

# SECTION III

## LINEAR SYSTEMS ANALYSIS

# LINEARIZATION OF NONLINEAR MODELS: THE STATE-SPACE FORMULATION

# 5

Many dynamic chemical processes are modeled by a set of nonlinear, first-order differential equations that generally arise from material and energy balances around the system. Common analysis techniques are based on linear systems theory and require a *state-space* model. Also, most control system design techniques are based on linear models. The purpose of this chapter is to provide an introduction to state-space models and linearization of nonlinear systems. After studying this chapter the reader should be able to:

- Write a linear model in state-space form.
- Linearize a nonlinear model and place in state-space form.
- Use the MATLAB `eig` function to analyze the stability of a state-space model.
- Develop the analytical solution of state-space models.
- Understand stability and transient response characteristics as a function of the eigenvalues.
- Understand the importance of initial condition “direction”.
- Be able to use the MATLAB routines `step` and `initial` for simulation of state-space models.

The major sections in this chapter are:

- 5.1 State-Space Models
- 5.2 Linearization of Nonlinear Models
- 5.3 Geometrical Interpretation of Linearization
- 5.4 Solution of the Zero-Input Form
- 5.5 Solution of the General State-Space Form
- 5.6 MATLAB Routines `step` and `initial`

## 5.1 STATE-SPACE MODELS

Thus far in this text we have discussed dynamic models of the general form:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \quad (5.1)$$

where  $\mathbf{f}(\mathbf{x}, \mathbf{u})$  is, in general, a nonlinear function vector.

A linear model is a subset of the more general modeling equation (5.1). The form of linear model that we discuss in this chapter is known as a *state-space* model. First, we show how to write state-space models for systems that are inherently linear. Then, we show how to approximate nonlinear systems with linear models.

Example 5.1 illustrates the form of a state-space model.

**EXAMPLE 5.1 Noninteracting Tanks**

Consider two tanks in series where the flow out of the first tank enters the second tank (Figure 5.1). Our objective is to develop a model to describe how the height of liquid in tank 2 changes with time, given the input flowrate  $F_o(t)$ . We assume that the flow out of each tank is a linear function of the height of liquid in the tank.

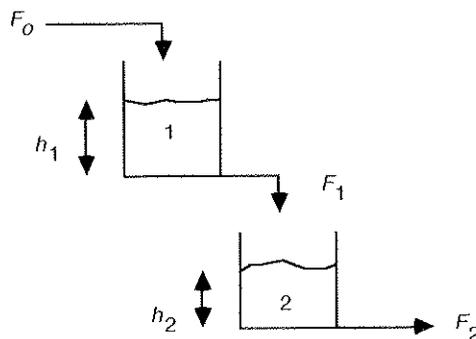


FIGURE 5.1 Noninteracting tanks.

A material balance around the first tank yields (assuming constant density and  $F_1 = \beta_1 h_1$ )

$$\frac{dh_1}{dt} = \frac{F_o}{A_1} - \frac{\beta_1}{A_1} h_1 \quad (5.2)$$

where  $A_1$  is the constant cross-sectional area (parameter),  $\beta_1$  is the flow coefficient (parameter),  $F_o$  is the flowrate into the tank (input), and  $h_1$  is the tank height (state).

Writing a material balance around the second tank (since  $F_2 = \beta_2 h_2$ )

$$\frac{dh_2}{dt} = \frac{F_1}{A_2} - \frac{\beta_2}{A_2} h_2$$

where  $A_2$  is the constant cross-sectional area for tank 2 (parameter),  $\beta_2$  is the flow coefficient (parameter),  $F_1$  is the flowrate into the tank, and  $h_2$  is the tank height (state). In this case,  $F_1$  is not an independent input variable that can be manipulated, since  $F_1 = \beta_1 h_1$ . We can write the previous equation as

$$\frac{dh_2}{dt} = \frac{\beta_1}{A_2} h_1 - \frac{\beta_2}{A_2} h_2 \quad (5.3)$$

Notice that we can write (5.2) and (5.3) in the following matrix form:

$$\begin{bmatrix} \dot{h}_1 \\ \dot{h}_2 \end{bmatrix} = \begin{bmatrix} -\frac{\beta_1}{A_1} & 0 \\ \frac{\beta_1}{A_2} & -\frac{\beta_2}{A_2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{A_1} \\ 0 \end{bmatrix} F_o \quad (5.4)$$

which has the general form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \quad (5.5)$$

where:

$$\mathbf{A} = \begin{bmatrix} \frac{\beta_1}{A_1} & 0 \\ \frac{\beta_1}{A_2} & -\frac{\beta_2}{A_2} \end{bmatrix} \quad \text{and} \quad \mathbf{B} = \begin{bmatrix} \frac{1}{A_1} \\ 0 \end{bmatrix}$$

The state and input vectors are (notice that the input is a scalar):

$$\mathbf{x} = \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \quad \text{and} \quad \mathbf{u} = F_o$$

The additional equation that is normally associated with a state space model is

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u} \quad (5.6)$$

where  $\mathbf{y}$  is a vector of output variables. Generally, output variables are variables that can be measured (at least conceptually) or are of particular interest in a simulation study. Here, we will consider the case where both tank heights are outputs. Let output 1 be the first tank height and output 2 be the second tank height

$$y_1 = h_1$$

$$y_2 = h_2$$

The matrix-vector form is:

$$\mathbf{y} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \mathbf{C} \mathbf{x}$$

where:

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

If we also consider the input,  $F_o$ , to be the third output variable, we have the following relationship:

$$\mathbf{y} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} [F_o]$$

which is the form of (5.6), with

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{D} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

### 5.5.1 General Form of State Space Models

Example 5.1 illustrated a specific case of a state-space model. In general, a state-space model has the following form:

$$\begin{aligned} \frac{dx_1}{dt} &= a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n + b_{11}u_1 + \dots + b_{1m}u_m \\ &\vdots \\ \frac{dx_n}{dt} &= a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n + b_{n1}u_1 + \dots + b_{nm}u_m \\ y_1 &= c_{11}x_1 + c_{12}x_2 + \dots + c_{1n}x_n + d_{11}u_1 + \dots + d_{1m}u_m \\ &\vdots \\ y_r &= c_{r1}x_1 + c_{r2}x_2 + \dots + c_{rn}x_n + d_{r1}u_1 + \dots + d_{rm}u_m \end{aligned}$$

which has  $n$  state variables ( $x$ ),  $m$  input variables ( $u$ ) and  $r$  output variables ( $y$ ). This relationship is normally written in the matrix form:

$$\begin{bmatrix} \dot{x}_1 \\ \vdots \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nm} \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & \dots & c_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{r1} & c_{r2} & \dots & c_{rn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} & \dots & d_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ d_{r1} & d_{r2} & \dots & d_{rm} \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix}$$

which has the general (*state-space*) form:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \\ \mathbf{y} &= \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}\end{aligned}\quad (5.7)$$

where the dot over a state variable indicates the derivative with respect to time. As shown in Section 5.4, the eigenvalues of the Jacobian matrix ( $\mathbf{A}$ ) determine the stability of the system of equations and the "speed" of response.

The  $a_{ij}$  coefficient relates state variable  $j$  to the rate of change of state variable  $i$ . Similarly, the  $b_{ij}$  coefficient relates input  $j$  to the rate of change of state variable  $i$ . Also,  $c_{ij}$  relates state  $j$  to output  $i$ , while  $d_{ij}$  relates input  $j$  to output  $i$ . We can also say that the  $k$ th row of  $\mathbf{C}$  relates all states to the  $k$ th output, while the  $k$ th column of  $\mathbf{C}$  relates state  $k$  to all outputs.

In this section we have shown how to write modeling equations that are naturally linear in the state-space form. In the next section we show how to linearize nonlinear models and write them in the state-space form. Linear models are easier to analyze for stability and expected dynamic behavior.

## 5.2 LINEARIZATION OF NONLINEAR MODELS

Most chemical process models are nonlinear, but they are often linearized to perform a stability analysis. Linear models are easier to understand (than nonlinear models) and are necessary for most control system design methods.

Before we generalize our results, we will illustrate linearization for a single variable problem.

### 5.2.1 Single Variable Example

A general single variable nonlinear model is:

$$\frac{dx}{dt} = f(x) \quad (5.8)$$

The function of a single variable,  $f(x)$ , can be approximated by a truncated Taylor series approximation around the steady-state operating point ( $x_s$ ):

$$f(x) = f(x_s) + \left. \frac{\partial f}{\partial x} \right|_{x_s} (x - x_s) + \frac{1}{2} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x_s} (x - x_s)^2 + \text{higher order terms} \quad (5.9)$$

Neglecting the quadratic and higher order terms, we obtain:

$$f(x) \approx f(x_s) + \left. \frac{\partial f}{\partial x} \right|_{x_s} (x - x_s) \quad (5.10)$$

Note that:

$$\left. \frac{dx_s}{dt} \right|_{x_s} = f(x_s) = 0 \quad (5.11)$$

by definition of a steady-state, so:

$$\frac{dx}{dt} = f(x) \approx \left. \frac{\partial f}{\partial x} \right|_{x_s} (x - x_s) \quad (5.12)$$

where the notation  $\left. \frac{\partial f}{\partial x} \right|_{x_s}$  is used to indicate the partial derivative of  $f(x)$  with respect to  $x$ , evaluated at the steady-state. Since the derivative of a constant ( $x_s$ ) is zero, we can write:

$$\frac{dx}{dt} = \frac{d(x - x_s)}{dt} \quad (5.13)$$

which leads to:

$$\frac{d(x - x_s)}{dt} \approx \left. \frac{\partial f}{\partial x} \right|_{x_s} (x - x_s) \quad (5.14)$$

The reason for using the expression above is that we are often interested in deviations in a state from a steady-state operating point. Sometimes the ' symbol is used to represent *deviation variables*,  $x' = x - x_s$ . We can see that a deviation variable represents the change or perturbation (deviation) from a steady-state value.

$$\frac{dx'}{dt} = \left. \frac{\partial f}{\partial x} \right|_{x_s} x' \quad (5.15)$$

This can be written in state-space form:

$$\frac{dx'}{dt} = a x' \quad (5.16)$$

where  $a = \left. \frac{\partial f}{\partial x} \right|_{x_s}$ .

We have shown how to linearize a single variable equation. Next, we consider a system with one state and one input.

## 5.2.2 One State Variable and One Input Variable

Similarly, consider a function with one state variable and one input variable

$$\dot{x} = \frac{dx}{dt} = f(x, u) \quad (5.17)$$

Using a Taylor Series Expansion for  $f(x, u)$ :

$$\begin{aligned} \dot{x} = & f(x_s, u_s) + \left. \frac{\partial f}{\partial x} \right|_{x_s, u_s} (x - x_s) + \left. \frac{\partial f}{\partial u} \right|_{x_s, u_s} (u - u_s) \\ & + \frac{1}{2} \left. \frac{\partial^2 f}{\partial x^2} \right|_{x_s, u_s} (x - x_s)^2 + \left. \frac{\partial^2 f}{\partial x \partial u} \right|_{x_s, u_s} (x - x_s)(u - u_s) + \frac{1}{2} \left. \frac{\partial^2 f}{\partial u^2} \right|_{x_s, u_s} (u - u_s)^2 \\ & + \text{higher order terms} \end{aligned}$$

and truncating after the linear terms, we have:

$$\dot{x} \approx f(x_s, u_s) + \left. \frac{\partial f}{\partial x} \right|_{x_s, u_s} (x - x_s) + \left. \frac{\partial f}{\partial u} \right|_{x_s, u_s} (u - u_s) \quad (5.18)$$

and realizing that  $f(x_s, u_s) = 0$  and  $dx/dt = d(x - x_s)/dt$ :

$$\frac{d(x - x_s)}{dt} \approx \left. \frac{\partial f}{\partial x} \right|_{x_s, u_s} (x - x_s) + \left. \frac{\partial f}{\partial u} \right|_{x_s, u_s} (u - u_s)$$

Using deviation variables,  $x' = x - x_s$  and  $u' = u - u_s$ :

$$\frac{dx'}{dt} \approx \left. \frac{\partial f}{\partial x} \right|_{x_s, u_s} x' + \left. \frac{\partial f}{\partial u} \right|_{x_s, u_s} u'$$

which can be written:

$$\frac{dx'}{dt} = a x' + b u' \quad (5.19)$$

where  $a = \partial f / \partial x|_{x_s, u_s}$  and  $b = \partial f / \partial u|_{x_s, u_s}$

If there is a single output that is a function of the states and inputs, then:

$$y = g(x, u) \quad (5.20)$$

Again, performing a Taylor series expansion and truncating the quadratic and higher terms:

$$g(x, u) \approx g(x_s, u_s) + \left. \frac{\partial g}{\partial x} \right|_{x_s, u_s} (x - x_s) + \left. \frac{\partial g}{\partial u} \right|_{x_s, u_s} (u - u_s) \quad (5.21)$$

Since  $g(x_s, u_s)$  is simply the steady-state value of the output ( $y_s$ ), we can write:

$$y \approx g(x_s, u_s) + \left. \frac{\partial g}{\partial x} \right|_{x_s, u_s} (x - x_s) + \left. \frac{\partial g}{\partial u} \right|_{x_s, u_s} (u - u_s) \quad (5.22)$$

or

$$y - y_s = c (x - x_s) + d (u - u_s)$$

where  $c = \partial g / \partial x|_{x_s, u_s}$  and  $d = \partial g / \partial u|_{x_s, u_s}$

Using deviation notation:

$$y' = c x' + d u' \quad (5.23)$$

Example 5.2 illustrates the application of linearization to a one-input, one-state nonlinear system.

**EXAMPLE 5.2 Consider a Nonlinear Tank Height Problem**

$$\frac{dh}{dt} = \frac{F}{A} - \beta \sqrt{h} \quad (5.24)$$

where  $h$  is the state variable,  $F$  is the input variable,  $\beta$  and  $A$  are parameters. The righthand side is:

$$f(h, F) = \frac{F}{A} - \beta \sqrt{h}$$

Using a truncated Taylor series expansion, we find:

$$f(h, F) = \left[ \frac{F_s}{A} - \beta \sqrt{h_s} \right] + \frac{1}{A} [F - F_s] - \frac{\beta}{2A\sqrt{h_s}} [h - h_s] \quad (5.25)$$

The first term on the righthand side is zero, because the linearization is about a steady-state point. That is,

$$\left. \frac{dh}{dt} \right|_{h, F} = \frac{F_s}{A} - \beta \sqrt{h_s} = 0$$

We can now write:

$$\frac{d(h - h_s)}{dt} = - \frac{\beta}{2A\sqrt{h_s}} [h - h_s] + \frac{1}{A} [F - F_s]$$

and using deviation variable notation ( $h' = h - h_s$  and  $u' = F - F_s$ ), and dropping the =

$$\frac{dh'}{dt} = - \frac{\beta}{2A\sqrt{h_s}} h' + \frac{1}{A} u'$$

For convenience (simplicity in notation) we often drop the ( $'$ ) notation and assume that  $x$  and  $u$  are deviation variables ( $x = h - h_s$ ,  $u = F - F_s$ ) and write:

$$\frac{dx}{dt} = - \frac{\beta}{2A\sqrt{h_s}} x + \frac{1}{A} u \quad (5.26)$$

which is in the state-space form

$$\frac{dx}{dt} = a x + b u \quad (5.27)$$

**5.2.3 Linearization of Multistate Models**

The previous examples showed how to linearize single-state variable systems. In this section we generalize the technique for any number of states. Before we generalize the technique, it is worthwhile to consider an example system with two states, one input and one output.

