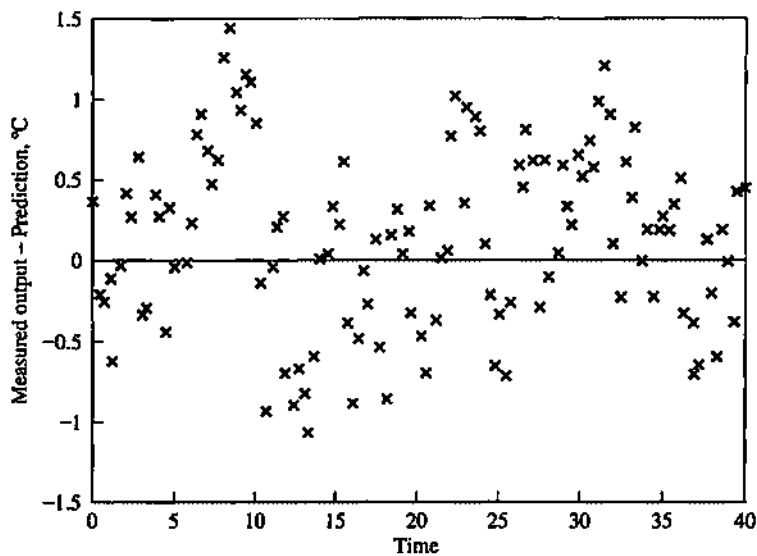


FIGURE 6.12

Plot of residuals between measured and predicted outputs from Example 6.6.

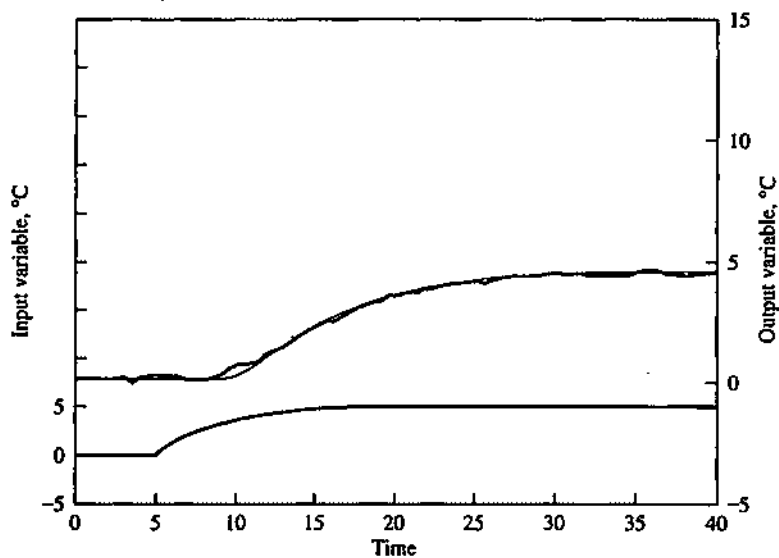


FIGURE 6.13

Experimental data and model prediction for an input that is not a perfect step, analyzed in Example 6.7.

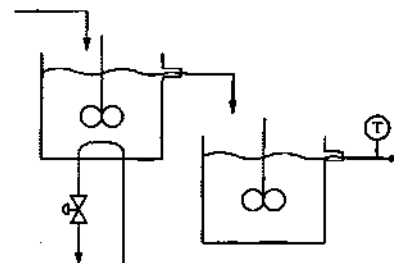
The model is compared with the data in Figure 6.13. The dynamic response is somewhat faster than the previous response, as might be expected because this model does not include the heat exchanger dynamics. The data in this example could not be analyzed using the graphical process reaction curve method because

input deviates substantially from a perfect step. However, the statistical method provided good parameter estimates from this data.

The linear regression identification method for a first-order-with-dead-time model is more general than the process reaction curve and can be used to fit important industrial processes. However, it also has limitations. Although it is easier to use and yields more accurate parameter values when the data has noise, it gives erroneous results when the noise is too large compared with the output change caused by the experiment—the same trend as with the process reaction curve.

