Development of Empirical Models From Process Data

Chapter 7

- In some situations it is not feasible to develop a theoretical (physically-based model) due to:

  1. Lack of information
  2. Model complexity
  3. Engineering effort required.

- **An attractive alternative:** Develop an empirical dynamic model from input-output data.

  - *Advantage:* less effort is required

  - *Disadvantage:* the model is only valid (at best) for the range of data used in its development.

    i.e., empirical models usually don’t extrapolate very well.

Simple Linear Regression: Steady-State Model

- As an illustrative example, consider a simple linear model between an output variable y and input variable u,

$$y = \beta_1 + \beta_2 u + \varepsilon$$

where β_1 and β_2 are the unknown model parameters to be estimated and ε is a random error.

- Predictions of y can be made from the regression model,

$$\hat{y} = \hat{\beta}_1 + \hat{\beta}_2 u \qquad (7\text{-}3)$$

where $\hat{\beta}_1$ and $\hat{\beta}_2$ denote the estimated values of β_1 and β_2, and $\hat{y}$ denotes the predicted value of y.

- Let Y denote the measured value of y. Each pair of (u_i, Y_i) observations satisfies:

$$Y_i = \beta_1 + \beta_2 u_i + \varepsilon_i \qquad (7\text{-}1)$$

The Least Squares Approach

- The least squares method is widely used to calculate the values of β_1 and β_2 that minimize the sum of the squares of the errors S for an arbitrary number of data points, N:

$$S = \sum_{i=1}^{N} \varepsilon_1^2 = \sum_{i=1}^{N} \left(Y_i - \beta_1 - \beta_2 u_i\right)^2 \qquad (7\text{-}2)$$

- Replace the unknown values of β_1 and β_2 in (7-2) by their estimates. Then using (7-3), S can be written as:

$$S = \sum_{i=1}^{N} e_i^2$$

where the i-th residual, e_i, is defined as,

$$e_i \triangleq Y_i - \hat{y}_i \qquad (7-4)$$

Chapter 7

The Least Squares Approach (continued)

- The least squares solution that minimizes the sum of squared errors, *S*, is given by:

$$\hat{\beta}_1 = \frac{S_{uu} S_y - S_{uy} S_u}{N S_{uu} - (S_u)^2} \qquad (7\text{-}5)$$

$$\hat{\beta}_2 = \frac{N S_{uy} - S_u S_y}{N S_{uu} - (S_u)^2} \qquad (7\text{-}6)$$

where:

$$S_u \triangleq \sum_{i=1}^{N} u_i \quad S_{uu} \triangleq \sum_{i=1}^{N} u_i^2 \quad S_y \triangleq \sum_{i=1}^{N} Y_i \quad S_{uy} \triangleq \sum_{i=1}^{N} u_i Y_i$$

Extensions of the Least Squares Approach

- Least squares estimation can be extended to more general models with:
  1. More than one input or output variable.
  2. Functionals of the input variables u, such as polynomials and exponentials, as long as the unknown parameters appear linearly.

- A general nonlinear steady-state model which is linear in the parameters has the form,

$$y = \sum_{j=1}^{p} \beta_j X_j + \varepsilon \qquad (7\text{-}7)$$

where each X_j is a nonlinear function of u.

The sum of the squares function analogous to (7-2) is

$$S = \sum_{i=1}^{N} \left(Y_i - \sum_{j=1}^{p} \beta_j X_{ij} \right)^2 \qquad (7\text{-}8)$$

which can be written as,

$$S = (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta})^T (\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}) \qquad (7\text{-}9)$$

where the superscript *T* denotes the matrix transpose and:

$$\boldsymbol{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

Chapter 7

$$\boldsymbol{X} = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1p} \\ X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{np} \end{bmatrix}$$

The least squares estimates $\hat{\beta}$ is given by,

$$\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y} \qquad (7\text{-}10)$$

providing that matrix $\boldsymbol{X}^T\boldsymbol{X}$ is nonsingular so that its inverse exists. Note that the matrix $\boldsymbol{X}$ is comprised of functions of u_j; for example, if:

$$y = \beta_1 + \beta_2 u + \beta_3 u^2 + \varepsilon$$

This model is in the form of (7-7) if $X_1 = 1$, $X_2 = u$, and $X_3 = u^2$.