**EXAMPLE 5.3 Two-state System**

$$\dot{x}_1 = \frac{dx_1}{dt} = f_1(x_1, x_2, u) \quad (5.28)$$

$$\dot{x}_2 = \frac{dx_2}{dt} = f_2(x_1, x_2, u) \quad (5.29)$$

$$y = g(x_1, x_2, u) \quad (5.30)$$

Performing a Taylor series expansion of the nonlinear functions, and neglecting the quadratic and higher terms:

$$\begin{aligned} f_1(x_1, x_2, u) &= f_1(x_{1s}, x_{2s}, u_s) + \left. \frac{\partial f_1}{\partial x_1} \right|_{x_{1s}, x_{2s}, u_s} (x_1 - x_{1s}) \\ &+ \left. \frac{\partial f_1}{\partial x_2} \right|_{x_{1s}, x_{2s}, u_s} (x_2 - x_{2s}) + \left. \frac{\partial f_1}{\partial u} \right|_{x_{1s}, x_{2s}, u_s} (u - u_s) + \text{higher order terms} \\ f_2(x_1, x_2, u) &= f_2(x_{1s}, x_{2s}, u_s) + \left. \frac{\partial f_2}{\partial x_1} \right|_{x_{1s}, x_{2s}, u_s} (x_1 - x_{1s}) \\ &+ \left. \frac{\partial f_2}{\partial x_2} \right|_{x_{1s}, x_{2s}, u_s} (x_2 - x_{2s}) + \left. \frac{\partial f_2}{\partial u} \right|_{x_{1s}, x_{2s}, u_s} (u - u_s) + \text{higher order terms} \\ g(x_1, x_2, u) &= g(x_{1s}, x_{2s}, u_s) + \left. \frac{\partial g}{\partial x_1} \right|_{x_{1s}, x_{2s}, u_s} (x_1 - x_{1s}) \\ &+ \left. \frac{\partial g}{\partial x_2} \right|_{x_{1s}, x_{2s}, u_s} (x_2 - x_{2s}) + \left. \frac{\partial g}{\partial u} \right|_{x_{1s}, x_{2s}, u_s} (u - u_s) + \text{higher order terms} \end{aligned}$$

From the linearization about the steady-state:

$$f_1(x_{1s}, x_{2s}, u_s) = f_2(x_{1s}, x_{2s}, u_s) = 0$$

and:

$$g(x_{1s}, x_{2s}, u_s) = y_s$$

Since the derivative of a constant is zero:

$$\frac{dx_1}{dt} = \frac{d(x_1 - x_{1s})}{dt} \quad \text{and} \quad \frac{dx_2}{dt} = \frac{d(x_2 - x_{2s})}{dt}$$

we can write the state-space model:

$$\begin{bmatrix} \frac{d(x_1 - x_{1s})}{dt} \\ \frac{d(x_2 - x_{2s})}{dt} \end{bmatrix} = \begin{bmatrix} \left. \frac{\partial f_1}{\partial x_1} \right|_{x_{1s}, x_{2s}, u_s} & \left. \frac{\partial f_1}{\partial x_2} \right|_{x_{1s}, x_{2s}, u_s} \\ \left. \frac{\partial f_2}{\partial x_1} \right|_{x_{1s}, x_{2s}, u_s} & \left. \frac{\partial f_2}{\partial x_2} \right|_{x_{1s}, x_{2s}, u_s} \end{bmatrix} \begin{bmatrix} x_1 - x_{1s} \\ x_2 - x_{2s} \end{bmatrix}$$

$$+ \begin{bmatrix} \frac{\partial f_1}{\partial u} \\ \frac{\partial f_2}{\partial u} \end{bmatrix}_{x_1, x_2, u} [u - u_s] \quad (5.31)$$

$$y - y_s = \begin{bmatrix} \frac{\partial g}{\partial x_1} \\ \frac{\partial g}{\partial x_2} \end{bmatrix}_{x_1, x_2, u} \begin{bmatrix} x_1 - x_{1s} \\ x_2 - x_{2s} \end{bmatrix} + \begin{bmatrix} \frac{\partial g}{\partial u} \end{bmatrix}_{x_1, x_2, u} [u - u_s] \quad (5.32)$$

which is the form of a state-space model:

$$\begin{aligned} \dot{\mathbf{x}}' &= \mathbf{A} \mathbf{x}' + \mathbf{B} \mathbf{u}' \\ \mathbf{y}' &= \mathbf{C} \mathbf{x}' + \mathbf{D} \mathbf{u}' \end{aligned}$$

where (') indicates deviation variables.

### 5.2.4 Generalization

Now consider the general nonlinear model where  $\mathbf{x}$  is a vector of  $n$  state variables,  $\mathbf{u}$  is a vector of  $m$  input variables and  $\mathbf{y}$  is a vector of  $r$  output variables:

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, \dots, x_n, u_1, \dots, u_m) \\ &\vdots \\ \dot{x}_n &= f_n(x_1, \dots, x_n, u_1, \dots, u_m) \\ y_1 &= g_1(x_1, \dots, x_n, u_1, \dots, u_m) \\ &\vdots \\ y_r &= g_r(x_1, \dots, x_n, u_1, \dots, u_m) \end{aligned}$$

In vector notation:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \quad (5.33)$$

$$\mathbf{y} = \mathbf{g}(\mathbf{x}, \mathbf{u}) \quad (5.34)$$

Elements of the linearization matrices are defined in the following fashion:

$$A_{ij} = \left. \frac{\partial f_i}{\partial x_j} \right|_{x_s, u_s} \quad (5.35)$$

$$B_{ij} = \left. \frac{\partial f_i}{\partial u_j} \right|_{x_s, u_s} \quad (5.36)$$

$$C_{ij} = \left. \frac{\partial g_i}{\partial x_j} \right|_{x^0, u^0} \quad (5.37)$$

$$D_{ij} = \left. \frac{\partial g_i}{\partial u_j} \right|_{x^0, u^0} \quad (5.38)$$

After linearization, we have the state-space form:

$$\dot{\mathbf{x}}' = \mathbf{A} \mathbf{x}' + \mathbf{B} \mathbf{u}'$$

$$\mathbf{y}' = \mathbf{C} \mathbf{x}' + \mathbf{D} \mathbf{u}'$$

Generally, the (') notation is dropped and it is understood that the model is in deviation variable form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}$$

Usually, the measured (output) variable is not a direct function of the input variable, so it is more common to see the following state-space model:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x}$$

This procedure is applied in Example 5.4.

#### EXAMPLE 5.4 Interacting Tanks

Consider the interacting tank height problem shown in Figure 5.2:

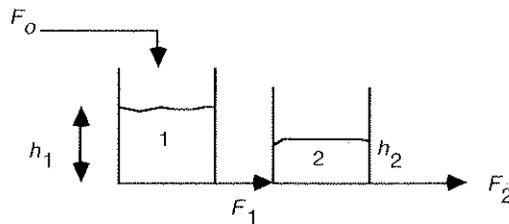


FIGURE 5.2 Interacting tanks.

Assume that the flowrate out of tanks is a nonlinear function of tank height. The flowrate out of tank one is a function of the difference in levels between tank 1 and tank 2.

$$\frac{dh_1}{dt} = f_1(h_1, h_2, F) = \frac{F}{A_1} - \frac{\beta_1}{A_1} \sqrt{h_1 - h_2}$$

$$\frac{dh_2}{dt} = f_2(h_1, h_2, F) = \frac{\beta_1}{A_2} \sqrt{h_1 - h_2} - \frac{\beta_2}{A_2} \sqrt{h_2}$$

Also, assume that only the second tank height is measured. The output, in deviation variable form is

$$y = h_2 - h_{2s}$$

Notice that there are two state variables, one input variable, and one output variable.

Let

$$\mathbf{h}_s = \begin{bmatrix} h_{1s} \\ h_{2s} \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} h_1 - h_{1s} \\ h_2 - h_{2s} \end{bmatrix}$$

$$\mathbf{u} = F - F_s$$

The elements of the **A** (Jacobian) and **B** matrices ((5.35) and (5.36)) are:

$$A_{11} = \left. \frac{\partial f_1}{\partial h_1} \right|_{\mathbf{h}, F_s} = - \frac{\beta_1}{2A_1 \sqrt{h_{1s} - h_{2s}}}$$

$$A_{12} = \left. \frac{\partial f_1}{\partial h_2} \right|_{\mathbf{h}, F_s} = \frac{\beta_1}{2A_1 \sqrt{h_{1s} - h_{2s}}}$$

$$A_{21} = \left. \frac{\partial f_2}{\partial h_1} \right|_{\mathbf{h}, F_s} = \frac{\beta_1}{2A_2 \sqrt{h_{1s} - h_{2s}}}$$

$$A_{22} = \left. \frac{\partial f_2}{\partial h_2} \right|_{\mathbf{h}, F_s} = - \frac{\beta_1}{2A_2 \sqrt{h_{1s} - h_{2s}}} - \frac{\beta_2}{2A_2 \sqrt{h_{2s}}}$$

$$B_{11} = \left. \frac{\partial f_1}{\partial F} \right|_{\mathbf{h}, F_s} = \frac{1}{A_1}$$

$$B_{21} = \left. \frac{\partial f_2}{\partial F} \right|_{\mathbf{h}, F_s} = 0$$

Since only the height of the second tank is measured,  $y = \mathbf{g}(h_1, h_2, F) = h_2 - h_{2s}$  (from (5.37)):

$$C_{11} = \left. \frac{\partial g}{\partial h_1} \right|_{\mathbf{h}, u_s} = 0$$

$$C_{12} = \left. \frac{\partial g}{\partial h_2} \right|_{\mathbf{h}, u_s} = 1$$

and the state-space model is:

$$\begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{\beta_1}{2A_1\sqrt{h_{1s}} - h_{2s}} & \frac{\beta_1}{2A_1\sqrt{h_{1s}} - h_{2s}} \\ \frac{\beta_1}{2A_2\sqrt{h_{1s}} - h_{2s}} & -\frac{\beta_1}{2A_2\sqrt{h_{1s}} - h_{2s}} - \frac{\beta_2}{2A_2\sqrt{h_{2s}}} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 1 \\ A_1 \\ 0 \end{bmatrix} [u]$$

$$y = [0 \quad 1] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

where:

$$y = x_2 = h_2 - h_{2s}$$

In this section we have shown how to linearize a nonlinear process model and put it in state-space form. The states in this model are in deviation (perturbation) variable form; that is, the states are perturbations from a nominal steady-state. A state-space model provides a good approximation to the physical system when the operating point is "close" to the linearization point (nominal steady-state).

### 5.3 INTERPRETATION OF LINEARIZATION

In Section 5.2 we illustrated the method of linearization of models into state-space form. The objective of this section is to illustrate what is meant by linearization of a function. Consider the single tank height problem, which has the following model:

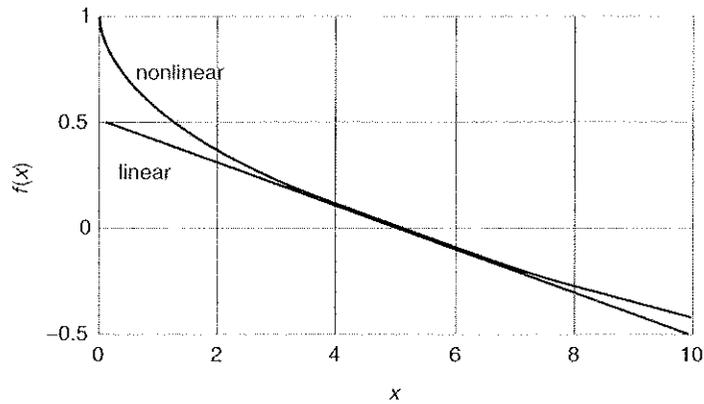
$$\frac{dh}{dt} = f(h, F) = \frac{F}{A} - \frac{\beta}{A} \sqrt{h} \quad (5.39)$$

for a system with  $A = 1 \text{ ft}^2$ ,  $h_s = 5 \text{ ft}$ , and  $\beta = 1/\sqrt{5} \text{ ft}^{2.5}/\text{min}$  the steady-state flowrate is  $F_s = 1 \text{ ft}^3/\text{min}$ . To focus our analysis on the meaning of the linearization with respect to the state variable, consider the case where the input is constant. Then, from (5.39) and the given parameter values:

$$f(h, F_s) = 1 - \frac{1}{\sqrt{5}} \sqrt{h} \quad (5.40)$$

performing the linearization:

$$f(h, F_s) \approx f(h_s, F_s) + \left. \frac{\partial f}{\partial h} \right|_{h_s, F_s} (h - h_s)$$



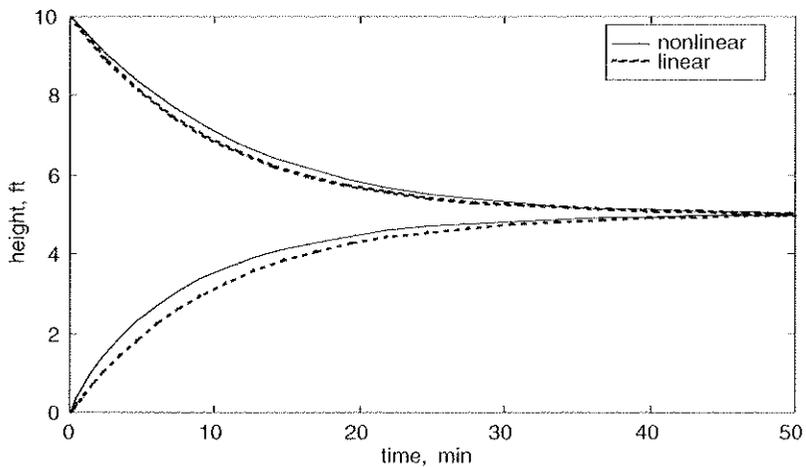
**FIGURE 5.3** Basic idea of linearization. The linear approximation is exact for the steady-state value of  $x = 5$ .

for our parameter values

$$f(h, F_s) \approx 0 + \frac{-1}{2\sqrt{5}\sqrt{h_s}}(h - h_s)$$

or

$$f(h, F_s) \approx 0 - \frac{1}{10}(h - h_s) \quad (5.41)$$



**FIGURE 5.4** Comparison of linear and nonlinear responses for two different initial conditions.

We can see how good the linear approximation is by plotting both the nonlinear function (5.40) and the linear function (5.41), as shown in Figure 5.3 on p. 118. Here we have used  $x$  to represent tank height and  $f(x)$  to represent the nonlinear and linear functions. Notice that the linear approximation works well between roughly 3.5 to 7 feet. Of course, the two functions are exactly equal at the steady-state value of 5 feet, which was the point at which the Taylor series expansion was performed. Realize that  $f(x)$  is  $dx/dt$ , which is the rate of change of tank height. It makes sense that the rate of change is positive at a tank height less than 5 feet, because the system “seeks” to achieve a steady-state level of 5 feet. Similarly, for a tank height greater than 5 feet, the rate of change of tank height is negative, because the level “desires” to decrease to 5 feet. We can also see that the linear system will be slower than the nonlinear system, if the tank height is less than 5 feet, but will be faster if the height is greater than 5 feet, as shown in Figure 5.4.

## 5.4 SOLUTION OF THE ZERO-INPUT FORM

We have previously written the general state space model in the following form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

where  $\mathbf{x}$  and  $\mathbf{u}$  are deviation variable vectors for the states and inputs, respectively. In this section we assume that the inputs are held constant at their steady-state values, but that the states may be initially perturbed from steady-state. The “zero-input” form of the state space model is then:

$$\begin{bmatrix} \dot{x}_1 \\ \cdot \\ \cdot \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdot & a_{1n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ a_{n1} & a_{n2} & \cdot & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix}$$

or

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} \quad (5.42)$$

This form is used to analyze the stability of a system and to understand the dynamic behavior of a system that has had its states perturbed from the steady-state values.

Recall that the single variable equation:

$$\dot{x} = a x$$

has the solution:

$$x(t) = e^{at} x(0)$$

which is stable if  $a < 0$ . In a similar fashion, the solution to (5.42) is

$$x(t) = e^{\mathbf{A}t} x(0) \quad (5.43)$$

and the solution to (5.43) is stable if all of the eigenvalues of  $\mathbf{A}$  are less than zero. The response of (5.43) is oscillatory if the eigenvalues are complex.

There are many different ways to calculate the exponential of a matrix; in this chapter we discuss only the *similarity transform* method.

Recall that the eigenvector/eigenvalue problem is written (see Module 2 for a review):

$$\mathbf{A} \mathbf{V} = \mathbf{V} \Lambda \quad (5.44)$$

For a  $2 \times 2$   $\mathbf{A}$  matrix we have the following eigenvector matrix:

$$\mathbf{V} = [\xi_1 \quad \xi_2] = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \quad (5.45)$$

where  $\xi_1 = \begin{bmatrix} v_{11} \\ v_{21} \end{bmatrix}$  = first eigenvector (associated with  $\lambda_1$ )

$\xi_2 = \begin{bmatrix} v_{12} \\ v_{22} \end{bmatrix}$  = second eigenvector (associated with  $\lambda_2$ )

and the following eigenvalue matrix:

$$\Lambda = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \quad (5.46)$$

Multiplying (5.44) on the right side by  $\mathbf{V}^{-1}$  we find:

$$\mathbf{A} = \mathbf{V} \Lambda \mathbf{V}^{-1} \quad (5.47)$$

multiplying by the scalar  $t$  and taking the matrix exponential, we find:

$$e^{\mathbf{A}t} = \mathbf{V} e^{\Lambda t} \mathbf{V}^{-1} \quad (5.48)$$

where

$$e^{\Lambda t} = \begin{bmatrix} e^{\lambda_1 t} & 0 \\ 0 & e^{\lambda_2 t} \end{bmatrix} \quad (5.49)$$

and we see immediately why  $\lambda_i < 0$  is required for a stable solution. The solution for  $\mathbf{x}(t)$  is

$$\mathbf{x}(t) = \mathbf{V} e^{\Lambda t} \mathbf{V}^{-1} \mathbf{x}(0) \quad (5.50)$$

An interesting result is that an initial condition vector in the same direction as  $\xi_i$  has a response in the direction of  $\xi_i$  with a "speed or response" of  $\lambda_i$ . This is shown by the following analysis.