EXAMPLE 6.8.

Figure 6.14 gives data recorded when a very small input change is introduced into the valve opening in the stirred tank system in Figure 6.2. The statistical method can be used, but the results ($\tau = 0.6$ min, $\theta = 3.66$ min, and $K_p = 2.3^\circ\text{C}/\%\text{open}$) deviate from the previously reported, more accurate results obtained with larger input disturbances. Clearly, a model from such a small input change is not reliable.



In addition, the simple statistical method used here is susceptible to unmeasured disturbances. The experimental design shown in Figure 6.9 is recommended to identify such disturbances. The statistical identification method described in this section is summarized in Table 6.3.

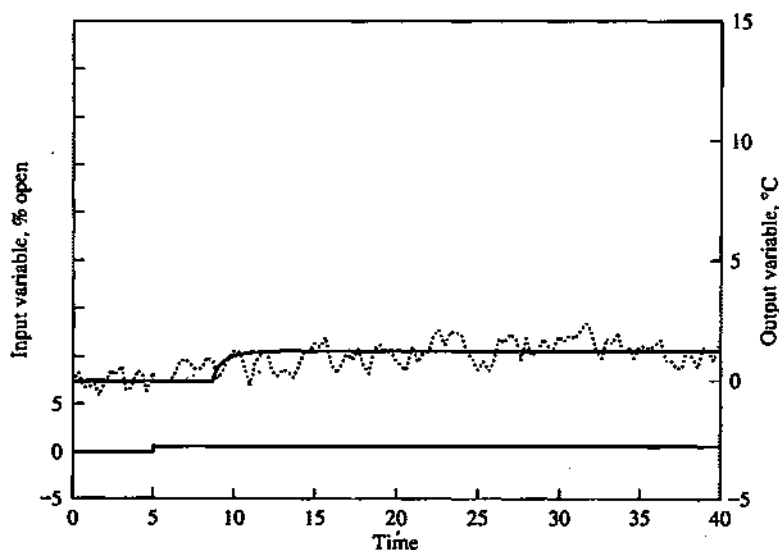


FIGURE 6.14

Example of empirical identification with an input perturbation that is too small.

6.6 ■ CONCLUSIONS

Transfer function models of most chemical processes can be identified empirically using the methods described in this chapter. The general, six-step experimental procedure should be employed, regardless of the calculation method used.

It is again worth emphasizing that the vast majority of control strategies are based on empirical models; thus, the methods in this chapter are of great practical importance.

Model Error

Model errors result from measurement noise, unmeasured disturbances, imperfect input adjustments, and applying simple linear models to truly nonlinear processes. The examples in this chapter give realistic results, which indicate that model parameters are known only within ± 20 percent at best for many processes. However, these models appear to capture the dominant dynamic behavior. Engineers must always consider the sensitivity of their decisions and calculations to expected model errors to ensure good performance of their designs. We will investigate the effects of model errors in later chapters and will learn that moderate errors do not substantially degrade the performance of single-loop controllers. A summary of a few sensitivity studies, which are helpful when reviewing modelling and control design, are given in Table 6.4.

TABLE 6.4

Summary of sensitivity of control stability and performance to modelling errors

Case	Issue studied
Example 9.2	The effect on performance of using controller tuning parameters based on an empirical model that is lower-order than the true process
Example 9.5	The effect on performance of using controller tuning parameters based on an empirical model that is substantially different from the true process
Example 10.15	The effect of modelling error on the stability of feedback control, showing the change of model parameters likely to lead to significant differences in dynamic behavior
Example 10.18	The effect of modelling error on the stability of feedback control, showing the critical frequency range of importance
Figure 13.16 and discussion	The effect of modelling error on the performance of feedback control, showing the frequency range of importance



Experimental Design

The design of the experimental conditions, especially the input perturbation, has a great effect on the success of empirical model identification. The perturbation must be large enough, compared with other effects on the output, to allow accurate model parameter estimation. Naturally, this requirement is in conflict with the desire to minimize process disturbances, and some compromise is required. Model accuracy depends strongly on the experimental procedure, and no amount of analysis can compensate for a very poor experiment.