Fitting First and Second-Order Models Using Step Tests

- Simple transfer function models can be obtained graphically from step response data.
- A plot of the output response of a process to a step change in input is sometimes referred to as a *process reaction curve.*
- If the process of interest can be approximated by a first- or second-order linear model, the model parameters can be obtained by inspection of the process reaction curve.
- The response of a first-order model, $Y(s)/U(s)=K/(\tau s+1)$, to a step change of magnitude M is:

$$y(t) = KM(1 - e^{-t/\tau}) \qquad (5\text{-}18)$$

- The initial slope is given by:

$$\frac{d}{dt}\left(\frac{y}{KM}\right)_{t=0} = \frac{1}{\tau} \qquad (7\text{-}15)$$

- The gain can be calculated from the steady-state changes in u and y:

$$K = \frac{\Delta y}{\Delta u} = \frac{\Delta y}{M}$$

where Δy is the steady-state change in y.

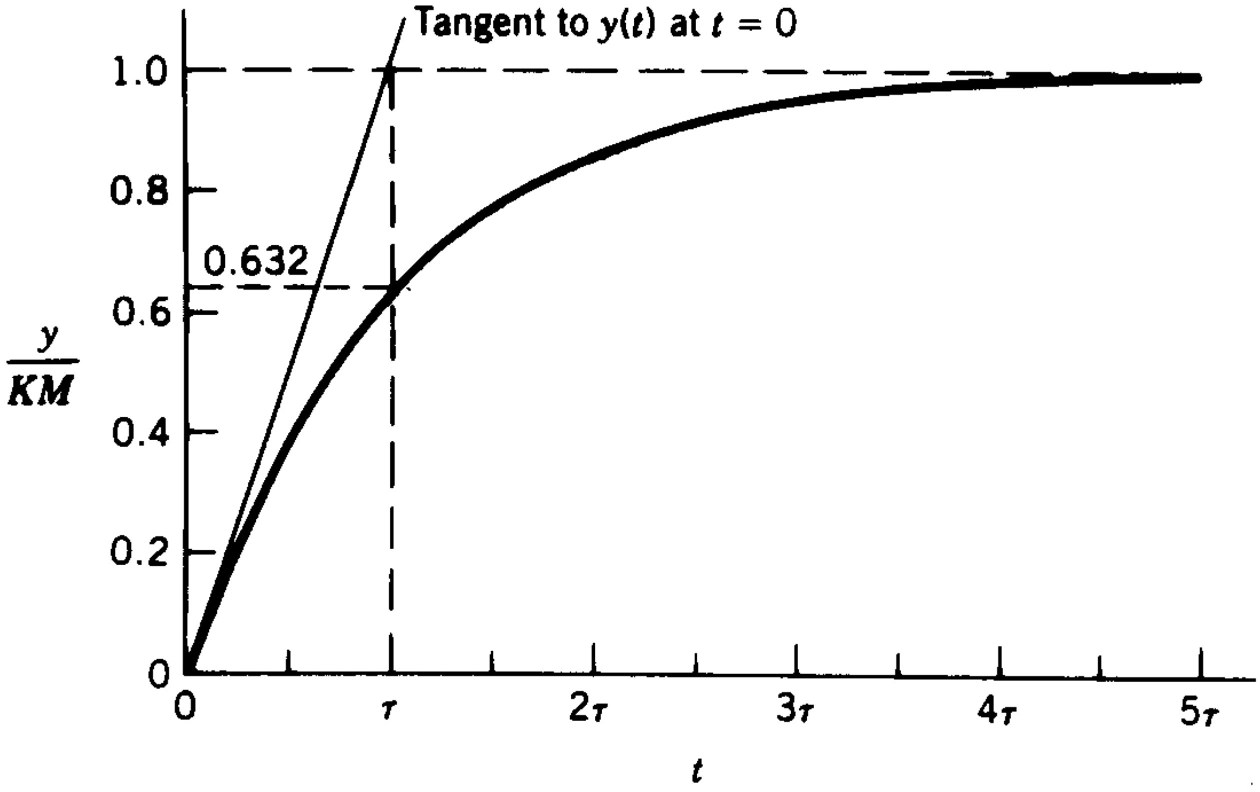

Figure 7.3 Step response of a first-order system and graphical constructions used to estimate the time constant, τ.