#### 5.4.1 Effect of Initial Condition Direction (Use of Similarity Transform)

Recall that we are solving the following model

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} \quad (5.42)$$

Define a new vector  $\mathbf{z}$ , such that

$$\mathbf{x} = \mathbf{V} \mathbf{z} \quad (5.51)$$

or

$$\mathbf{z} = \mathbf{V}^{-1} \mathbf{x} \quad (5.52)$$

and notice that (from (5.51)):

$$\dot{\mathbf{x}} = \mathbf{V} \dot{\mathbf{z}} \quad (5.53)$$

Substituting (5.53) and (5.51) into (5.42):

$$\mathbf{V} \dot{\mathbf{z}} = \mathbf{A} \mathbf{V} \mathbf{z} \quad (5.54)$$

or, left multiplying by  $\mathbf{V}^{-1}$

$$\dot{\mathbf{z}} = \mathbf{V}^{-1} \mathbf{A} \mathbf{V} \mathbf{z} \quad (5.55)$$

But, from (5.44)  $\mathbf{A} \mathbf{V} = \mathbf{V} \mathbf{\Lambda}$

so we can write:

$$\mathbf{V}^{-1} \mathbf{A} \mathbf{V} = \mathbf{\Lambda} \quad (5.56)$$

which yields (from (5.55) and (5.56)):

$$\dot{\mathbf{z}} = \mathbf{\Lambda} \mathbf{z} \quad (5.57)$$

But  $\mathbf{\Lambda}$  is a diagonal matrix (see (5.46)), so we have:

$$\begin{bmatrix} \dot{z}_1 \\ \dot{z}_2 \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} \quad (5.58)$$

Notice that (5.58) represents two independent equations:

$$\dot{z}_1 = \lambda_1 z_1 \quad (5.59)$$

$$\dot{z}_2 = \lambda_2 z_2 \quad (5.60)$$

which have the solutions:

$$z_1(t) = z_1(0) e^{\lambda_1 t} \quad (5.61)$$

$$z_2(t) = z_2(0) e^{\lambda_2 t} \quad (5.62)$$

and we can write:

$$\begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix} = \begin{bmatrix} e^{\lambda_1 t} & 0 \\ 0 & e^{\lambda_2 t} \end{bmatrix} \begin{bmatrix} z_1(0) \\ z_2(0) \end{bmatrix} \quad (5.63)$$

or

$$\mathbf{z}(t) = e^{\mathbf{\Lambda} t} \mathbf{z}(0) \quad (5.64)$$

Notice that, if the  $\mathbf{z}(0)$  vector has the form:

$$\mathbf{z}(0) = \begin{bmatrix} z_1(0) \\ 0 \end{bmatrix} \quad (5.65)$$

then:

$$\mathbf{z}(t) = \begin{bmatrix} z_1(0)e^{\lambda_1 t} \\ 0 \end{bmatrix} \quad (5.66)$$

and, if the  $\mathbf{z}(0)$  vector has the form:

$$\mathbf{z}(0) = \begin{bmatrix} 0 \\ z_2(0) \end{bmatrix} \quad (5.67)$$

then,

$$\mathbf{z}(t) = \begin{bmatrix} 0 \\ z_2(0)e^{\lambda_2 t} \end{bmatrix} \quad (5.68)$$

that is, initial conditions of  $\mathbf{z}(0) = \begin{bmatrix} z_1(0) \\ 0 \end{bmatrix}$  will yield a “speed of response” associated with  $\lambda_1$ , while initial conditions of  $\mathbf{z}(0) = \begin{bmatrix} 0 \\ z_2(0) \end{bmatrix}$  will yield a “speed of response” associated with  $\lambda_2$ .

This means that state variable initial conditions in the “direction” of the first eigenvector will have a speed or response associated with the first eigenvalue:

$$\mathbf{x}(t) = \mathbf{V} \mathbf{z}(t) = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix} = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \begin{bmatrix} z_1(0)e^{\lambda_1 t} \\ 0 \end{bmatrix} \quad (5.69)$$

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} v_{11}z_1(0)e^{\lambda_1 t} \\ v_{21}z_1(0)e^{\lambda_1 t} \end{bmatrix}$$

and state variable initial conditions in the “direction” of the second eigenvector will have a speed or response associated with the second eigenvalue

$$\mathbf{x}(t) = \mathbf{V} \mathbf{z}(t) = \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix} \approx \begin{bmatrix} v_{11} & v_{12} \\ v_{21} & v_{22} \end{bmatrix} \begin{bmatrix} 0 \\ z_2(0)e^{\lambda_2 t} \end{bmatrix} \quad (5.70)$$

$$\mathbf{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} v_{12}z_2(0)e^{\lambda_2 t} \\ v_{22}z_2(0)e^{\lambda_2 t} \end{bmatrix}$$

Knowing the effect of the initial condition “direction” is important. If a random case study approach was taken, then we might arbitrarily select initial conditions that were “fast,” while other (missed) initial conditions could cause a much slower response.

We will show two examples of the effect of initial condition: Example 5.5, where the system is stable, and Example 5.6, where the system is unstable.

**EXAMPLE 5.5 A Stable System**

Consider the following system of equations

$$\dot{x}_1 = -0.5x_1 + x_2 \quad (5.71)$$

$$\dot{x}_2 = -2x_2 \quad (5.72)$$

Using standard state-space notation

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} \quad (5.42)$$

The Jacobian matrix is

$$\mathbf{A} = \begin{bmatrix} -0.5 & 1 \\ 0 & -2 \end{bmatrix} \quad (5.73)$$

the eigenvalues are the solution to  $\det(\lambda \mathbf{I} - \mathbf{A}) = 0$ , which yields

$$\det \left( \begin{bmatrix} \lambda + 0.5 & -1 \\ 0 & \lambda + 2 \end{bmatrix} \right) = (\lambda + 0.5)(\lambda + 2) = 0$$

so

$$\lambda_1 = -0.5 \quad \lambda_2 = -2$$

and the eigenvectors are

$$\xi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \xi_2 = \begin{bmatrix} -0.5547 \\ 0.8321 \end{bmatrix}$$

Note that  $\xi_1$  is the "slow" subspace, since it corresponds to  $\lambda_1 = -0.5$  and  $\xi_2$  is the "fast" subspace, since it corresponds to  $\lambda_2 = -2$ .

The numerical values of (5.50) for this problem are

$$\mathbf{x}(t) = \mathbf{V} e^{\Lambda t} \mathbf{V}^{-1} \mathbf{x}(0)$$

$$\mathbf{x}(t) = \begin{bmatrix} 1 & -0.5547 \\ 0 & 0.8321 \end{bmatrix} \begin{bmatrix} e^{-0.5t} & 0 \\ 0 & e^{-2t} \end{bmatrix} \begin{bmatrix} 1 & 0.6667 \\ 0 & 1.2019 \end{bmatrix} \mathbf{x}(0) \quad (5.74)$$

If the initial condition is in the direction of  $\xi_1$ , that is

$$\mathbf{x}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad (5.75)$$

we find the following state solution (from (5.74) and (5.75)):

$$\mathbf{x}(t) = \begin{bmatrix} 1 e^{-0.5t} \\ 0 \end{bmatrix} \quad (5.76)$$

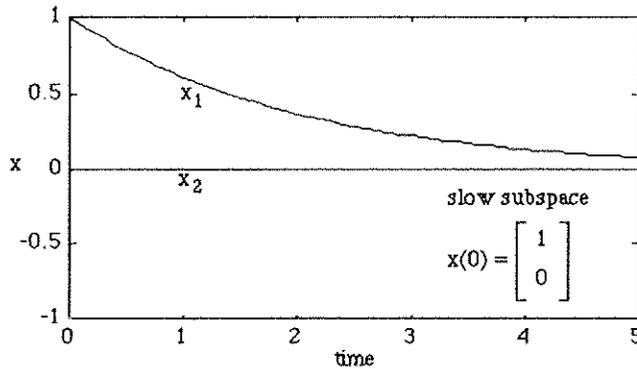
If the initial condition is in the direction of  $\xi_2$ , that is,

$$\mathbf{x}(0) = \begin{bmatrix} -0.5547 \\ 0.8321 \end{bmatrix} \quad (5.77)$$

we find the following state solution (from (5.74) and (5.77)):

$$\mathbf{x}(t) = \begin{bmatrix} -0.5547 e^{-2t} \\ 0.8321 e^{-2t} \end{bmatrix} \quad (5.78)$$

Note that  $\mathbf{x}(0) = \xi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$  is the slow initial condition and  $\mathbf{x}(0) = \xi_2 = \begin{bmatrix} -0.5547 \\ 0.8321 \end{bmatrix}$  is the fast initial condition, as shown in Figures 5.4 and 5.5. The initial conditions in the fast subspace have reached the steady-state in roughly 2.5 minutes (Figure 5.5), while the initial conditions in the slow subspace are roughly 75% complete in 2.5 minutes (Figure 5.6).



**FIGURE 5.5** Transient response for initial condition in the slow subspace.

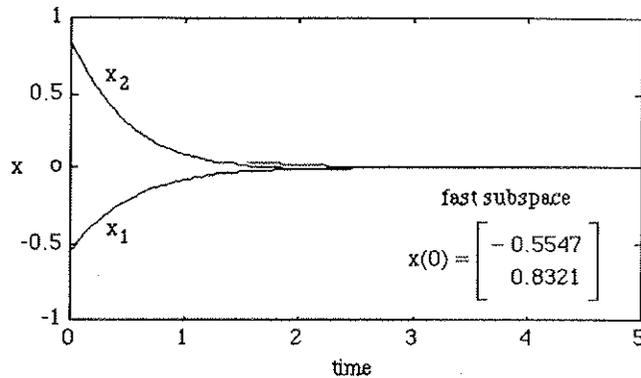
The `expm` (matrix exponential) function from MATLAB can be used to verify these simulations. Using  $t = 0.5$  and the fast initial condition, we find

```

>>a = [-0.5, 1; 0, -2];
>>x = expm(a*0.5) * [-0.5547 ; 0.8321]
x =
    -0.2040
     0.3061

```

which agrees with the plot shown in Figure 5.6.



**FIGURE 5.6** Transient response for initial condition in the fast subspace.

The previous example was a stable system. The next example is an unstable system.

**EXAMPLE 5.6 An Unstable System (Saddle)**

Consider the following system of equations:

$$\dot{x}_1 = 2x_1 + x_2$$

$$\dot{x}_2 = 2x_1 - x_2$$

The Jacobian matrix is

$$\mathbf{A} = \begin{bmatrix} 2 & 1 \\ 2 & -1 \end{bmatrix}$$

the eigenvalues are

$$\lambda_1 = -1.5616 \quad \lambda_2 = 2.5616$$

and the eigenvectors are

$$\xi_1 = \begin{bmatrix} 0.2703 \\ -0.9628 \end{bmatrix} \quad \xi_2 = \begin{bmatrix} 0.8719 \\ 0.4896 \end{bmatrix}$$

since  $\lambda_1 < 0$ ,  $\xi_1$  is a stable subspace; since  $\lambda_2 > 0$ ,  $\xi_2$  is an unstable subspace.

The solution for this system is:

$$\mathbf{x}(t) = \begin{bmatrix} 0.2703 & 0.8719 \\ -0.9628 & 0.4896 \end{bmatrix} \begin{bmatrix} e^{-1.5616t} & 0 \\ 0 & e^{2.5616t} \end{bmatrix} \begin{bmatrix} 0.5038 & -0.8972 \\ 0.9907 & 0.2782 \end{bmatrix} \mathbf{x}(0)$$

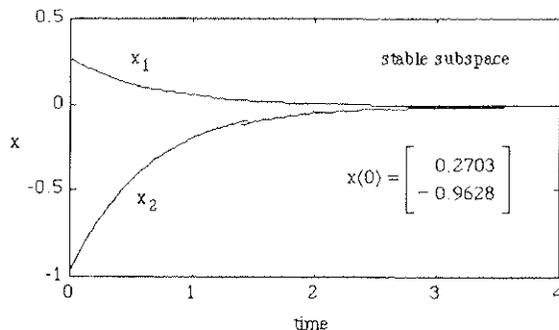
If the initial condition is in the direction of  $\xi_1$ , that is:

$$\mathbf{x}(0) = \begin{bmatrix} 0.2703 \\ -0.9628 \end{bmatrix}$$

we find the following state solution

$$\mathbf{x}(t) = \begin{bmatrix} 0.2703 e^{-1.5616t} \\ -0.9628 e^{-1.5616t} \end{bmatrix}$$

which is a stable solution, as shown in Figure 5.7.



**FIGURE 5.7** Initial condition in the stable subspace.

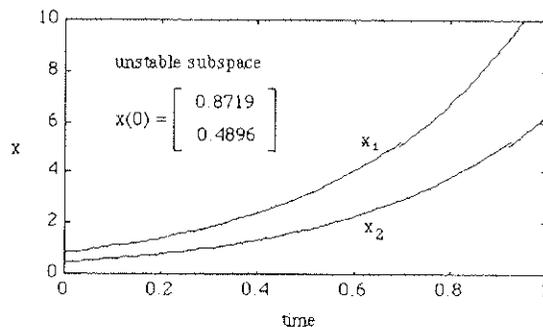
If the initial condition is in the direction of  $\xi_2$ , that is,

$$\mathbf{x}(0) = \begin{bmatrix} 0.8719 \\ 0.4896 \end{bmatrix}$$

we find the following state solution:

$$\mathbf{x}(t) = \begin{bmatrix} 0.8719 e^{2.5616t} \\ 0.4896 e^{2.5616t} \end{bmatrix}$$

which is an unstable solution, as shown in Figure 5.8.



**FIGURE 5.8** Initial condition in the unstable subspace.

It should be noted that if the initial condition is not *exactly* in the stable subspace, the solution will begin to diverge and become unstable. That is, if the initial condition is off by, say  $10^{-10}$ , the response will eventually become unbounded.

## 5.5 SOLUTION OF THE GENERAL STATE-SPACE FORM

Now, consider the general form:

$$\begin{bmatrix} \dot{x}_1 \\ \cdot \\ \cdot \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdot & a_{1n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ a_{n1} & a_{n2} & \cdot & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & \cdot & b_{1m} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ b_{n1} & b_{n2} & \cdot & b_{nm} \end{bmatrix} \begin{bmatrix} u_1 \\ \cdot \\ \cdot \\ u_m \end{bmatrix}$$

or

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \quad (5.79)$$

Recall that the single variable equation:

$$\dot{x} = ax + bu \quad (5.80)$$

has the solution:

$$x(t) = e^{at}x(0) + (e^{at} - 1)\frac{b}{a}u(0) \quad (5.81)$$

when  $u(t) = \text{constant} = u(0)$ .

In a similar fashion, the solution to (5.79), for a constant input ( $\mathbf{u}(t) = \mathbf{u}(0)$ ) from  $t = 0$  to  $t$  is

$$\mathbf{x}(t) = \mathbf{P} \mathbf{x}(0) + \mathbf{Q} \mathbf{u}(0) \quad (5.82)$$

where

$$\mathbf{P} = e^{\mathbf{A}t} \quad (5.83)$$

and

$$\mathbf{Q} = (\mathbf{P} - \mathbf{I}) \mathbf{A}^{-1} \mathbf{B} \quad (5.84)$$

Equation (5.82) can be used to solve for a system where the inputs change from time step to time step by using:

$$\mathbf{x}(t + \Delta t) = \mathbf{P} \mathbf{x}(t) + \mathbf{Q} \mathbf{u}(t) \quad (5.85)$$

More often this is written as

$$\mathbf{x}(k + 1) = \mathbf{P} \mathbf{x}(k) + \mathbf{Q} \mathbf{u}(k) \quad (5.86)$$

where  $k$  represents the  $k$ th time step. Often a general purpose numerical integration technique (such as one presented in Chapter 4) will be used to solve (5.79).

## 5.6 MATLAB ROUTINES `step` AND `initial`

We show the use of `step` and `initial` by way of the following example.

**EXAMPLE 5.7 A Linearized Bioreactor Model**

Consider the following linearized form of a bioreactor model with substrate inhibition kinetics (see Module 8 for details):

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}$$

where:

$$\mathbf{A} = \begin{bmatrix} 0 & 0.9056 \\ -0.7500 & -2.5640 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} -1.5302 \\ 3.8255 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Enter the state space model:

```
>> a = [0, 0.9056;-0.7500,-2.5640]
```

```
a =
```

```
    0    0.9056
 -0.7500 -2.5640
```

```
>> b = [-1.5302;3.8255]
```

```
b =
```

```
 -1.5302
  3.8255
```

```
>> c = [1, 0 ; 1 , 0]
```

```
c =
```

```
    1    0
    0    1
```

```
>> d = [0;0]
```

```
d =
```

```
    0
    0
```

Check the stability

```
> eig(a)
ans =
    -0.3000
   -2.2640
```

The system is stable.

Assume the process is initially at steady-state. Since this model is in deviation variable form, the initial condition is the zero vector.

### 5.6.1 The MATLAB `step` Function

The MATLAB `step` function assumes a deviation variable form (the initial conditions are zero). The commands are:

```
> [y,x,t] = step(a,b,c,d,1);
> plot(t,y)
```

which yields the plot shown in Figure 5.9.

Notice that the `step` function automatically determined the length of the time vector. You may also provide an equal-spaced time vector and use the following command

```
[y,x] = step(a,b,c,d,1,t)
```

### 5.6.2 The MATLAB `initial` Function

The MATLAB `initial` function assumes a deviation variable form, with the initial conditions perturbed from zero. The commands are:

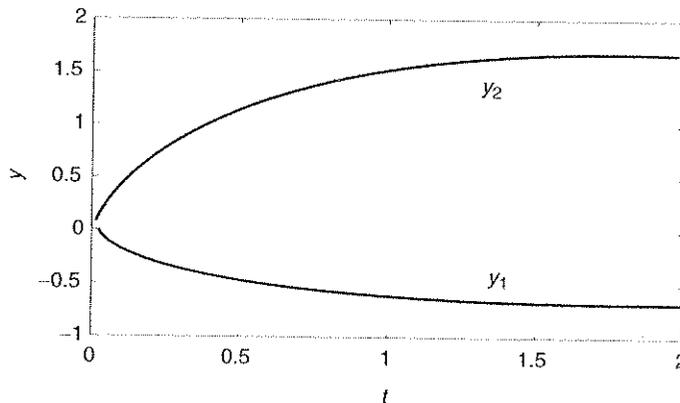


FIGURE 5.9 Plot of outputs, for a step input change.

```

> [y,x,t] = initial(a,b,c,d,1);
> plot(t,y)

```

Notice that the  $b$  and  $d$  matrices are not really used by the initial function, since it is assumed that there is no input change.