Six-Step Procedure

Empirical model identification is an iterative procedure that may involve several experiments and potential model structures before a satisfactory model has been determined. The procedure in Figure 6.1 clearly demonstrates the requirement for a priori information about the process to design the experiment. Since this information may be inexact, the experimental procedure may have to be repeated, perhaps using a larger perturbation, to obtain useful data. Also, the results of the analysis should be evaluated with diagnostic procedures to ensure that the model is accurate enough for control design. It is essential for engineers to recognize that the calculation procedure always yields parameter values and that they must judge the validity of the results based on diagnostics and knowledge of the process behavior based on fundamental models.

No process is known exactly! Good results using models with (unavoidable) errors is not simply fortuitous; process control methods have been developed over the years to function well in realistic situations.

In conclusion, empirical models can be determined by a rather straightforward experimental procedure combined with either a graphical or a statistical parameter estimation method. Usually, the models take the form of low-order transfer functions with dead time, which, although not capable of perfect prediction of all aspects of the process performance, provide the essential input-output relationships required for process control. The important topic of model error is considered in many of the subsequent chapters, where it is shown that models of the accuracy achieved with these empirical methods are adequate for many control design calculations. However, the selection of algorithms and determination of adjustable parameters must be performed with due consideration for the likely model errors. Therefore, lessons learned in this chapter about accuracy are applied in many later chapters.

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ADDITIONAL RESOURCES

Advanced statistical model identification methods are widely used in practice. The following reference provides further insight into some of the more popular approaches.

Vandaele, W., *Applied Time Series and Box-Jenkins Models*, Academic Press, New York, 1983.

The following proceedings give a selection of model identification applications.

Ekyhoff, P., *Trends and Progress in System Identification*, Pergamon Press, Oxford, 1981.

Computer programs are available to ease the application of statistical methods. The programs noted below can be applied to simple linear regression (Excel and Corel Quattro), to general statistical model fitting (SAS), and to empirical dynamic modelling for process control (MATLAB).

Excel®, Microsoft
MATLAB® and Identification Toolbox, The MathWorks
Corel Quattro®, Corel
SAS®, SAS Institute

International standards have been established for testing and reporting dynamic models for process control equipment. A good summary is provided in

ISA-S26-1968 and ANSI MC4.1-1975, *Dynamic Response Testing of Process Control Instrumentation*, Instrument Society of America, Research Triangle Park, NC, 1968.

Good results from the empirical method depend on proper engineering practices in experimental design and results analysis. The engineer must always cross-check the empirical model against the possible models based on physical principles.

Questions

QUESTIONS

- 6.1. An experiment has been performed on a fired heater (furnace). The fuel valve was opened an additional increment of 2 percent in a step, giving the resulting temperature response in Figure Q6.1. Determine the model parameters using both process reaction curve methods and estimate the inaccuracies in the parameter values due to the data and calculation methods.

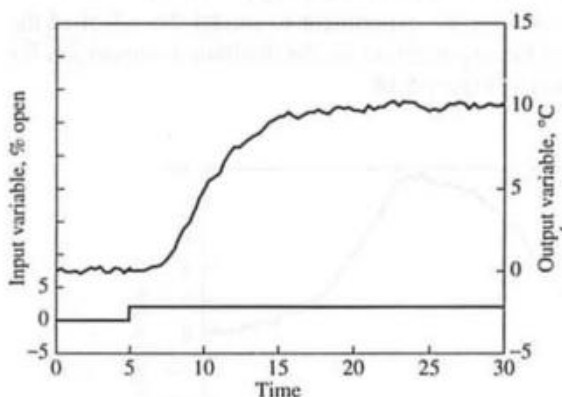


FIGURE Q6.1

- 6.2. Data has been collected from a chemical reactor. The inlet concentration was the only input variable that changed when the data was collected. The input and output data is given in Table Q6.2.