First-Order Plus Time Delay Model

$$G(s) = \frac{Ke^{-\theta s}}{\tau s + 1}$$

For this FOPTD model, we note the following characteristics of its step response:

1. The response attains 63.2% of its final response at time, $t = \tau + \theta$.

2. The line drawn tangent to the response at maximum slope ($t = \theta$) intersects the $y/KM = 1$ line at ($t = \tau + \theta$).

3. The step response is essentially complete at $t = 5\tau$. In other words, the settling time is $t_s = 5\tau$.

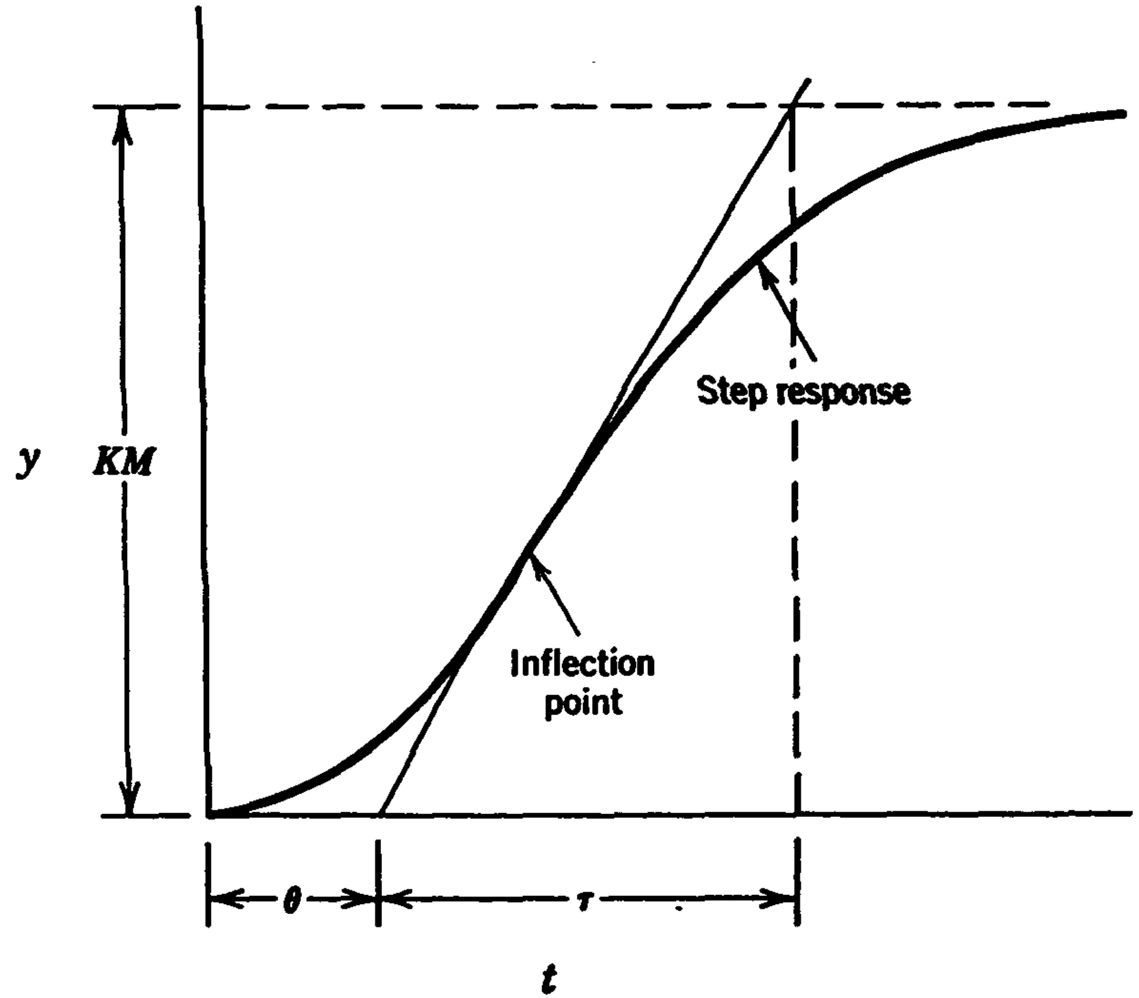

Figure 7.5 Graphical analysis of the process reaction curve to obtain parameters of a first-order plus time delay model.