## SUMMARY

In this chapter we have developed a state-space model of a chemical process that is inherently linear (e.g., the tank height example). We have also shown how to linearize models that are nonlinear. The models obtained in this fashion are based on *deviation variables*, that is, the states and inputs are *perturbations* from the steady-state operating point where the linearization is performed. The stability of a nonlinear system is determined from the eigenvalues of the Jacobian matrix in the linearized model (state-space form).

Several important concepts were presented in this chapter.

- For unforced systems (zero input), the initial condition vector will determine the “speed” of response. For stable systems (all  $\lambda < 0$ ), the eigenvector associated with the largest magnitude  $\lambda$  is the fast direction, while the eigenvector associated with the smallest  $\lambda$  is the slow direction.
- Although it is possible for a system with both negative (stable) and positive (unstable) eigenvalues to have stable behavior if the initial condition is in the stable subspace, this is impossible in practice. Any perturbation from the stable trajectory will cause the solution to become unbounded (unstable).

The MATLAB routines that were used include:

```

expm: Matrix exponential
step: Step response of a state-space (or transfer function) model

```

State-space models can be transformed to Laplace transfer function form, which is particularly useful for control system design. Applications of Laplace transforms will be presented in Chapters 7 through 10.

Eigenvector/eigenvalue analysis will be useful in performing phase-plane analysis, which is covered in Chapter 13.

The reader should understand the following terms:

```

state-space
Jacobian
deviation or perturbation variable
eigenvalue

```

eigenvector  
 linearization  
 stability  
 Taylor series

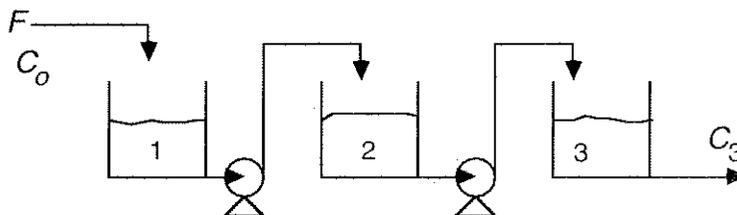
## FURTHER READING

Linearization is discussed briefly in most books on process control, including:

- Luyben, W.L. (1990). *Process Modeling, Simulation and Control for Chemical Engineers*, 2nd Ed., New York: McGraw-Hill.
- Marlin, T.E. (1995). *Process Control. Designing Processes and Control Systems for Dynamic Performance*, New York: McGraw-Hill.
- Ogunnaike, B.A. and W. H. Ray (1994). *Process Dynamics, Modeling and Control*, New York: Oxford University Press.
- Seborg, D.E., T.F. Edgar, and D.A. Mellichamp (1989). *Process Dynamics and Control*, New York: Wiley.
- Stephanopoulos, G. (1984). *Chemical Process Control: An Introduction to Theory and Practice*, Englewood Cliffs, NJ: Prentice-Hall.

## STUDENT EXERCISES

- As a process development engineer you are working on a process with three continuous-stirred-tank reactors (CSTRs) in series. A constant volumetric flowrate (flowrate does not vary with time) is maintained throughout the system, however the volume in each reactor is different (but constant). Since the temperature varies from reactor to reactor (but is constant in an individual reactor) the reaction rate parameter is different for each reactor. The molar concentration of the inlet stream varies.



Assume that the density of the streams remains constant (independent of concentration). The reaction is a first-order (irreversible) decomposition ( $A \rightarrow B$ ). Molar rate of decomposition of A (per unit volume) =  $k CA$

- a. Write the 3 dynamic model equations.
- b. Write the state-space model  $o(\dot{x}) = A x + B u$
- c. The values of the parameters and variables are

$$F = 1 \text{ ft}^3/\text{min} \quad C_o = 1 \text{ lbmol}/\text{ft}^3$$

$$V_1 = 10 \text{ ft}^3 \quad V_2 = \text{ft}^3 \quad V_3 = 5 \text{ ft}^3$$

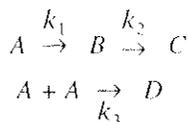
$$k_1 = 0.0333 \text{ min}^{-1} \quad k_2 = 0.2 \text{ min}^{-1} \quad k_3 = 0.55 \text{ min}^{-1}$$

- i. Find the steady-state concentrations in each reactor
  - ii. Evaluate the A matrix (Jacobian) and find the eigenvalues
2. Consider a chemical reactor with bypass, as shown below. Assume that the reaction rate (per unit volume) is first-order ( $r = kC_1$ ) and  $C_1$  is the concentration in the reactor (the reactor is perfectly mixed). Assume that the volume in the reactor ( $V$ ) and the feed flowrate ( $F$ ) remain constant. The fraction of feed bypassing the reactor is  $(1-a)F$  and that entering the reactor is  $aF$ . Assume that the fraction bypassing the reactor does not change. The inlet concentration ( $C_{in}$ ) is the input variable and the mixed outlet stream composition ( $C_2$ ) is the output variable. Write this model in state-space form (this model is inherently linear, so deviation variables are not needed).

$$o(\dot{x}) = A x + B u$$

$$y = C x + D u$$

3. Consider the following set of series and parallel reactions



Material balances on components  $A$  and  $B$  yield the following two equations

$$\frac{dC_A}{dt} = \frac{F}{V} (C_M - C_A) - k_1 C_A - k_3 C_A^2$$

$$\frac{dC_B}{dt} = \frac{F}{V} (-C_B) + (k_1 C_A - k_2 C_B)$$

where  $k_1 = \frac{5}{6} \text{ min}^{-1}$   $k_2 = \frac{5}{3} \text{ min}^{-1}$   $k_3 = \frac{1}{6} \frac{\text{liters}}{\text{mol min}}$

$$C_M = 10 \frac{\text{mol}}{\text{liter}} \quad C_{As} = 3 \frac{\text{mol}}{\text{liter}}$$

- a. Find the steady-state dilution rate ( $F/V$ ) and concentration of  $B$  (show all units).
- b. Linearize and put in state-space form (find the numerical values of the  $A$ ,  $B$ , and  $C$  matrices), assuming that the manipulated variable is dilution rate ( $F/V$ ), and the output variable is  $C_B$ .
- c. Find the eigenvalues (show units).
- d. Find perturbations in initial conditions that are in the fastest and slowest directions.

4. A chemical reactor that has a single second-order reaction and an outlet flowrate that is a linear function of height has the following model:

$$\frac{dVC}{dt} = F_{in}C_{in} - FC - kVC^2 \quad (5.87)$$

$$\frac{dV}{dt} = F_{in} - F \quad (5.88)$$

where the outlet flowrate is linearly related to the volume of liquid in the reactor ( $F = \beta V$ ). The parameters, variables and their steady-state values are shown below.

- $F_{in}$  = inlet flowrate (1 liter/min)
- $C_{in}$  = inlet concentration (1 gmol/liter)
- $C$  = tank concentration (0.5 gmol/liter)
- $V$  = tank volume (1 liter)
- $k$  = reaction rate constant (2 liter/(gmol min))
- $\beta$  =  $1 \text{ min}^{-1}$

Equations (5.87) and (5.88) can be written in physical state variable form as

$$\frac{dC}{dt} = \frac{F_{in}}{V} (C_{in} - C) - kC^2 \quad (5.89)$$

$$\frac{dV}{dt} = F_{in} - \beta V \quad (5.90)$$

- a. List the states, outputs, inputs and parameters for the nonlinear equations (5.89) and (5.90).
  - b. Linearize (5.89) and (5.90) and write the state space model (find the numerical values for the A, B, and C matrices), assuming that the inlet flowrate is the input variable and that both states are output variables. Define the deviation variables for states, inputs, and outputs.
5. Find the “fast” and “slow” initial conditions for the following model

$$\dot{x}_1 = -x_1$$

$$\dot{x}_2 = -4x_2$$

6. Find the stable and unstable subspaces for the following system of equations

$$\dot{x}_1 = -x_1$$

$$\dot{x}_2 = 4x_2$$

Plot the transient responses for initial conditions in both the stable and unstable subspaces. Show that a small perturbation from the stable initial condition will lead to an unstable solution.

7. The noninteracting tank model is (see Example 5.1)

$$\begin{bmatrix} \dot{h}_1 \\ \dot{h}_2 \end{bmatrix} = \begin{bmatrix} -\frac{\beta_1}{A_1} & 0 \\ \beta_1 & -\frac{\beta_2}{A_2} \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + \begin{bmatrix} \frac{1}{A_1} \\ 0 \end{bmatrix} F_o$$

Consider a system where the steady-state flowrates are 5 ft<sup>3</sup>/min, and the following cross-sectional areas and steady-state heights:

$$A_1 = 2 \text{ ft}^2 \quad A_2 = 10 \text{ ft}^2$$

$$h_1 = 2.5 \text{ ft} \quad h_2 = 5 \text{ ft}$$

We find (from  $F_1 = \beta_1 h_1$  and  $F_2 = \beta_2 h_2$ ), then, that:

$$\beta_1 = 2 \frac{\text{ft}^2}{\text{min}} \quad \beta_2 = 1 \frac{\text{ft}^2}{\text{min}}$$

and the state-space model (in physical variables) becomes:

$$\begin{bmatrix} \dot{h}_1 \\ \dot{h}_2 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0.2 & -0.1 \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + \begin{bmatrix} 0.5 \\ 0 \end{bmatrix} F_o$$

$$\begin{bmatrix} h_1 \\ h_2 \\ F_2 \\ F_o \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} [F_o]$$

- Work in deviation variable form and find the fast and slow subspaces. Use `initial` to simulate the unforced deviation variable system (input deviation remains constant at 0), from initial conditions in both the fast and slow subspaces.
  - Use the results from part a, and convert to the actual physical variables.
  - Work in physical variable form. Use `initial` to simulate the unforced deviation variable system (input remains constant), from initial conditions in both the fast and slow subspaces. Show that the results obtained are the same as those in part b.
8. As a chemical engineer in the pharmaceutical industry you are responsible for a process that uses a bacteria to produce an antibiotic. The reactor has been contaminated with a protozoan that consumes the bacteria. The predator-prey equations are used to model the system ( $b$  = bacteria (prey),  $p$  = protozoa (predator)). The time unit is days.

$$\frac{db}{dt} = \alpha b - \gamma bp$$

$$\frac{dp}{dt} = \epsilon \gamma bp - \beta p$$

- a. Show that the steady-state values are

$$b_s = \frac{\beta}{\varepsilon\gamma} \quad p_s = \frac{\alpha}{\gamma}$$

- b. Use the scaled variables,  $w$  and  $z$ , to find the following scaled modeling equations

$$w = \frac{b}{b_s} \quad z = \frac{p}{p_s}$$

$$\frac{dw}{dt} = \alpha(1-z)w$$

$$\frac{dz}{dt} = -\beta(1-w)z$$

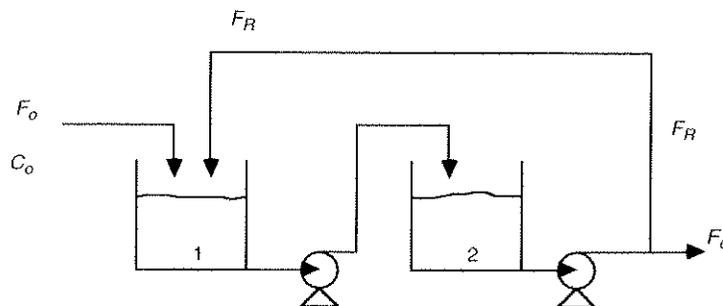
- c. Find the eigenvalues of the Jacobian matrix for the scaled equations, evaluated at  $w_s$  and  $z_s$ . Realize that  $w_s$  and  $z_s$  are 1.0 by definition. Find the eigenvalues in terms of  $\alpha$  and  $\beta$ .
- d. The parameters are  $\alpha = \beta = 1.0$  and the initial conditions are  $w(0) = 1.5$  and  $z(0) = 0.75$ .
- Linearize and write the state-space form (let the state variables be  $x_1 = w - w_s$  and  $x_2 = z - z_s$ ). Find the initial condition vector  $x_0 = \begin{bmatrix} x_1(0) \\ x_2(0) \end{bmatrix}$ , to use with `initial`.
  - Solve the state space model from (i) using `lsim` and plot the transient response of  $x_1$  and  $x_2$  as a function of time (plot these curves on the same graph), simulating to at least  $t = 20$ .
  - Show a phase-plane plot, placing  $x_1$  on the  $x$ -axis and  $x_2$  on the  $y$ -axis.
  - What is the “peak-to-peak” time for the bacteria? By how much time does the protozoan “lag” the bacteria?

9. Consider the state-space model

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -1.0 & 0.0 \\ 4.0 & -5.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- a. Find the “fast” and “slow” initial condition directions.

10. Consider the following system of two reactors.



Assume a first-order decomposition of  $A \rightarrow B$ . Assume that all flowrates are constant (volumes are constant).

- Write the modeling equations for concentration of  $A$ , using either the instantaneous or integral method.
- Write these in state-space form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

- Given the following constants, calculate the steady-state concentrations:

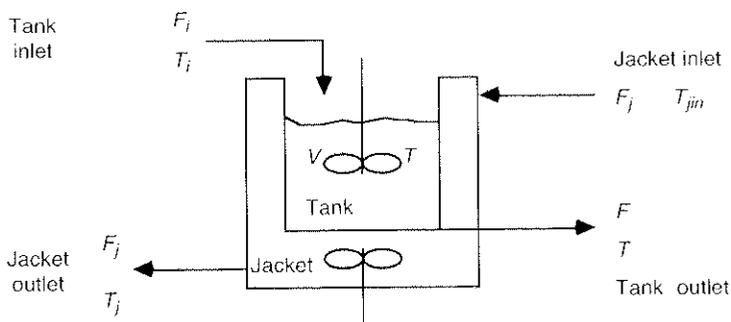
$$F_o = 1.25 \frac{\text{m}^3}{\text{hr}} \quad F_R = 1.75 \frac{\text{m}^3}{\text{hr}}$$

$$C_o = 1.5 \frac{\text{kgmol}}{\text{m}^3} \quad k_1 = 0.10833 \text{ hr}^{-1} \quad k_2 = 0.33333 \text{ hr}^{-1}$$

$$V_1 = 15 \text{ m}^3 \quad V_2 = 9 \text{ m}^3$$

- Find the eigenvalues of the  $\mathbf{A}$  matrix. Discuss the stability of this system.
  - The inlet concentration,  $C_o$ , is changed from 1.5 to 1.75 at  $t = 0$ . Use step to simulate the behavior of this system.
11. A stirred tank heater is used to supply a chemical process with a fluid at a constant temperature. The heater receives fluid from an upstream process unit, which may cause the flowrate or temperature to change.

Consider the diagram of the stirred tank heater shown below, where the tank inlet stream is received from another process unit. A heat transfer fluid is circulated through a jacket to heat the fluid in the tank. Assume that no change of phase occurs in either the tank liquid or the jacket liquid.



### Part 1

- Write the dynamic modeling equations to find the tank and jacket temperatures. Do not use any numerical values—leave these equations in terms of the process parameters and variables. State any additional assumptions needed to solve the problem.

Assume: Constant level.

Perfect mixing in both the tank and jacket.

The tank inlet flowrate, jacket flowrate, tank inlet temperature, and jacket inlet temperature may change.

The rate of heat transfer from the jacket to the tank is governed by the equation  $Q = UA(T_j - T)$ , where  $U$  is the overall heat transfer coefficient and  $A$  is the area for heat exchange.

- State the major objective of this process.
- What do you consider the most important measured variable?
- What is a likely input variable variable that you would use to maintain a desired tank temperature?

## Part 2

Assume that both the tank fluid and the jacket fluid are water. The steady-state values of this system variables and some parameters are:

$$F = 1 \frac{\text{ft}^3}{\text{min}} \quad \rho C_p = 61.3 \frac{\text{Btu}}{\text{°F ft}^3} \quad \rho_j C_{pj} = 61.3 \frac{\text{Btu}}{\text{°F ft}^3}$$

$$T_i = 50\text{°F} \quad T = 125\text{°F} \quad V = 10 \text{ft}^3$$

$$T_{jm} = 200\text{°F} \quad T_j = 150\text{°F} \quad V_j = 1 \text{ft}^3$$

- Find  $F_j$  and  $UA$  (show units) at steady-state.
- Linearize the set of two nonlinear ODEs obtained in problem a, to obtain the state space form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x}$$

where  $\mathbf{x} = \begin{bmatrix} T - T_s \\ T_j - T_{js} \end{bmatrix}$  = state variables

$$\mathbf{u} = \begin{bmatrix} F_j - F_{js} \\ F - F_s \\ T_i - T_{is} \\ T_{jm} - T_{jms} \end{bmatrix} = \text{input variables}$$

$$\mathbf{y} = \begin{bmatrix} T - T_s \\ T_j - T_{js} \end{bmatrix} = \text{output variables}$$

Determine the  $\mathbf{A}$ ,  $\mathbf{B}$ , and  $\mathbf{C}$  matrices (symbolically and numerically)

- Find the eigenvalues of  $\mathbf{A}$ .

**Part 3**

- h. Simulate the system of state-space equations for a step change in the jacket flowrate from  $F_j = 1.5 \text{ ft}^3/\text{min}$  to  $F_j = 1.75 \text{ ft}^3/\text{min}$  at time = 5 minutes (work in deviation variables, but remember to convert back to physical variables before plotting). What is the final value of the states, in the physical variables ( $T$  and  $T_j$ )? Plot the response.
- i. Perform some simulations with step changes on some of the other input variables. Comment on any different behavior that you may observe.