TABLE Q6.2

Time (min)	Input (% open)	Output (°C)	Time (min)	Input (% open)	Output (°C)	Time (min)	Input (% open)	Output (°C)
0	30	69.65	36	38	70.22	72	38	75.27
4	30	69.7	40	38	71.32	76	38	75.97
8	30	70.41	44	38	72.33	80	38	76.30
12	30	70.28	48	38	72.92	84	38	76.30
16	30	69.55	52	38	73.45	88	38	75.51
20	30	70.32	56	38	74.09	92	38	74.86
24	38	69.97	60	38	75.00	96	38	75.86
28	38	69.96	64	38	75.25	100	38	76.20
32	38	69.68	68	38	74.78	104	38	76.0

CHAPTER 6 Empirical Model Identification

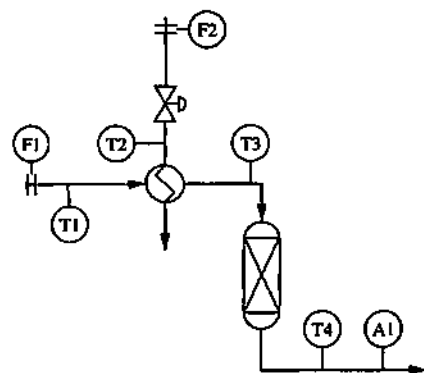


FIGURE Q6.3

- Use the statistical identification method to estimate parameters for a first-order-with-dead-time model.
- Determine whether the model structure is adequate for this data.
- Estimate the inaccuracies in the parameter values due to the data and calculation method.

You may use a spreadsheet or statistical computer program. Note that the number of data points is smaller than desired for good estimation; this is solely to reduce the effort of typing the data into your program.

- 6.3. (a) The chemical reactor system in Figure Q6.3 is to be modelled. The relationship between the steam valve on the preheat exchanger and the outlet concentration is to be determined. Develop a complete experimental plan for a process reaction curve experiment. Include in your plan all actions, variables to be recorded or monitored, and any a priori information required from the plant operating personnel.
- (b) Repeat the discussion for the experiment to model the effect of the flow of the reboiler heating medium on the distillate composition for the distillation tower in Figure 5.18.