There are two generally accepted graphical techniques for determining model parameters τ, θ, and K.

Method 1: *Slope-intercept method*

First, a slope is drawn through the inflection point of the process reaction curve in Fig. 7.5. Then τ and θ are determined by inspection.

Alternatively, τ can be found from the time that the normalized response is 63.2% complete or from determination of the settling time, t_s. Then set $\tau = t_s/5$.

Method 2. *Sundaresan and Krishnaswamy's Method*

This method avoids use of the point of inflection construction entirely to estimate the time delay.

Sundaresan and Krishnaswamy's Method

- They proposed that two times, t_1 and t_2, be estimated from a step response curve, corresponding to the 35.3% and 85.3% response times, respectively.
- The time delay and time constant are then estimated from the following equations:

$$\theta = 1.3t_1 - 0.29t_2$$
$$\tau = 0.67\left(t_2 - t_1\right) \qquad (7\text{-}19)$$

- These values of θ and τ approximately minimize the difference between the measured response and the model, based on a correlation for many data sets.

Estimating Second-order Model Parameters Using Graphical Analysis

- In general, a better approximation to an experimental step response can be obtained by fitting a second-order model to the data.

- Figure 7.6 shows the range of shapes that can occur for the step response model,

$$G(s) = \frac{K}{(\tau_1 s + 1)(\tau_2 s + 1)} \qquad (5\text{-}39)$$

- Figure 7.6 includes two limiting cases: $\tau_2 / \tau_1 = 0$, where the system becomes first order, and $\tau_2 / \tau_1 = 1$, the critically damped case.

- The larger of the two time constants, τ_1, is called the dominant time constant.