12. Consider the following model of 2-stage absorption column:

$$\frac{dw}{dt} = -\left(\frac{L + Va}{M}\right)w + \left(\frac{Va}{M}\right)z$$

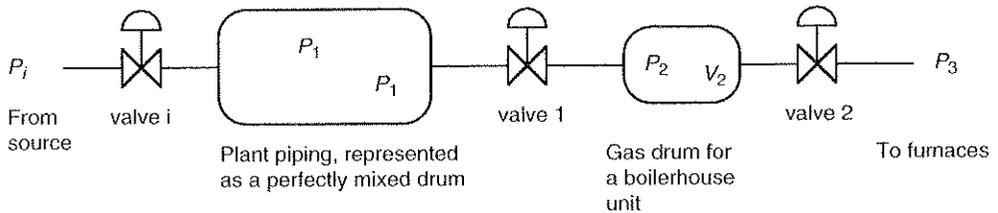
$$\frac{dz}{dt} = \left(\frac{L}{M}\right)w - \left(\frac{L + Va}{M}\right)z + \frac{V}{M}z_f$$

where  $w$  and  $z$  are the liquid concentrations on stage 1 and stage 2, respectively.  $L$  and  $V$  are the liquid and vapor molar flowrates.  $z_f$  is the concentration of the vapor stream entering the column.

The steady-state input values are  $L = 80 \text{ gmol inert liquid/min}$  and  $V = 100 \text{ gmol inert vapor/min}$ .

The parameter values are  $M = 20 \text{ gmol inert liquid}$ ,  $a = 0.5$ , and  $z_f = 0.1 \text{ gmol solute/gmol inert vapor}$ .

- a. Find the steady-state values of  $w$  and  $z$ .
  - b. Linearize and find the state space model, assuming that  $L$  and  $V$  are the inputs.
  - c. Find the eigenvalues and eigenvectors of  $\mathbf{A}$  (Jacobian).
  - d. Find the expected “slowest” and “fastest” initial conditions (perturbations from steady-state).
13. Most chemical process plants have a natural gas header that circulates through the process plant. A simplified version of such a header is shown below.



Here, the natural gas enters the process plant from a source (the natural gas pipeline) through a control valve. It flows through the plant piping, which we have represented as a perfectly mixed drum for simplicity. Another valve connects the

plant piping to the gas drum for a boilerhouse unit. Gas passes through another valve to the boilerhouse furnaces.

The objective of this problem is to develop a linear model that relates changes in valve position to changes in drum pressures.

- Write modeling equations assuming that the pressures in drums 1 and 2 are the state variables. Let the input variables be (1) valve position 1, (2) valve position 2, and (3) source pressure.
- Solve for the steady-state conditions and write the modeling equations in linear, deviation variable form.

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x}$$

$$\mathbf{x} = \begin{bmatrix} P_1 - P_{1s} \\ P_2 - P_{2s} \end{bmatrix} = \text{state variables}$$

$$\mathbf{u} = \begin{bmatrix} h_1 - h_{1s} \\ h_2 - h_{2s} \\ P_i - P_{is} \end{bmatrix} = \begin{bmatrix} \text{change in valve position 1} \\ \text{change in valve position 2} \\ \text{change in source pressure} \end{bmatrix} = \text{input variables}$$

$$\mathbf{y} = \begin{bmatrix} P_1 - P_{1s} \\ P_2 - P_{2s} \end{bmatrix} = \text{output variables}$$

- Study the effect of step changes in each input on each tank pressure.

**HINTS:** For simplicity, assume that the following equations can be used for the flow through the valves:

$$q_i = \alpha_i h_i (p_i - p_1) = \text{flow through valve } i$$

$$q_1 = \alpha_1 h_1 (p_1 - p_2) = \text{flow through valve 1}$$

$$q_2 = \alpha_2 h_2 (p_2 - p_3) = \text{flow through valve 2}$$

where the flowrate is in lbmol/min,  $h$  is the fraction that a valve is open (varies between 0 and 1), and  $\alpha$  is a valve coefficient.

#### STEADY STATE DATA:

gas flowrate = 1000 std ft<sup>3</sup>/min

$P_{is} = 250$  psig,  $P_{1s} = 50$  psig,  $P_{2s} = 30$  psig,  $P_{3s} = 5$  psig

assume that each valve is 1/2 open under these conditions ( $h_{is} = h_{1s} = h_{2s} = 0.5$ )

## CONSTANTS:

$$V_1 = 1135 \text{ ft}^3, V_2 = 329 \text{ ft}^3, \text{Temperature} = 32 \text{ }^\circ\text{F}$$

$$R \text{ (gas constant)} = 10.73 \frac{\text{psia ft}^3}{\text{lbmol } ^\circ\text{R}}$$

## MAGNITUDE OF STEP CHANGES:

Make separate step changes of 0.1 (10%) in the valve openings, and 10 psia in the inlet pressure. Simulate for  $t = 0$  to  $t = 15$  minutes.

14. A stream contains a waste chemical, W, with a concentration of 1 mol/liter. To meet EPA and state standards, at least 90% of the chemical must be removed by reaction. The chemical decomposes by a second-order reaction with a rate constant of 1.5 liter/(mol hr). The stream flowrate is 100 liter/hr and two available reactors (400 and 2000 liters) have been placed in series (the smaller reactor is placed before the larger one).

- a. Write the modeling equations for the concentration of the waste chemical. Assume constant volume and constant density. Let

$C_{w1}$  = concentration in reactor 1, mol/liter

$C_{w2}$  = concentration in reactor 2, mol/liter

$F$  = volumetric flowrate, liter/hr

$V_1$  = liquid volume in reactor 1, liters

$V_2$  = liquid volume in reactor 2, liters

$k$  = second-order rate constant, liter/(mol hr)

- b. Show that the steady-state concentrations are 0.33333 mol/liter (reactor 1) and 0.09005 mol/liter (reactor 2), so the specification is met.

(Hint: You need to solve quadratic equations to obtain the concentrations.)

- c. Linearize at steady-state and develop the state space model (analytical), of the form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

where:

$$\mathbf{x} = \begin{bmatrix} C_{w1} - C_{w1s} \\ C_{w2} - C_{w2s} \end{bmatrix} \quad \mathbf{u} = \begin{bmatrix} F - F_s \\ C_{win} - C_{wins} \end{bmatrix}$$

- d. Show that the  $\mathbf{A}$  and  $\mathbf{B}$  matrices are:

$$\mathbf{A} = \begin{bmatrix} -1.25 & 0 \\ 0.05 & -0.32015 \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} 0.0016667 & 0.25 \\ 0.0001216 & 0 \end{bmatrix}$$

(also, show the units associated with each coefficient)

- e. i. Find the eigenvalues and eigenvectors using the MATLAB eig function.  
ii. Find the eigenvalues by hand, by solving  $\det(\lambda \mathbf{I} - \mathbf{A}) = 0$ .

- f. The system is not initially at steady-state. Solve the following for the linearized model, using the MATLAB function `initial` (first, convert the physical variables to deviation variables)
- If  $C_{w1}(0) = 0.3833$  and  $C_{w2}(0) = 0.09005$ , find how the concentrations change with time.
  - If  $C_{w1}(0) = 0.3333$  and  $C_{w2}(0) = 0.14005$ , find how the concentrations change with time.

Relate these responses to the eigenvalues/eigenvector analysis of  $e$ . Discuss the differences in speeds of response (you should find that a perturbation in the first reactor concentration responds more rapidly and a perturbation in the second reactor concentration).

The MATLAB `initial` function needs you to create the following matrices before using it:

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$$

- Solve  $\mathbf{f}$  for the nonlinear equations, using `ode45`. Compare the linear and nonlinear variables on the same plots (make certain you convert from deviation to physical variables for the linear results).
- Now, consider a step change in the flowrate from 100 liters/hour to 110 liters/hour. Assume the initial concentrations are the steady-state values (0.3333 and 0.09005). Compare the linear and nonlinear responses of the reactor concentrations. Is the removal specification still obtained?
- Would better steady-state removal of W be obtained if the order of the reaction vessels was reversed? Why or why not? (Show your calculations.)

# SOLVING LINEAR $n$ TH ORDER ODE MODELS

# 6

The purpose of this chapter is to review methods to solve linear  $n$ th order ODEs. After studying this material, the student will be able to:

- Transform a linear state-space model with  $n$  states to a single  $n$ th order ordinary differential equation.
- Solve an  $n$ th order constant coefficient homogeneous ODE.
- Solve an  $n$ th order constant coefficient heterogeneous ODE.
- Solve a first-order ODE with a time-varying coefficient.
- Use the Routh stability criterion for stability analysis.

The major sections in this chapter are:

- 6.1 Background
- 6.2 Solving Homogeneous, Linear ODEs with Constant Coefficients
- 6.3 Solving Nonhomogeneous, Linear ODEs with Constant Coefficients
- 6.4 Equations with Time-Varying Parameters
- 6.5 Routh Stability Criterion—Determining Stability without Calculating Eigenvalues

## 6.1 BACKGROUND

A model composed of a single,  $n$ th order linear ordinary differential equation has the following form:

$$\begin{aligned} a_n(t) \frac{d^n x}{dt^n} + a_{n-1}(t) \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1(t) \frac{dx}{dt} + a_0(t) x \\ = b_m(t) \frac{d^m u}{dt^m} + b_{m-1}(t) \frac{d^{m-1} u}{dt^{m-1}} + \dots + b_1(t) \frac{du}{dt} + b_0(t) u \end{aligned} \quad (6.1)$$

where the state variable is  $x$  and the input variable is  $u$ . This general model is linear because the state ( $x$ ) and input ( $u$ ) and all of their derivatives with respect to time appear linearly. Notice that the coefficients do not have to be linear functions of time, however.

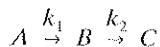
Models of the form of (6.1) do not arise naturally when chemical processes are modeled. As shown in previous chapters, dynamic chemical process models are generally sets of first-order (either linear or nonlinear ordinary differential equations). The advantage of the form of (6.1) is that there exist a number of techniques to obtain analytical solutions.

In this chapter we show how to transform sets of linear, first-order differential equations to a single  $n$ th order differential equation. We then review several techniques for solving this type of equation. For motivation, we use a batch reactor example to illustrate each of the techniques. It should be noted that there are many good mathematics texts that cover each of these techniques in more depth (see Boyce and DiPrima, 1992, for example). Our goal here is to provide a concise overview of some more useful techniques to solve dynamic chemical process problems.

### EXAMPLE 6.1 Batch Chemical Reactor

Consider a batch chemical reactor, where there is no flow in or out of the vessel. The reactor is initially charged with a liquid of volume  $V$  and an initial concentration (mol/liter) of reactant  $A$  of  $C_{A0}$ .

We consider a series reaction where component  $A$  reacts to form the desired component  $B$ . Component  $B$  can further react to form the undesired component  $C$ . Each of the reactions is irreversible, so  $A$  can react to form  $B$ , but  $B$  does not react to form  $A$ .



Here  $k_1$  represents kinetic rate constant ( $\text{time}^{-1}$ ) for the conversion of  $A$  to  $B$ , while  $k_2$  represents the rate constant for the conversion of  $B$  to  $C$ .

Since component  $B$  is the desired product, we would like to know how long to run the reaction in order to maximize the amount of  $B$  produced. If the reaction time is too long, all of  $B$  will eventually be converted to  $C$ .

**Develop the Modeling Equations.** Assume that each of the reactions is first-order. Since the volume is constant ( $dV/dt = 0$ ), and there is no flow in or out, the modeling equations are (the reader should be able to derive these, based on material balances on each component):

$$\frac{dC_A}{dt} = -k_1 C_A \quad (6.2)$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B \quad (6.3)$$

$$\frac{dC_C}{dt} = k_2 C_B \quad (6.4)$$

where  $C_A$ ,  $C_B$ , and  $C_C$  represent the concentrations (mol/volume) of components A, B, and C, respectively. The units for the rate constants ( $k_1$  and  $k_2$ ) are  $\text{time}^{-1}$ .

Notice that the time rate of change of component A is only a function of the concentration of A. Then equation (6.2) can be solved, since  $C_A$  and  $t$  are separable, to find

$$C_A(t) = C_{A0} e^{-k_1 t} \quad (6.5)$$

where  $C_{A0}$  is the initial condition for the concentration of A. If we define the conversion of A as  $x = (C_{A0} - C_A)/C_{A0}$  and the dimensionless time  $\tau = k_1 t$ , (6.5) can be represented by the single curve shown in Figure 6.1 ( $x = 1 - e^{-\tau}$ ).

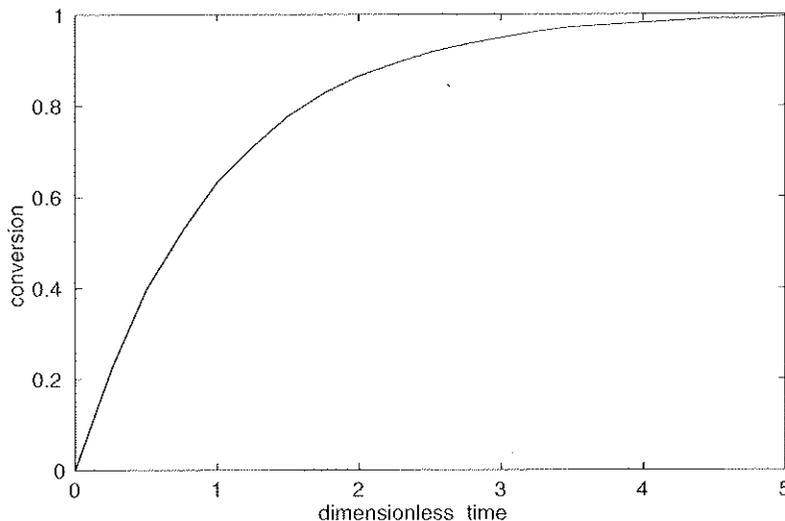


FIGURE 6.1 Conversion of A as a function of the dimensionless time.

Now we wish to find a single differential equation to solve for  $C_B$ .

**Reduce to a Single Equation for CB.** Here we have two different ways to solve for  $C_B$ .

*Method 1.* Substitute (6.5) into (6.3) to obtain the expression

$$\frac{dC_B}{dt} + k_2 C_B = k_1 C_{A0} e^{-k_1 t} \quad (6.6)$$

Equation (6.6) is a linear, constant coefficient, *heterogeneous* differential equation. It is heterogeneous because of the “forcing function” on the righthand side. Heterogeneous equations are solved in Section 6.3.

*Method 2.* Here we can rewrite (6.3) to solve for  $C_A$  in terms of  $C_B$ :

$$C_A = \frac{1}{k_1} \frac{dC_B}{dt} + \frac{k_2}{k_1} C_B \quad (6.7)$$

Taking the first derivative of (6.7) with respect to time, we find:

$$\frac{dC_A}{dt} = \frac{1}{k_1} \frac{d^2C_B}{dt^2} + \frac{k_2}{k_1} \frac{dC_B}{dt} \quad (6.8)$$

Substituting (6.7) and (6.8) into (6.2), we find the second-order equation:

$$\frac{d^2C_B}{dt^2} + (k_1 + k_2) \frac{dC_B}{dt} + k_1 k_2 C_B = 0 \quad (6.9)$$

Notice that (6.9) has the form

$$a_2 \frac{d^2x}{dt^2} + a_1 \frac{dx}{dt} + a_0 x = 0 \quad (6.10)$$

Equation (6.10) is known as a linear, constant coefficient, homogeneous differential equation. The term homogeneous means that there is no “forcing function” on the righthand side. In Section 6.2 we cover the solution of these equations.

## 6.2 SOLVING HOMOGENEOUS, LINEAR ODES WITH CONSTANT COEFFICIENTS

Homogeneous  $n$ th order linear differential equations have the form

$$a_n \frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = 0 \quad (6.11)$$

To solve equation (6.11) we replace all  $d^i x/dt^i$  terms by  $\lambda^i$

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \dots + a_1 \lambda + a_0 = 0 \quad (6.12)$$

Equation (6.12) is called the *characteristic equation*. The  $n$  roots of the characteristic equation are called *eigenvalues* (in control textbooks the roots are often called *poles*). The eigenvalues are used to solve (6.11). Two related methods are used, depending on whether the eigenvalues are distinct (all are different) or repeated (some are the same).

### 6.2.1 Distinct Eigenvalues

We see that (6.12) is an  $n$ th order polynomial that will have  $n$  roots,  $\lambda_i$ . If all of the roots are distinct (not repeated), the solution to (6.11) is

$$x(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} + \dots + c_n e^{\lambda_n t} \quad (6.13)$$

where each of the constants  $c_1$  through  $c_n$  is found from the initial conditions,  $x(0)$ ,  $\dots$ ,  $d^n x^{(n-1)}(0)/dt^{n-1}$ .

In order to find the coefficients,  $c_i$ , we must know the *initial conditions* for  $x$  and its derivatives.

#### EXAMPLE 6.1 Continued. Solution for Component A

We see from equation (6.2) that the concentration of  $A$  does not depend on the values of  $B$  and  $C$ .

$$\frac{dC_A}{dt} + k_1 C_A = 0 \quad (6.14)$$

The characteristic equation is

$$\lambda + k_1 = 0 \quad (6.15)$$

and the eigenvalue is  $\lambda = -k_1$ . The solution is then

$$C_A(t) = c_1 e^{-k_1 t} \quad (6.16)$$

and we can solve for  $c_1$  from initial condition  $C_A(0) = C_{A0}$  to obtain

$$C_A(t) = C_{A0} e^{-k_1 t} \quad (6.17)$$

which is the same result obtained in (6.5) using separation of variables and integration.

Now, let's continue and use the general procedure to solve a second-order differential equation.