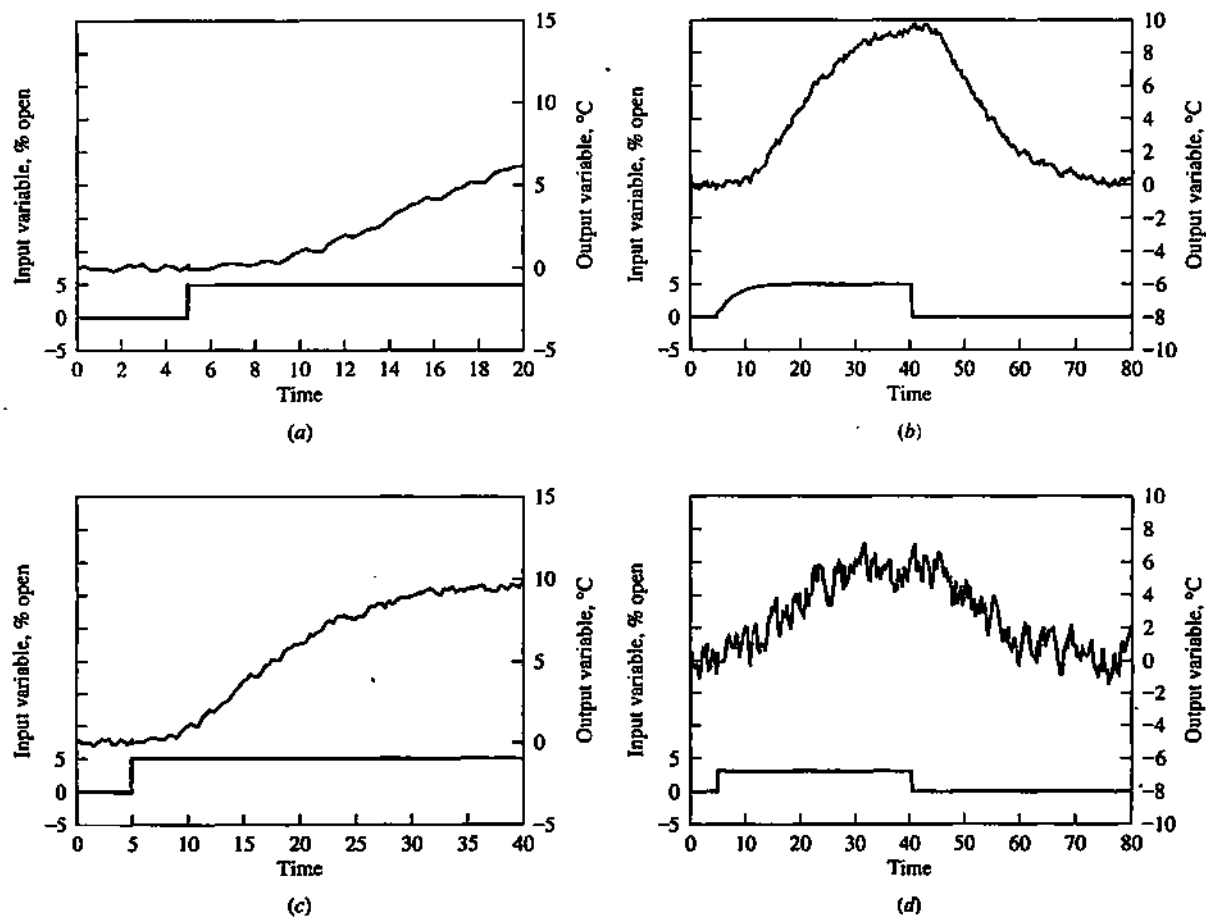


FIGURE Q6.4



4. Several experiments were performed on the chemical reactor shown in Figure Q6.3. In each experiment, the heat exchanger valve was changed and the reactor outlet temperature T_4 was recorded. The dynamic data are given in Figure Q6.4a through d. Discuss the results of each experiment, noting any deficiencies and stating whether the data can be used for estimation and if so, which estimation method(s)—process reaction curve, statistical, or both—could be used.
- 6.5. Individual experiments have been performed on the process in Figure Q6.3. The following transfer function models were determined from these experiments:

$$\frac{T_3(s)}{T_2(s)} = \frac{0.55e^{-0.5s}}{2s + 1} \quad \frac{T_4(s)}{T_3(s)} = \frac{3.4e^{-2.1s}}{2.7s + 1}$$

- (a) What are the units of the gains and do they make sense? Is the reaction exothermic or endothermic?
 - (b) Determine an approximate first-order-with-dead-time transfer function model for $T_4(s)/T_2(s)$.
 - (c) With better planning, could the model requested in (b) have been determined directly from the experimental data used to determine the models given in the problem statement?
- 6.6. This question addresses dynamics of the mixing process in Figure Q6.6a, which has a mixing point, a pipe, and three identical, well-mixed tanks. Some information about the process follows.
- (i) The flow of pure component A is linear with the valve % open; $F_A = K_A v$.
 - (ii) The flow of pure component A is very small compared with the flow of B; $F_A \ll F_B$. Also, no component A exists in the B stream.
 - (iii) Delays in the pipes designated by single lines are all negligible.
 - (iv) The two materials have the same density, and x_A is the volume percent (or weight %).
 - (v) F_B is not influenced by the valve opening.
- (a) An experimental process reaction curve is given in Figure Q6.6b for a step change in the valve of +5% at time = 7.5 minutes.
- (i) Discuss the good and poor aspects of this experimental data that affect its usefulness for empirical modelling.
 - (ii) Determine the model parameters for a model between the valve and the concentration in the third tank.
- (b) In this question, you are to model the physical process and determine whether the response in Figure Q6.6b is possible, i.e., consistent with the fundamental model you derive.
- (i) Develop the time-domain models for each process element in linear (or linearized) form in deviation variables.
 - (ii) Take the Laplace transform of each model and combine into an overall transfer function between $v'(s)$ and $x'_{A3}(s)$.
 - (iii) Compare the model with the data and conclude whether the fundamental model and data are or are not consistent. You must provide an explanation!