Chapter 7

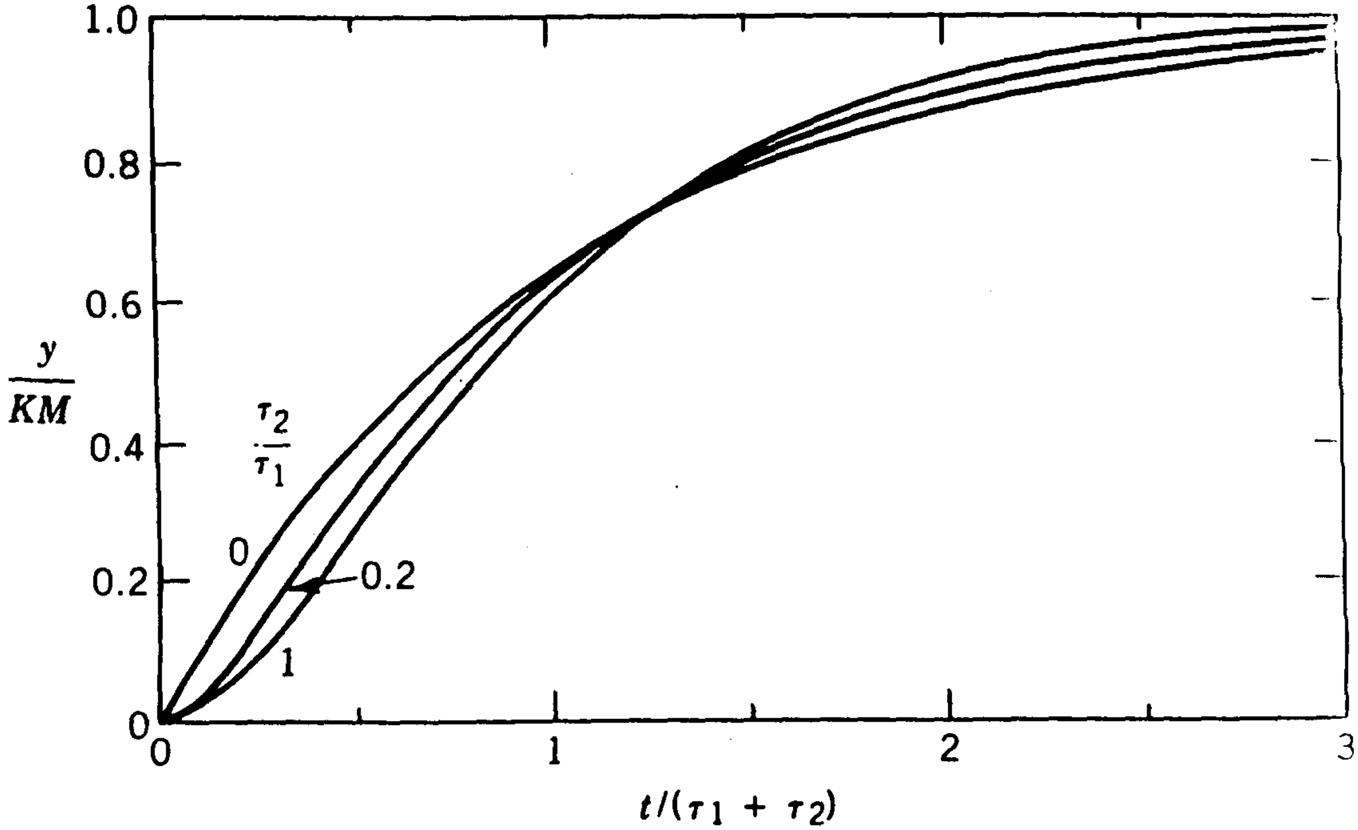

Figure 7.6 Step response for several overdamped second-order systems.

Smith's Method

- **Assumed model:**

$$G(s) = \frac{Ke^{-\theta s}}{\tau^2 s^2 + 2\zeta\tau s + 1}$$

- **Procedure:**

1. Determine t_{20} and t_{60} from the step response.
2. Find ζ and t_{60}/τ from Fig. 7.7.
3. Find t_{60}/τ from Fig. 7.7 and then calculate τ (since t_{60} is known).

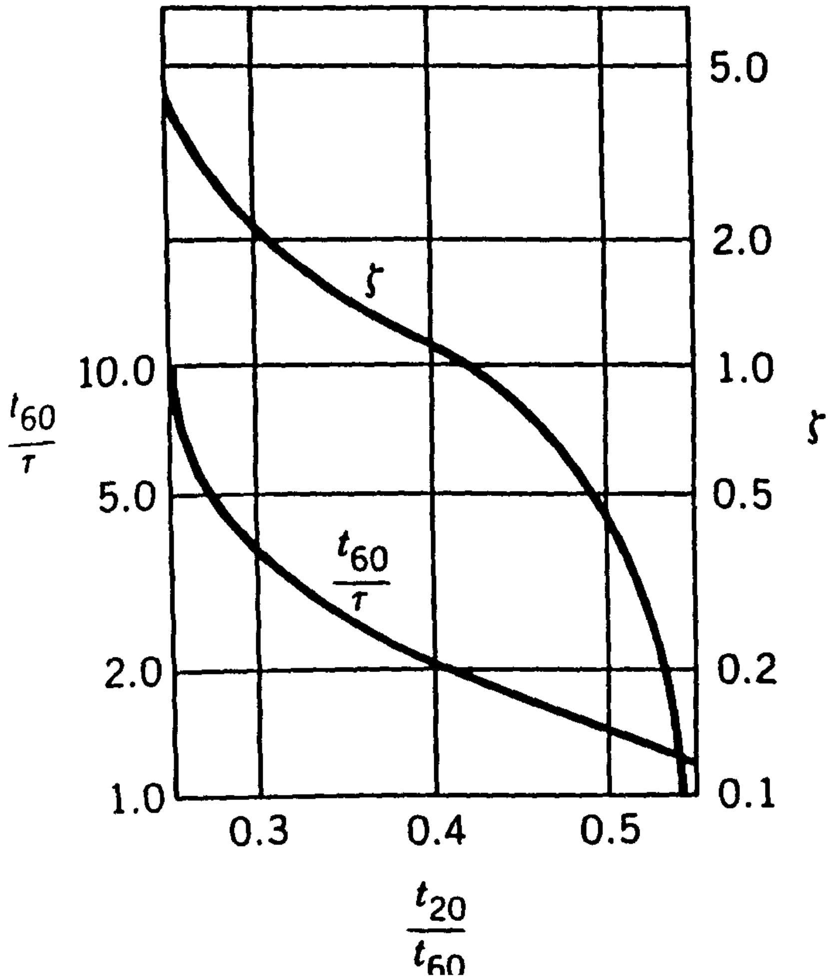

Figure 7.7. Smith's method: relationship of ζ and τ to t_{20} and t_{60}.