#### EXAMPLE 6.1 Continued. Solution for Component B

Recall that the equation for the concentration of  $B$  is:

$$\frac{d^2 C_B}{dt^2} + (k_1 + k_2) \frac{dC_B}{dt} + k_1 k_2 C_B = 0 \quad (6.9)$$

and the characteristic equation is:

$$\lambda^2 + (k_1 + k_2) \lambda + k_1 k_2 = 0 \quad (6.18)$$

which can be written:

$$(\lambda + k_1)(\lambda + k_2) = 0 \quad (6.19)$$

So the eigenvalues are:

$$\lambda_1 = -k_1 \quad \text{and} \quad \lambda_2 = -k_2$$

and the solution can be written:

$$C_B(t) = c_1 \exp(-k_1 t) + c_2 \exp(-k_2 t) \quad (6.20)$$

We need two initial conditions,  $C_B(0)$  and  $dC_B(0)/dt$ , to evaluate the constants,  $c_1$  and  $c_2$ .

We assumed that there is no component  $B$  in the reactor initially, so  $C_B(0) = 0$ . From (6.20) we then find:

$$c_1 = -c_2 \quad (6.21)$$

From (3) we see that:

$$\frac{dC_B(0)}{dt} = k_1 C_{A0} \quad (6.22)$$

Taking the derivative of (6.20) and using (6.21) and (6.22), we find:

$$C_B(t) = \frac{k_1 C_{A0}}{k_2 - k_1} [\exp(-k_1 t) - \exp(-k_2 t)] \quad (6.23)$$

This expression can be used, for example, to solve for the amount of time that will yield the maximum amount of  $C_B$  (see student exercise 15).

**Dimensionless Equation.** It should also be noted that (6.23) can be made dimensionless by defining the following variables:

$$x = C_B/C_{A0} = \text{conversion of } A \text{ to } B$$

$$\tau = k_1 t = \text{dimensionless time}$$

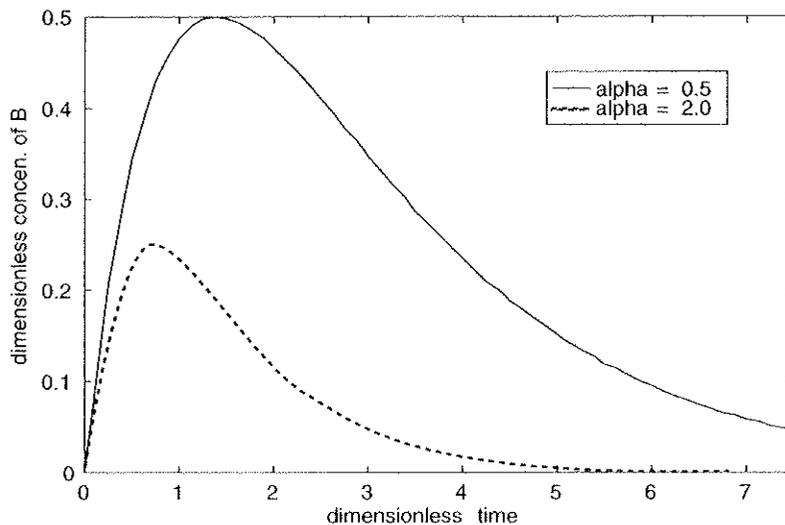
$$\alpha = k_2/k_1 = \text{rate constant ratio}$$

to find:

$$x(\tau) = \frac{1}{\alpha - 1} [\exp(-\tau) - \exp(-\alpha\tau)]$$

which is shown in Figure 6.2, for  $\alpha = 0.5$  and 2. Notice that when the first reaction is faster than the second ( $\alpha = 0.5$ ), there is a higher concentration of  $B$  than when the first reaction is slower

than the second ( $\alpha = 2$ ). When the second reaction is faster than the first, component  $B$  reacts further to form  $C$ , before a substantial amount of  $B$  is formed.



**FIGURE 6.2** Concentration of  $B$  as a function of time. When the rate for the second reaction is faster than the first ( $\alpha = 2$ ), the peak concentration of  $B$  is lower.

We notice in the previous example that (6.23) cannot be used if  $k_2 = k_1$ . This is a case where the eigenvalues are repeated. The procedure for repeated eigenvalues is shown next.

### 6.2.2 Repeated Eigenvalues

If a particular root in the solution of (6.12),  $\lambda_i$ , occurs  $r$  times, then the corresponding terms in the solution to (6.11) are:

$$(c_i + c_{i+1}t + c_{i+2}t^2 + \dots + c_{i+r-1}t^{r-1})e^{\lambda_i t} \quad (6.24)$$

#### EXAMPLE 6.1 Continued. Repeated Roots

The equation for the concentration of  $B$  is when  $k_2 = k_1 = k$  is:

$$\frac{d^2 C_B}{dt^2} + 2k \frac{dC_B}{dt} + k^2 C_B = 0 \quad (6.25)$$

and the characteristic equation is:

$$\lambda^2 + 2k\lambda + k^2 = 0 \quad (6.26)$$

which can be factored as:

$$(\lambda + k)(\lambda + k) = 0$$

so the eigenvalues (roots) are:

$$\lambda_1 = \lambda_2 = -k$$

The solution can be written:

$$C_B(t) = (c_1 + c_2 t) \exp(-kt) \quad (6.27)$$

Notice that we can find  $c_1$  from the initial condition for  $C_B$ . From (6.27) at  $t = 0$ ,

$$c_1 = C_B(0)$$

But  $C_B(0) = 0$ , since there is no  $B$  initially, so:

$$C_B(t) = c_2 t \exp(-kt) \quad (6.28)$$

The derivative of (6.28) with respect to time is:

$$\dot{C}_B(t) = c_2 e^{-kt} - c_2 k t e^{-kt}$$

at  $t = 0$ ,

$$c_2 = \dot{C}_B(0)$$

We also know from (6.3) that:

$$\frac{dC_B(t)}{dt} = k C_{A0}$$

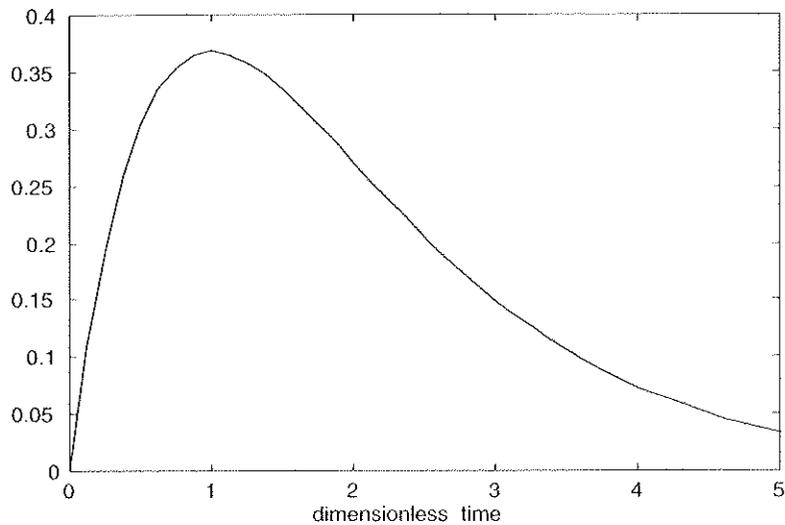
so:

$$C_B(t) = k C_{A0} t \exp(-kt) \quad (6.29)$$

If we define the conversion of  $A$  to  $B$  as  $x = C_B/C_{A0}$ , and the dimensionless time as  $\tau = kt$ , then (6.29) can be written:

$$x(\tau) = \tau \exp(-\tau) \quad (6.30)$$

which is shown in Figure 6.3. The reader should be able to find the maximum value for the conversion of  $A$  to  $B$  and the reaction time required for this conversion.



**FIGURE 6.3** Conversion of  $A$  to  $B$  as a function of dimensionless time ( $\tau = kt$ ), for the case of equal rate constants.

The previous example illustrated the solution for systems with real roots. The next example illustrates a system with complex roots.

### EXAMPLE 6.2 Complex Roots

Consider the second-order equation:

$$\frac{d^2x}{dt^2} + \frac{dx}{dt} + x = 0 \quad (6.31)$$

The characteristic equation is:

$$\lambda^2 + \lambda + 1 = 0 \quad (6.32)$$

Solving for the roots using the quadratic formula, we find that the roots are complex:

$$\lambda = \frac{-1 \pm \sqrt{1-4}}{2}$$

$$\lambda = -\frac{1}{2} \pm \frac{\sqrt{3}}{2}j$$

where  $j = \sqrt{-1}$ . The solution is

$$x(t) = c_1 e^{\left(-\frac{1}{2} + \frac{\sqrt{3}}{2}j\right)t} + c_2 e^{\left(-\frac{1}{2} - \frac{\sqrt{3}}{2}j\right)t} \quad (6.33)$$

We can use the following Euler identities:

$$e^{j\theta} = \cos \theta + j \sin \theta \quad (6.34)$$

$$e^{-j\theta} = \cos \theta - j \sin \theta \quad (6.35)$$

and the property that  $e^{x+y} = e^x e^y$  to write (6.33) as:

$$x(t) = c_1 e^{-t/2} \left[ \cos \frac{\sqrt{3}}{2}t + j \sin \frac{\sqrt{3}}{2}t \right] + c_2 e^{-t/2} \left[ \cos \frac{\sqrt{3}}{2}t - j \sin \frac{\sqrt{3}}{2}t \right] \quad (6.36)$$

$$x(t) = e^{-t/2} \left[ c_1 \cos \frac{\sqrt{3}}{2}t + c_2 \cos \frac{\sqrt{3}}{2}t + c_1 j \sin \frac{\sqrt{3}}{2}t - c_2 j \sin \frac{\sqrt{3}}{2}t \right] \quad (6.37)$$

which can be written:

$$x(t) = e^{-t/2} \left[ (c_1 + c_2) \cos \frac{\sqrt{3}}{2}t + (c_1 - c_2)j \sin \frac{\sqrt{3}}{2}t \right] \quad (6.38)$$

Defining  $c_3 = c_1 + c_2$  and  $c_4 = (c_1 - c_2)j$ ,

$$x(t) = e^{-t/2} \left[ c_3 \cos \frac{\sqrt{3}}{2}t + c_4 \sin \frac{\sqrt{3}}{2}t \right] \quad (6.39)$$

Again, initial conditions for  $x(0)$  and  $\dot{x}(0)$  can be used to determine  $c_3$  and  $c_4$ . The student should verify that if  $x(0) = 1$  and  $\dot{x}(0) = 1$ , then  $c_3 = 1.0$  and  $c_4 = 1.5$ . A plot is shown in Figure 6.4.

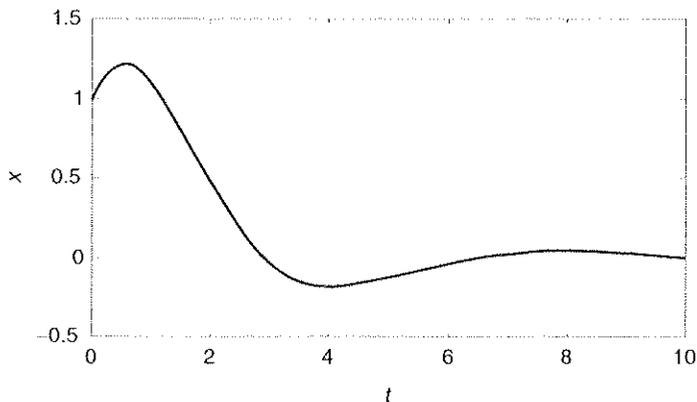


FIGURE 6.4 Plot of (6.39) with  $x(0) = 1$  and  $\dot{x}(0) = 1$ .

Chemical process system models with complex roots include some exothermic chemical reactors. Also, models including feedback control will often have complex roots (leading to oscillatory behavior).

### 6.2.3 General Result for Complex Roots

We can now generalize the results of Example 6.2 for any equation that has pairs of complex roots. For each pair of complex roots,  $\lambda = \lambda_r \pm j \lambda_i$ , where  $\lambda_r$  and  $\lambda_i$  are the real and imaginary portions, the solution is:

$$x(t) = e^{\lambda_r t} [c_1 \cos \lambda_i t + c_2 \sin \lambda_i t] \quad (6.40)$$

In the previous example the real part of the complex roots was negative (stable). Notice that the state variables decayed to zero with time. Notice from (6.40) that there will be no decay (simply a continuous oscillation) if the real portion is 0. We can also see from (6.40) that a positive real portion of the complex root will lead to an ever growing (unstable) solution. This behavior is shown by student exercise 19.

Most chemical processes are stable; however, some exothermic chemical reactors have unstable operating points. Also, improperly tuned feedback control systems can be unstable.

Thus far in this chapter we have solved the *homogeneous* problems. Homogeneous problems result from models that are “unforced,” that is, there is no input. This usually occurs when the process model is in deviation variable form, and there is no change in the input variable. They are based on a perturbation from steady-state in the state variable values.

In Section 6.3 we will solve *nonhomogeneous* problems using the method of undetermined coefficients. These types of problems arise when there are input changes to a process.

## 6.3 SOLVING NONHOMOGENEOUS, LINEAR ODES WITH CONSTANT COEFFICIENTS

In Section 6.2 we solved homogeneous problems with constant coefficients:

$$\frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = 0 \quad (6.41)$$

In this section we will solve nonhomogeneous problems with the following form:

$$\frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = q(t) \quad (6.42)$$

using the *method of undetermined coefficients*, which is outlined below.

### Method of Undetermined Coefficients

The method of undetermined coefficients consists of the following steps:

1. Solve the *homogeneous* problem to find

$$x_H(t)$$

2. Solve for the particular solution by determining the coefficients of a trial function (see Table 6.1) that satisfy the *nonhomogeneous* equation

$$x_P(t)$$

3. Combine the two solutions for

$$x(t) = x_H(t) + x_P(t)$$

**TABLE 6.1 Trial Functions for Method of Undetermined Coefficients (Boyce and DiPrima, 1992)**

Forcing Function	Trial Function
$A$ (a constant)	$B$ (a constant)
$Ae^{\alpha t}$	$Be^{\alpha t}$
$A \cos \alpha t$ or $A \sin \alpha t$	$B_1 \cos \alpha t + B_2 \sin \alpha t$
$A t^n$	$B_n t^n + B_{n-1} t^{n-1} + \dots + B_0$

We illustrate the method by use of an illustrative example.

#### EXAMPLE 6.1 Continued. First Order Heterogeneous System

Notice that we can take the solution for  $C_A$  as a function of time

$$c_A(t) = C_{A0} e^{-k_1 t} \quad (6.14)$$

and substitute it into (6.3) to obtain

$$\frac{dC_B}{dt} + k_2 C_B = k_1 C_{A0} e^{-k_1 t} \quad (6.43)$$

**Step 1.** The homogeneous solution to (6.43) is

$$x_H(t) = c_1 e^{-k_2 t} \quad (6.44)$$

**Step 2.** Since the forcing function is  $k_1 C_{A0} e^{-k_1 t}$ , we use  $c_2 e^{-k_1 t}$  (Table 6.1) as our trial function for the particular solution:

$$x_P(t) = c_2 e^{-k_1 t} \quad (6.45)$$

substituting this solution into the original equation (6.47),

$$-k_1 c_2 e^{-k_1 t} + k_2 c_2 e^{-k_1 t} = k_1 C_{A0} e^{-k_1 t} \quad (6.46)$$

which we can solve for  $c_2$ :

$$c_2 = \frac{k_1 C_{A0}}{k_2 - k_1} \quad (6.47)$$

**Step 3.** Now find the complete solution as  $x(t) = x_H(t) + x_P(t)$

$$C_A(t) = c_1 e^{-k_1 t} + \frac{k_1 C_{A0}}{k_2 - k_1} e^{-k_2 t} \quad (6.48)$$

We can evaluate  $c_1$  from the initial conditions,  $C_{B0} = 0$ :

$$c_1 = -\frac{k_1 C_{A0}}{k_2 - k_1}$$

and the total solution is:

$$C_B(t) = \frac{k_1 C_{A0}}{k_2 - k_1} [\exp(-k_1 t) - \exp(-k_2 t)]$$

which, of course, is the same result obtained previously (6.23) by solving the second-order homogeneous equation in  $C_B$ .

We have used a single first-order equation to illustrate the procedure for heterogeneous equations. The same procedure is used for higher-order equations.

## 6.4 EQUATIONS WITH TIME-VARYING PARAMETERS

Consider a first-order equation with the following form:

$$\frac{dx}{dt} + p(t)x = q(t) \quad (6.49)$$

Notice that the coefficient is time-varying and the equation is heterogeneous. One approach to solve this type of problem is to use an *integrating factor*.