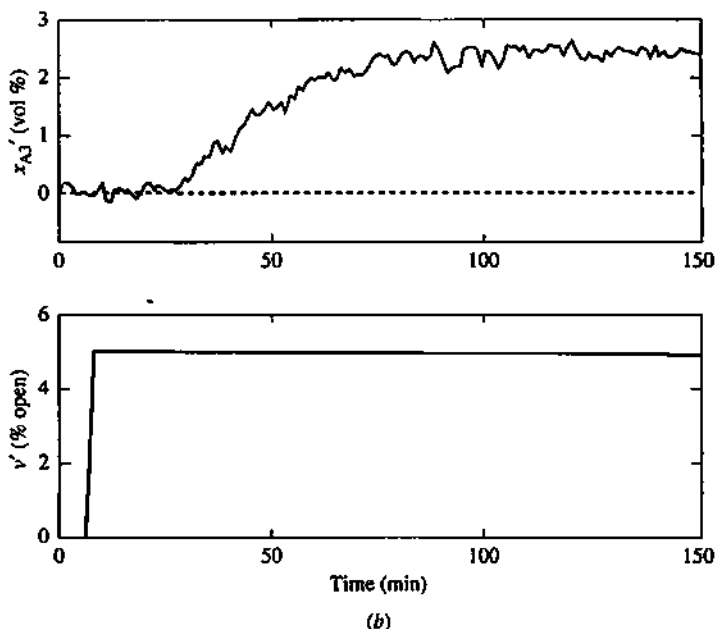
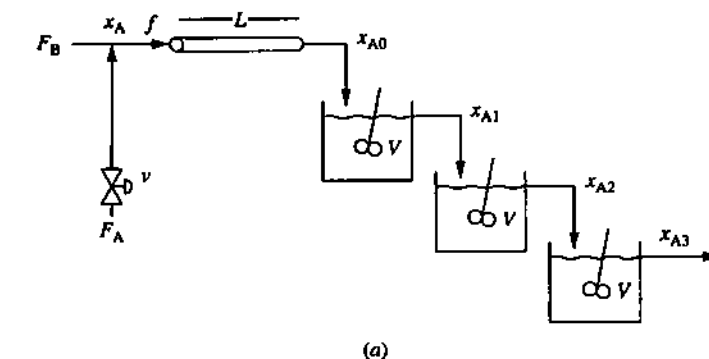


FIGURE Q6.6

(a) Mixing, delay, and series reactors; (b) process reaction curve.

- 6.7. The difference equation for a first-order system was derived from the continuous differential equation in Section 6.4 by assuming that the input was constant over the sample period Δt . An alternative approach would be to approximate the derivative(s) by finite differences. Apply the finite difference approach to a first-order and a second-order model. Discuss how you would estimate the model parameters from a set of experimental data using least squares.
- 6.8. Although such experiments are not common for a process, frequency response modelling is specified for some instrumentation (ISA, 1968). Assume that the data in Table Q6.8 was determined by changing the fluid temperature about a thermocouple and thermowell in a sinusoidal manner. (Refer to Figure 4.9 for the meaning of frequency response.) Determine an approximate model by answering the following:



- (a) Plot the amplitude ratio, and estimate the order of the model from this plot.
- (b) Estimate the steady-state gain and time constant(s) from the results in (a).
- (c) Plot the phase angle from the data and determine the value of the dead time, if any, from the plot.