Fitting an Integrator Model to Step Response Data

In Chapter 5 we considered the response of a first-order process to a step change in input of magnitude *M*:

$$y_1(t) = KM\left(1 - e^{-t/\tau}\right) \qquad (5\text{-}18)$$

For short times, $t < \tau$, the exponential term can be approximated by

$$e^{-t/\tau} \approx 1 - \frac{t}{\tau}$$

so that the approximate response is:

$$y_1(t) \approx KM\left[1 - \left(1 - \frac{t}{\tau}\right)\right] = \frac{KM}{\tau}t \qquad (7\text{-}22)$$

is virtually indistinguishable from the step response of the integrating element

$$G_2(s) = \frac{K_2}{s} \qquad (7\text{-}23)$$

In the time domain, the step response of an integrator is

$$y_2(t) = K_2 M t \qquad (7\text{-}24)$$

Hence an approximate way of modeling a first-order process is to find the single parameter

$$K_2 = \frac{K}{\tau} \qquad (7\text{-}25)$$

that matches the early ramp-like response to a step change in input.

If the original process transfer function contains a time delay (cf. Eq. 7-16), the approximate short-term response to a step input of magnitude M would be

$$y(t) = \frac{KM}{t}(t-\theta)S(t-\theta)$$

where $S(t-\theta)$ denotes a delayed unit step function that starts at $t=\theta$.