Let the integrating factor be represented by  $\mu(t)$

$$\mu(t) = \exp \left[ \int p(t) dt \right] \quad (6.50)$$

Equation (6.49) is solved by multiplying each term by the integrating factor:

$$\mu(t) \frac{dx}{dt} + \mu(t) p(t) x = \mu(t) q(t) \quad (6.51)$$

$$\exp \left[ \int p(t) dt \right] \frac{dx}{dt} + \exp \left[ \int p(t) dt \right] p(t) x = \exp \left[ \int p(t) dt \right] q(t) \quad (6.52)$$

Notice that the lefthand side of (6.52) is simply the expansion of:

$$\frac{d}{dt} \left[ x(t) \exp \left\{ \int p(t) dt \right\} \right] = \exp \left[ \int p(t) dt \right] \frac{dx}{dt} + \exp \left[ \int p(t) dt \right] p(t) x \quad (6.53)$$

so we can write:

$$\frac{d}{dt} \left[ x(t) \exp \left\{ \int p(t) dt \right\} \right] = \exp \left[ \int p(t) dt \right] q(t) \quad (6.54)$$

which is a separable equation. Separating and integrating, we find:

$$x(t) \exp \left[ \int p(t) dt \right] = \int q(t) \exp \left[ \int p(t) dt \right] dt + c \quad (6.55)$$

and, evaluating  $c$  using the initial conditions,

$$x(t) = \exp \left[ - \int p(t) dt \right] \left\{ x(0) + \int q(t) \exp \left[ \int p(t) dt \right] dt \right\} \quad (6.56)$$

### EXAMPLE 6.3 Semi-batch Reactor

Consider the case where the batch reactor is being filled. Assume a single, first-order reaction ( $A \rightarrow B$ ) and a constant volumetric flowrate into the reactor ( $F$ ), with no flow out of the reactor.

The modeling equations are:

$$\frac{dV}{dt} = F \quad (6.57)$$

$$\frac{dVC_A}{dt} = -k_1 V C_A + FC_{AF} \quad (6.58)$$

Expanding the LHS of (6.58) as:

$$\frac{dVC_A}{dt} = C_A \frac{dV}{dt} + V \frac{dC_A}{dt} \quad (6.59)$$

we find:

$$\frac{dC_A}{dt} + \left[ \frac{F}{V} + k_1 \right] C_A = \frac{F}{V} C_{AF} \quad (6.60)$$

If the flowrate is constant and the initial volume is 0, then:

$$V = Ft \quad (6.61)$$

and:

$$\frac{dC_A}{dt} + \left[ \frac{1}{t} + k_1 \right] C_A = \frac{C_{AF}}{t} \quad (6.62)$$

Let:

$$\int p(t) dt = \int \left( \frac{1}{t} + k_1 \right) dt = \ln t + k_1 t + c_1 \quad (6.63)$$

$$\begin{aligned} \exp \left[ \int p(t) dt \right] &= \exp [\ln t + k_1 t + c_1] = \exp [\ln t] \exp [k_1 t] \exp [c_1] \\ &= c_2 t \exp [k_1 t] \end{aligned} \quad (6.64)$$

Multiplying through on each side of (6.64) by  $c_2 t \exp [k_1 t]$  and dividing by  $c_2$

$$t \exp [k_1 t] \frac{dC_A}{dt} + \exp [k_1 t] [1 + k_1 t] C_A = \exp [k_1 t] C_{AF} \quad (6.65)$$

and noting that the lefthand side is simply

$$\frac{d [t \exp [k_1 t] C_A]}{dt} \quad (6.66)$$

we multiply by  $dt$  and integrate to find

$$\exp [k_1 t] C_A t = \frac{C_{AF}}{k_1} [\exp [k_1 t] - 1] \quad (6.67)$$

multiplying by  $\exp [-k_1 t]$  and dividing by  $t$ , we find the solution

$$C_A = \frac{C_{AF}}{k_1 t} \{1 - \exp [-k_1 t]\} \quad (6.68)$$

The division by  $t$  is bothersome at  $t = 0$ ; the reader should use L'Hospital's rule to show that the correct initial condition is obtained with this expression.

Notice that we can define a dimensionless concentration and time as

$$y = C_A / C_{AF} \quad \text{and} \quad \tau = k_1 t$$

to find

$$y(\tau) = \frac{1}{\tau} \{1 - \exp [-\tau]\} \quad (6.69)$$

which is shown in Figure 6.5.

Notice that this solution holds while the reactor is being "fed". After the feed is stopped the model is simply  $dC_A/dt = -k_1 C_A$  with appropriate initial conditions (see student exercise 20).

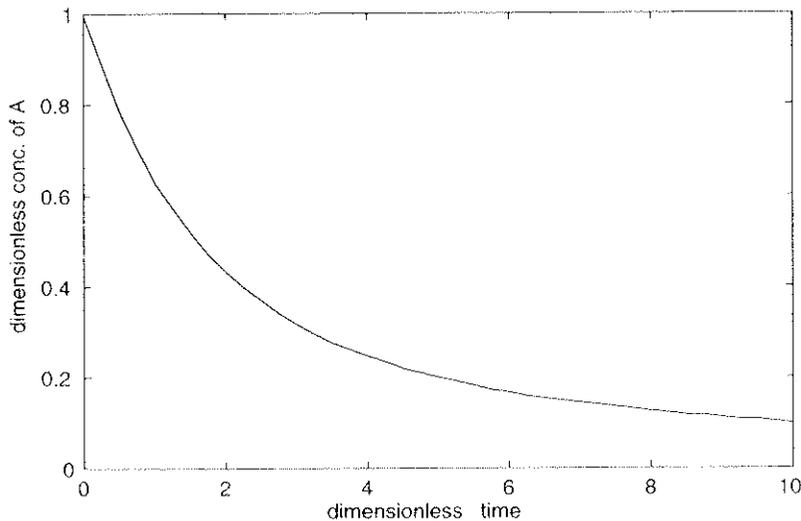


FIGURE 6.5 Solution, dimensionless semibatch reactor problem.

## 6.5 ROUTH STABILITY CRITERION—DETERMINING STABILITY WITHOUT CALCULATING EIGENVALUES

The stability of the characteristic equation is determined from the values of its roots (eigenvalues). This is easy for first and second order equations (and not too hard for third) since there is an analytical solution for the roots of polynomials through third order. If the polynomial is fourth order or higher, the roots must be determined numerically. There is a method for determining if any of the roots are positive (unstable) without actually calculating the roots (Routh, 1905). This method involves an analysis of the coefficients of the characteristic polynomial by setting up the *Routh Array*. The test of the coefficients in the Routh Array is called the *Routh Stability Criterion*.

The Routh Stability Criterion is based on the characteristic equation that has the following polynomial form

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \dots + a_1 \lambda + a_0 = 0 \quad (6.70)$$

We can arbitrarily assume that  $a_n > 0$ . If  $a_n < 0$  then multiply (6.73) by  $-1$ . A *necessary* condition for stability is that all of the coefficients in (6.70) must be positive. If any of the coefficients are negative or zero then at least one eigenvalue (root of the characteristic equation) is positive or zero, indicating that the equation is unstable. Even if all of the coefficients are positive, we cannot state that the system is stable. What is needed is a *sufficient* condition for stability. To determine that the system is stable, we must construct the Routh array and use the Routh stability criterion, which provides necessary and sufficient conditions for stability.

Sometimes we simply wish to determine if a particular system is stable or not, without actually evaluating the eigenvalues. This is particularly true if we wish to determine values of system parameters that will cause a system to lose stability. This approach will be useful in performing a bifurcation analysis in later chapters, and in tuning control systems in chemical process control.

### 6.5.1 Routh Array

If all of the coefficients of the characteristic equation (6.70) are positive, the *necessary* condition for stability is satisfied. The following Routh array (Seborg, Edgar, & Mellichamp, 1989) is developed to test for the *sufficient* conditions for stability:

Row				
1	$a_n$	$a_{n-2}$	$a_{n-4}$	...
2	$a_{n-1}$	$a_{n-3}$	$a_{n-5}$	...
3	$b_1$	$b_2$	$b_3$	...
4	$c_1$	$c_2$	...	
.	.			
$n+1$				

where  $n$  is the order of the characteristic polynomial. Notice that the first two rows consist of the coefficients of the characteristic polynomial. The elements of the third row are calculated in the following fashion:

$$b_1 = \frac{a_{n-1}a_{n-2} - a_n a_{n-3}}{a_{n-1}} \quad b_2 = \frac{a_{n-1}a_{n-4} - a_n a_{n-5}}{a_{n-1}}$$

and so on. Elements of the fourth and larger rows are calculated in a similar fashion:

$$c_1 = \frac{b_1 a_{n-3} - a_{n-1} b_2}{b_1} \quad c_2 = \frac{b_1 a_{n-5} - a_{n-1} b_3}{b_1}$$

and so on.

### Routh Stability Criterion

A necessary and sufficient condition for all roots of the characteristic polynomial to have negative real parts is that all of the coefficients of the polynomial are positive and all of the elements in the left column of the Routh array are positive.

#### EXAMPLE 6.4 Second-order Characteristic Equations

Consider the second-order ODE:

$$a_2 \frac{d^2x}{dt^2} + a_1 \frac{dx}{dt} + a_0 x = 0 \quad (6.71)$$

The characteristic polynomial is:

$$a_2 \lambda^2 + a_1 \lambda + a_0 = 0 \quad (6.72)$$

If all of the coefficients  $a_2$ ,  $a_1$ , and  $a_0$  are positive, then the necessary condition is satisfied. We can form the Routh array to test for the sufficient condition:

Row		
1	$a_2$	$a_0$
2	$a_1$	
3	$a_0$	

Since the left column consists of the polynomial coefficients, if all of the coefficients in the second order system are positive, the system is stable.

Notice that, for second-order systems, a test for positive coefficients is necessary *and* sufficient for stability.

**EXAMPLE 6.5**    Third-order System

The system:

$$\frac{d^3x}{dt^3} + 2 \frac{d^2x}{dt^2} + 3 \frac{dx}{dt} + x = 0$$

has the characteristic polynomial:

$$\lambda^3 + 2\lambda^2 + 3\lambda + 1 = 0$$

and the following Routh array:

<i>Row</i>			
1	1		3
2	2		1
3	5/2		
4	1		

All of the coefficients of the characteristic polynomial are positive and all of the elements in the left column of the Routh array are positive, so the system is stable.

The Routh array is particularly useful for determining how much a parameter can vary before a system loses stability. The following example illustrates such a system.

**EXAMPLE 6.6**    Third-order, System With a Variable Parameter

The system:

$$\frac{d^3x}{dt^3} + 2 \frac{d^2x}{dt^2} + 3 \frac{dx}{dt} + \mu x = 0$$

has the characteristic polynomial:

$$\lambda^3 + 2\lambda^2 + 3\lambda + \mu = 0$$

where  $\mu$  is a parameter that may vary. The Routh array is:

<i>Row</i>			
1	1		3
2	2		$\mu$
3	$b_1$		
4	$c_1$		

where  $b_1 = 3 - \mu/2$  and  $c_1 = \mu$ . From the characteristic polynomial, we see that  $\mu > 0$  is required. The same result holds true for the requirement of  $c_1 > 0$ . We notice that  $b_1$  will be positive only if  $\mu < 6$ .

From these conditions, we find that the stability requirement is  $0 < \mu < 6$ .

For complex, high order (3 or greater), it is not uncommon for a system to have parameters that stabilize the system only over a certain range of parameter values. This is particularly true of feedback control systems.

## SUMMARY

We have reviewed techniques to solve homogeneous and nonhomogeneous (heterogeneous)  $n$ th order ODEs.

- Homogeneous problems are solved using the roots of the characteristic equation, forming the solution as a sum of exponential terms. Homogeneous equations generally occur if the system is unforced, but there is an initial deviation from steady-state in the state variables.
- The *method of undetermined coefficients* is useful for solving nonhomogeneous (heterogeneous) problems. These generally occur if the system is forced by a changing input.
- The *integrating factor* method was useful for solving a first-order heterogeneous equation with a time-varying coefficient.
- The *Routh array* was used to test for the stability of a differential equation. This is useful for finding values of a parameter that cause a system to lose stability, such as in feedback control system design or bifurcation analysis.
- The type of dynamic behavior of an  $n$ th order differential equation is a function of the eigenvalues (roots of the characteristic equation). Eigenvalues that are further in the left half plane are “fast.” The larger the ratio of the imaginary portion to real portion of a complex eigenvalue, the more oscillatory the response. Stability is determined by the real portion of the complex eigenvalue. If all eigenvalues have a real portion that is negative, then the system is stable. If any single eigenvalue has a real portion that is positive, then the system is unstable.

Often engineers study the dynamic behavior of processes by starting out at steady-state, then applying a changing input to the process. Although the method of undetermined coefficients can be used to solve these problems, the Laplace transform technique is used more often. The Laplace transform method is introduced in Chapter 7.

## FURTHER READING

- Boyce, W., & R. DiPrima. (1992). *Ordinary Differential Equations and Boundary Value Problems*, 5th ed. New York: Wiley.
- Routh, F.J. (1905). *Dynamics of a System of Rigid Bodies, Part II*. London: Macmillan.
- Seborg, D.E., T.F. Edgar, & D.A. Mellichamp. (1989). *Process Dynamics and Control*. New York: Wiley.

## STUDENT EXERCISES

1. Consider the state-space model:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -1 & -2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- a. Find the second order ODE in terms of  $x_1$ .
  - b. Find the second order ODE in terms of  $x_2$ .
  - c. For  $x_1(0) = -1$  and  $x_2(0) = 1$ , obtain the analytical solution for  $x_1(t)$  and  $x_2(t)$ .
  - d. Use `ode45` or `initial` to solve the set of two differential equations, given the initial conditions in part c.
2. Consider the following linearized form of a bioreactor model with substrate inhibition kinetics (see Module 8 for details):

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \\ \mathbf{y} &= \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u} \end{aligned}$$

where:

$$\begin{aligned} \mathbf{A} &= \begin{bmatrix} 0 & 0.9056 \\ -0.7500 & -2.5640 \end{bmatrix} & \mathbf{B} &= \begin{bmatrix} -1.5302 \\ 3.8255 \end{bmatrix} \\ \mathbf{C} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & \mathbf{D} &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \end{aligned}$$

- a. Find the second-order ODE in terms of  $x_1$ , assuming  $u = 0$ .
  - b. Find the second-order ODE in terms of  $x_2$ , assuming  $u = 0$ .
  - c. For  $x_1(0) = -1$  and  $x_2(0) = 1$ , obtain the analytical solution for  $x_1(t)$  and  $x_2(t)$ .
  - d. Use `ode45` or `initial` to solve the set of two differential equations, given the initial conditions in part c.
3. Consider the state space model for a two-state system:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{A} \mathbf{x} \\ \begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} &= \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \end{aligned}$$

- a. Let  $y = x_1$ , and derive the following relationship:

$$\ddot{y} - [a_{11} + a_{22}]\dot{y} + [a_{11}a_{22} - a_{21}a_{12}]y = 0$$

which has the characteristic equation:

$$\lambda^2 - [a_{11} + a_{22}]\lambda + [a_{11}a_{22} - a_{21}a_{12}] = 0$$

Recall that the eigenvalues of the  $\mathbf{A}$  matrix are calculated by:

$$\det(\lambda\mathbf{I} - \mathbf{A}) = 0$$

Show that  $\det(\lambda\mathbf{I} - \mathbf{A}) = 0$  applied to this general two-state example, yields:

$$\lambda^2 - [a_{11} + a_{22}]\lambda + [a_{11}a_{22} - a_{21}a_{12}] = 0$$

4. Solve the following differential equation with the given initial conditions:

$$\frac{d^2y}{dx^2} + 5\frac{dy}{dx} + 6y = 0$$

$$y(0) = 0 \quad \text{and} \quad \frac{dy(0)}{dx} = 1$$

5. Find the particular solution of the differential equation:

$$\frac{d^2y}{dx^2} - 3\frac{dy}{dx} - 4y = 2\sin x$$

6. Consider the following second-order homogeneous ODE:

$$\frac{d^2x}{dt^2} - 3\frac{dx}{dt} + 3x = 0$$

- Write the characteristic equation for this ODE.
  - Find the solution (solve for any constants),  $x(t)$ , if the initial conditions are  $x(0) = 2.0$  and  $\dot{x}(0) = 3.0$ .
  - Discuss the stability of this system.
7. Consider the following first-order heterogeneous ODE:

$$3\frac{dx}{dt} + x = 2(1 - e^{-4t})$$

- Write the characteristic equation for the homogeneous part of this ODE.
  - Find the solution to the heterogeneous problem. Show all steps. The initial condition is  $x(0) = 2.0$ .
8. Consider the following state-space model that results from a linearization of the predator-prey equations:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & -1.0 \\ 1.0 & 0.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

with initial conditions  $x_1(0) = 0.5$  and  $x_2(0) = -0.25$ .

- a. What are the eigenvalues of the  $\mathbf{A}$  matrix? Use both MATLAB and your own analytical solution.
  - b. Write the second-order ODE that corresponds to  $x_1$ . Use the method of Section 6.2 to solve for  $x_1(t)$ . Plot  $x_1(t)$ .
  - c. Write the second-order ODE that corresponds to  $x_2$ . Use the method of Section 6.2 to solve for  $x_2(t)$ . Plot  $x_2(t)$ .
  - d. Compare the results from **b** and **c** with those obtained by integrating the state-space equations using either `ode45` or `initial`.
  - e. Show a phase-plane plot ( $x_1$  versus  $x_2$ ), placing  $x_1$  on the  $x$ -axis and  $x_2$  on the  $y$ -axis.
9. Consider a system described by the following third-order ODE:

$$\frac{d^3y}{dt^3} + 1.5 \frac{d^2y}{dt^2} + \frac{dy}{dt} + 2y = 0$$

Is the system described by this equation stable? Why or why not?

10. For a general third-order polynomial:

$$a_3 \lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0 = 0$$

show that  $a_i > 0$  and  $a_1 a_2 - a_0 a_3 > 0$  are necessary and sufficient for stability.

11. For a general fourth-order polynomial:

$$a_4 \lambda^4 + a_3 \lambda^3 + a_2 \lambda^2 + a_1 \lambda + a_0 = 0$$

show that  $a_i > 0$ ,  $a_2 a_3 - a_1 a_4 > 0$ , and  $a_1 a_2 a_3 - a_4 a_1^2 - a_0 a_3^2 > 0$  are necessary and sufficient for stability.