TABLE Q6.8

Frequency	Amplitude ratio	Phase angle (°)
0.0001	1.0	-1
0.001	0.99	-7
0.005	0.85	-32
0.010	0.62	-51
0.015	0.44	-63
0.050	0.16	-80

6.9. It is important to use our knowledge of the process to design experiments and determine the range of applicability of the empirical models. Assume that the dynamic models for the following processes have been identified, for the input and output stated, using methods described in this chapter about some nominal operating conditions. After the experiments, the nominal operating conditions change as defined in the following table by a “substantial” amount, say 50 percent. You are to determine

- (a) whether the input-output dynamic behavior would change as a result of the change in nominal conditions
- (b) if so, which parameters would change and by how much
- (c) whether the empirical procedure should be repeated to identify a model at the new nominal operating conditions

Process (all are worked examples)	Input variable	Output variable	Process variable that changes for the new nominal operating condition
Example 3.1: Mixing tank	C_{A0}	C_A	$(C_{A0})_s$
Example 3.1: Mixing tank	C_{A0}	C_A	F
Example 3.2: Isothermal CSTR	C_{A0}	C_A	T
Example 3.5: Isothermal CSTR	C_{A0}	C_A	$(C_{A0})_s$
Section 5.3: Noninteracting mixing tanks	C_{A0}	C_A	$(C_{A0})_s$
Section 5.3: Interacting levels	F_0	L_2	$(F_0)_s$

6.10. Use Method II of the process reaction curve to evaluate empirical models from the dynamic responses in Figure 5.17a. Explain why you can obtain two models from one experiment.

- 6.11. The graphical methods could be extended to other models. Develop a method for estimating the parameters in a second-order transfer function with dead time and a constant numerator for a step input forcing function. The method should be able to fit both overdamped and underdamped systems. State all assumptions and explain all six steps.
- 6.12. The graphical methods could be extended to other forcing functions. For both first- and second-order systems with dead time, develop methods for fitting parameters from an impulse response.
- 6.13. We will be using first-order-with-dead-time models often. Sketch an ideal process that is exactly first-order with dead time. Derive the fundamental model and relate the equipment and operating conditions to the model parameters. Discuss how well this model approximates more complex processes.
- 6.14. Develop a method for testing whether the empirical data can be fitted using equation (6.2). The method should involve comparing calculated values to a straight-line model.
- 6.15. Both process reaction curve methods require that the process achieve a steady state after the step input. For both methods, suggest modifications that would relieve the requirement for a final steady state. Discuss the relative accuracy of these modified methods to those presented in the chapter. Could you apply your method to the first part of the transient response in Figure 3.10c?
- 6.16. Often, more than one input to a process changes during an experiment. For the process reaction curve and the statistical method:
 - (a) If possible, show how models for two inputs could be determined from such experiments. Clearly state the requirements of the experimental design and calculations.
 - (b) Assume that the model between one of the inputs and the output is known. Show how to fit the parameters for the remaining input.
- 6.17. For each of the processes and dynamic data, state whether the process reaction curve, the statistical model fitting method, or both can be used. Also, state the model form necessary to model the process adequately. The systems are Examples 3.3, 5.1, and Figure 5.5 (with $n = 10$).
- 6.18. The residual plot provides a visual display of goodness of fit. How could you use the calculated residuals to test the hypothesis that the model has provided a good fit? What could you do if the result of this test indicates that the model is not adequate?
- 6.19.
 - (a) Experiments were performed to obtain the process reaction curves in Figure 5.20a and b. How do you think that the results would change if
 - (1) The step magnitudes were halved? doubled?
 - (2) The step signs were inverted?
 - (3) Both steps were made simultaneously?
 - (b) Describe how the inventories (liquid levels) were controlled during the experiments.
 - (c) Would the results change if the inventories were controlled differently?