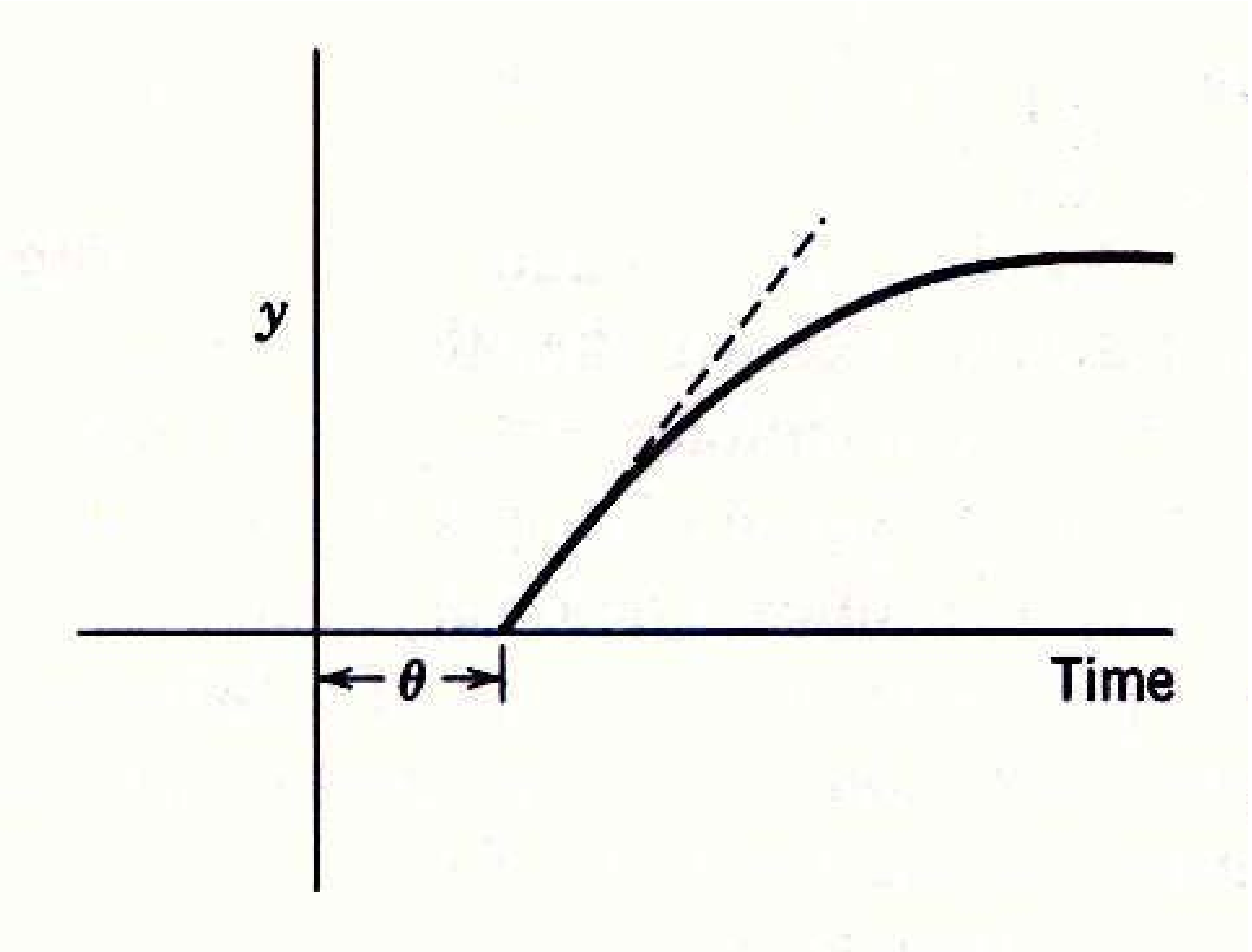

Figure 7.10. Comparison of step responses for a FOPTD model (solid line) and the approximate integrator plus time delay model (dashed line).

Development of Discrete-Time Dynamic Models

- A digital computer by its very nature deals internally with discrete-time data or numerical values of functions at equally spaced intervals determined by the sampling period.
- Thus, discrete-time models such as *difference equations* are widely used in computer control applications.
- One way a continuous-time dynamic model can be converted to discrete-time form is by employing a finite difference approximation.
- Consider a nonlinear differential equation,

$$\frac{dy(t)}{dt} = f(y, u) \tag{7-26}$$

where y is the output variable and u is the input variable.

- This equation can be numerically integrated (though with some error) by introducing a finite difference approximation for the derivative.
- For example, the first-order, backward difference approximation to the derivative at $t = k\Delta t$ is

$$\frac{dy}{dt} \cong \frac{y(k) - y(k-1)}{\Delta t} \qquad (7\text{-}27)$$

where Δt is the integration interval specified by the user and $y(k)$ denotes the value of $y(t)$ at $t = k\Delta t$. Substituting Eq. 7-26 into (7-27) and evaluating $f(y, u)$ at the previous values of y and u (i.e., $y(k-1)$ and $u(k-1)$) gives:

$$\frac{y(k) - y(k-1)}{\Delta t} \cong f\left(y(k-1), u(k-1)\right) \qquad (7\text{-}28)$$

$$y(k) = y(k-1) + \Delta t f\left(y(k-1), u(k-1)\right) \qquad (7\text{-}29)$$

Second-Order Difference Equation Models

- Parameters in a discrete-time model can be estimated directly from input-output data based on linear regression.
- This approach is an example of *system identification* (Ljung, 1999).
- As a specific example, consider the second-order difference equation in (7-36). It can be used to predict $y(k)$ from data available at time $(k-1)\Delta t$ and $(k-2)\Delta t$.

$$y(k) = a_1 y(k-1) + a_2 y(k-2) + b_1 u(k-1) + b_2 u(k-2) \qquad (7\text{-}36)$$

- In developing a discrete-time model, model parameters a_1, a_2, b_1, and b_2 are considered to be unknown.

- This model can be expressed in the standard form of Eq. 7-7,

$$y = \sum_{j=1}^{p} \beta_j X_j + \varepsilon \qquad (7\text{-}7)$$

by defining:

$$\beta_1 \triangleq a_1, \quad \beta_2 \triangleq a_2, \quad \beta_3 \triangleq b_1, \quad \beta_4 \triangleq b_2$$
$$X_1 \triangleq y(k-1), \quad X_2 \triangleq y(k-2),$$
$$X_3 \triangleq u(k-1), \quad X_4 \triangleq u(k-2)$$

- The parameters are estimated by minimizing a least squares error criterion:

$$S = \sum_{i=1}^{N} \left(Y_i - \sum_{j=1}^{p} \beta_j X_{ij} \right)^2 \qquad (7\text{-}8)$$

Chapter 7

Equivalently, S can be expressed as,

$$S = \left(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\right)^T \left(\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{\beta}\right) \qquad (7\text{-}9)$$

where the superscript T denotes the matrix transpose and:

$$\boldsymbol{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_n \end{bmatrix} \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

The least squares solution of (7-9) is:

$$\hat{\boldsymbol{\beta}} = \left(\boldsymbol{X}^T \boldsymbol{X}\right)^{-1} \boldsymbol{X}^T \boldsymbol{Y} \qquad (7\text{-}10)$$