12. Consider the following third-order ODE:

$$\frac{d^3y}{dt^3} + 2 \frac{d^2y}{dt^2} + (\alpha - 1) \frac{dy}{dt} + \alpha y = 0$$

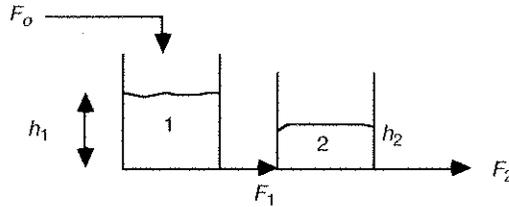
where  $\alpha$  is a parameter. Find the range of  $\alpha$  that will cause this equation to be stable.

13. Consider the following second-order ODE:

$$\frac{d^2y}{dt^2} + 2 \frac{dy}{dt} + 2y = 0$$

which has eigenvalues of  $-1 \pm 1j$  and initial conditions  $y(0) = 2$  and  $\dot{y}(0) = -2$ . Find  $y(t)$ .

14. Consider the series of two tanks, where the levels interact.

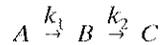


- a. Assuming that the flow from the first tank is linearly proportional to the difference in the tank heights ( $F_1 = \beta_1 (h_1 - h_2)$ ), the flowrate from tank 2 is proportional to the height in tank 2 ( $F_2 = \beta_2 h_2$ ), and the tanks are of constant cross-sectional area ( $A_1$  and  $A_2$ ) show that the modeling equations are

$$\frac{dh_1}{dt} = \frac{F_o}{A_1} - \frac{\beta_1}{A_1} (h_1 - h_2)$$

$$\frac{dh_2}{dt} = \frac{\beta_1}{A_2} (h_1 - h_2) - \frac{\beta_2}{A_2} h_2$$

- b. Reduce these two equations to a single second-order equation in  $h_2$ .
- c. Assume that the steady-state flowrate is 3 ft<sup>3</sup>/min, and the steady-state tank heights for tanks 1 and 2 are 7 and 3 feet, respectively. The constant cross-sectional area is 5 ft<sup>2</sup> for each tank. The initial conditions are  $h_1(0) = 6$  feet and  $h_2(0) = 5$  feet. Solve for the heights of tanks 1 and 2 as a function of time. Plot the tank heights as a function of time. Discuss your results.
- d. Write a MATLAB m-file and use `ode45` to integrate the two equations shown above. Show that the numerical integration agrees with your solution in part c.
15. For the batch series reaction (Example 6.1):



- a. Find the reaction time that maximizes the production of  $B$ . Recall that the solution for the concentration of  $B$  is:

$$C_B(t) = \frac{k_1 C_{A0}}{k_2 - k_1} [\exp(-k_1 t) - \exp(-k_2 t)]$$

and that the maximum occurs when the condition  $dC_B/dt = 0$  is satisfied.

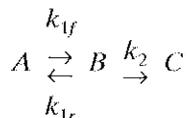
- b. For  $k_1 = 1$  and  $k_2 = 5 \text{ min}^{-1}$ , find the maximum conversion of  $A$  to  $B$  (express as  $C_B/C_{A0}$ ) and the time required for this conversion.
- c. In practice there is uncertainty in the rate constants. If the actual value of  $k_2$  is  $7.5 \text{ min}^{-1}$ , and the reaction time from **b** is used, find the actual conversion of  $A$  to  $B$ .
- d. Use the MATLAB routine `ode45` to integrate the three state variable equations and solve for  $C_A$ ,  $C_B$ , and  $C_C$  as a function of time, for the parameter values in

b, with  $C_{A0} = 1.5$  and  $C_{B0} = C_{C0} = 0$  mol/liter. Make a comparative plot for the parameter values in c. What do you observe about the concentrations of A, B, and C?

16. For the batch series reaction with irreversible reactions ( $A \rightarrow B \rightarrow C$ ):
- Find the reaction time ( $t_{\max}$ ) that maximizes the conversion of A to B for the case where  $k_2 = k_1 = k$ . Also find the value for the maximum conversion of A to B. Recall that the solution for the conversion is

$$x(t) = C_B(t)/C_{A0} = k t \exp(-kt)$$

- Assume that the reactor is run for the period  $t_{\max}$  found in a. Now consider the effect of an error in the reaction rate constant of +50%. What is the actual conversion of A to B obtained at  $t_{\max}$ ?
17. Consider a batch reactor with a series reaction where component A reacts to form the desired component B *reversibly*. Component B can also react to form the undesired component C. The reaction scheme can be characterized by:



Here  $k_{1f}$  and  $k_{1r}$  represent the kinetic rate constants for the forward and reverse reactions for the conversion of A to B, while  $k_2$  represents the rate constant for the conversion of B to C.

Assuming that each of the reactions is first-order and constant volume, the modeling equations are

$$\begin{aligned} \frac{dC_A}{dt} &= -k_{1f} C_A + k_{1r} C_B \\ \frac{dC_B}{dt} &= k_{1f} C_A - k_{1r} C_B \\ \frac{dC_C}{dt} &= k_2 C_B \end{aligned}$$

where  $C_A$ ,  $C_B$ , and  $C_C$  represent the concentrations (mol/volume) of components A, B, and C, respectively. Using the following definitions:

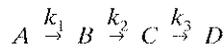
Dimensionless time,	$\tau = k_1 t$
Conversion of A,	$x_1 = (C_{A0} - C_A)/C_{A0}$
Dimensionless concentration of B,	$x_2 = C_B/C_{A0}$
Ratio of rate constants,	$\alpha = k_2/k_{1f}$
Ratio of forward and reverse rate constants,	$\beta = k_{1r}/k_{1f}$

- a. Show that the equation for the dimensionless concentration of  $B$  is

$$\frac{d^2 x_2}{d\tau^2} + (\beta + \alpha + 1) \frac{dx_2}{d\tau} + \alpha x_2 = 0$$

and that the roots of the characteristic equation can never be complex or unstable (assuming that the rate constants are positive).

- b. Solve the previous equation to find  $x_2$  as a function of  $\tau$  and  $\alpha$  and  $\beta$ .  
 c. For  $k_{1f} = 2$ ,  $k_{1r} = 1$ , and  $k_2 = 1.25 \text{ hr}^{-1}$ , find the maximum conversion of  $A$  to  $B$  and the reaction time required for this conversion.  
 d. Usually there is some uncertainty in the rate constants. If the real value of  $k_2$  is  $1.5 \text{ hr}^{-1}$  and the reaction is run for the time found in c, what will be the actual conversion of  $A$  to  $B$ ?
18. Consider the series reaction:



The modeling equations for a constant volume batch reactor are

$$\begin{aligned} \frac{dC_A}{dt} &= -k_1 C_A \\ \frac{dC_B}{dt} &= k_1 C_A - k_2 C_B \\ \frac{dC_C}{dt} &= k_2 C_B - k_3 C_C \end{aligned}$$

- a. Show that the third-order ODE describing the concentration of  $C$  is:

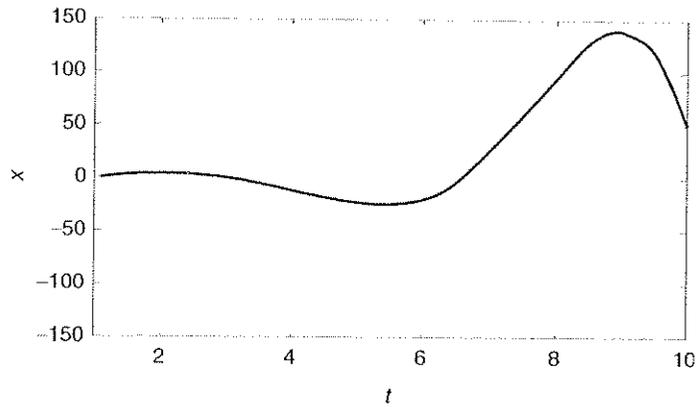
$$\frac{d^3 C_C}{dt^3} + [k_1 + k_2 + k_3] \frac{d^2 C_C}{dt^2} + [k_1 k_2 + k_1 k_3 + k_2 k_3] \frac{dC_C}{dt} + k_1 k_2 k_3 C_C = 0$$

[Hint: Solve for  $C_B$  from the third equation and take the derivative to find  $dC_B/dt$ .]

- b. Assuming that all of the kinetic parameters are positive, show that this system is stable.
19. Consider the second-order equation:

$$\frac{d^2 x}{dt^2} - \frac{dx}{dt} + x = 0$$

For initial conditions  $x(0) = 1$  and  $\dot{x}(0) = 1$ , find the analytical solution and show that the following plot describes how  $x$  changes with time.



20. Consider a semibatch reactor (Example 6.3) with a first-order kinetic parameter of  $k = 1 \text{ hr}^{-1}$ . For a flowrate of 10 liters/hour, a feed concentration of 5 mol/liter, and a feed time of 2 hours, find (and plot) how the concentration changes from 0 to 10 hours.

# AN INTRODUCTION TO LAPLACE TRANSFORMS

# 7

After studying this chapter, the reader should be able to:

- Define the Laplace transform and apply it to several example functions.
- Use Laplace transforms to convert an  $n$ th order ODE to the Laplace domain.
- Manipulate the algebraic equations by performing a partial fraction expansion.
- “Invert” the Laplace domain functions to obtain the time domain solution.
- Use the final value theorem to compute the long-term behavior of a system.

The important sections of this chapter are:

- 7.1 Motivation
- 7.2 Definition of the Laplace Transform
- 7.3 Examples of Laplace Transforms
- 7.4 Final and Initial Value Theorems
- 7.5 Application Examples
- 7.6 Table of Laplace Transforms

## 7.1 MOTIVATION

In this chapter we introduce a mathematical tool, the *Laplace transform*, which is very useful in the analysis of linear dynamic systems. The purpose of the Laplace transform, as used in this textbook, is to convert linear differential equations into algebraic equa-

tions. Algebraic equations are much easier to manipulate than differential equations. An analogy is the use of logarithms to change the operation of multiplication into that of addition. Laplace transforms are useful for solving linear dynamic systems problems, particularly nonhomogeneous (heterogeneous) problems (i.e., where the input to the process system is changed), and are commonly used in process control system design and analysis.

## 7.2 DEFINITION OF THE LAPLACE TRANSFORM

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### Definition: Laplace transform

Consider the time domain function  $f(t)$ . The Laplace transform of  $f(t)$  is represented by  $L[f(t)]$  and is defined as

$$L[f(t)] \equiv F(s) = \int_0^{\infty} f(t) e^{-st} dt \quad (7.1)$$


---

This operation transforms a variable from the time domain to the  $s$  (or Laplace) domain. Note that some texts use an overbar or capital letters for the transformed variable. In this initial development we will let  $f(t)$  represent the time domain function and  $F(s)$  represent the Laplace domain function. Later we may be more relaxed in our notation and let  $f(s)$  represent the Laplace domain function.

The Laplace transform is a linear operation, as shown below.

$$\begin{aligned} L[a_1 f_1(t) + a_2 f_2(t)] &= \int_0^{\infty} [a_1 f_1(t) + a_2 f_2(t)] e^{-st} dt \\ &= \int_0^{\infty} a_1 f_1(t) e^{-st} dt + \int_0^{\infty} a_2 f_2(t) e^{-st} dt \\ &= a_1 \int_0^{\infty} f_1(t) e^{-st} dt + a_2 \int_0^{\infty} f_2(t) e^{-st} dt \end{aligned} \quad (7.2)$$

$$L[a_1 f_1(t) + a_2 f_2(t)] = a_1 L[f_1(t)] + a_2 L[f_2(t)]$$

Equation (7.2) satisfies the definition of a linear operation.

In (7.1) we used  $L[f(t)] \equiv F(s)$  to define the transform of a time domain function. If we wish to transform a Laplace domain (sometimes called the  $s$ -domain) function to the time domain, we use the notion of an inverse transform

$$L^{-1}[F(s)] = f(t)$$

Although not emphasized in this text, Laplace transforms can also be used to solve linear partial differential equations (PDEs).

### 7.3 EXAMPLES OF LAPLACE TRANSFORMS

In this section we develop transforms of some functions that commonly occur in the solution of linear dynamic problems. These functions are: (i) exponential function, (ii) step function, (iii) time-delay, (iv) derivatives, (v) integrals, and (vii) impulse.

#### 7.3.1 Exponential Function

Exponential functions commonly arise in the solutions of linear, constant coefficient, ordinary differential equations:

$$f(t) = e^{-at}$$

A plot of this function is shown in Figure 7.1.

Recall that the transform is defined for  $t > 0$  (we also use the identity that  $e^{x+y} = e^x e^y$ )

$$\begin{aligned} L[e^{-at}] &= \int_0^{\infty} f(t) e^{-st} dt = \int_0^{\infty} e^{-at} e^{-st} dt = \int_0^{\infty} e^{-(s+a)t} dt \\ &= -\frac{1}{s+a} [e^{-(s+a)t}]_0^{\infty} = -\frac{1}{s+a} [0 - 1] = \frac{1}{s+a} \end{aligned}$$

$L[e^{-at}] = \frac{1}{s+a}$ <p style="text-align: right; margin-right: 50px;"><i>Exponential</i></p> $L^{-1}\left[\frac{1}{s+a}\right] = e^{-at}$
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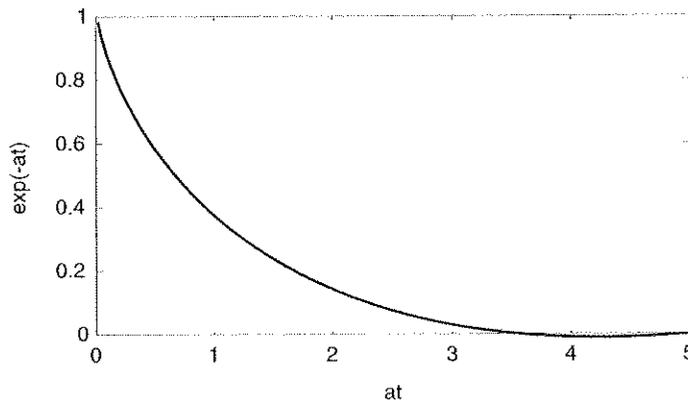


FIGURE 7.1 Exponential function.

Notice that the way we have solved for the limits of integration is only rigorously true for  $a > 0$ . For  $a < 0$  the solution still holds for  $s > -a$ ; we will assume that this condition is always satisfied.

### 7.3.2 Step Function

The step function is used to solve dynamic problems where a sudden change in an input variable occurs (a flowrate could be rapidly changed from one value to another, for example). The step function is defined as 0 before  $t = 0$  and  $A$  after  $t = 0$ , as shown in Figure 7.2.

$$f(t) = \begin{cases} 0 & \text{for } t < 0 \\ A & \text{for } t > 0 \end{cases}$$

We must use the "more precise" definition of the Laplace transform, because of the discontinuity at  $t = 0$ :

$$L[f(t)] = \lim_{\epsilon \rightarrow 0} \int_{\epsilon}^T f(t) e^{-st} dt$$

Since the transform is defined for  $t > 0$ ,

$$L[A] = \int_{0^+}^{\infty} A e^{-st} dt = -\frac{A}{s} [e^{-st}]_0^{\infty} = -\frac{A}{s} [0 - 1] = \frac{A}{s}$$

$L[A] = \frac{A}{s}$ $L^{-1}\left[\frac{A}{s}\right] = A$ <div style="text-align: right; margin-top: 10px;"><i>Step</i></div>
---

Notice that the same expression is used for the Laplace transform of a constant.

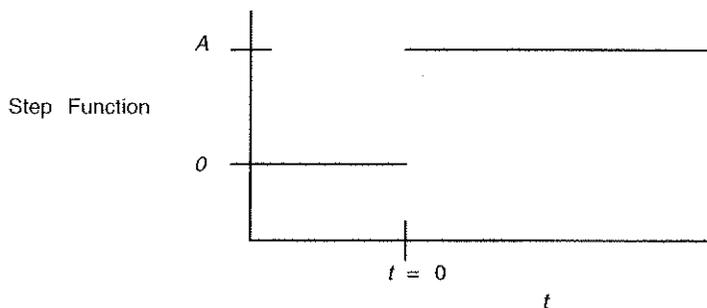


FIGURE 7.2 Step function.

### 7.3.3 Time-Delay (Dead Time)

This is important for systems with transport delays (flow through pipes, etc.), or delays due to measurements. Let  $t_d$  represent the time delay. If the undelayed time domain function is  $f(t)$ , then the delayed function is  $f(t - t_d)$ , as shown in Figure 7.3.

The Laplace transform of the delayed function is:

$$\begin{aligned} L[f(t - t_d)] &= \int_0^{\infty} f(t - t_d) e^{-st} dt = \int_0^{\infty} f(t - t_d) e^{-s(t - t_d + t_d)} dt = \int_0^{\infty} f(t - t_d) e^{-s(t - t_d)} e^{-st_d} dt \\ &= \int_0^{\infty} f(t - t_d) e^{-s(t - t_d)} e^{-st_d} d(t - t_d) = e^{-st_d} \int_0^{\infty} f(t - t_d) e^{-s(t - t_d)} d(t - t_d) \\ &= e^{-st_d} \int_0^{\infty} f(t') e^{-st'} dt' = e^{-st_d} F(s) \end{aligned}$$

Notice that the lower limit of integration did not change with the change of variable, because the function  $f(t)$  is defined as  $f(t) = 0$  for  $t < 0$ .

$L[f(t - t_d)] = e^{-st_d} F(s)$	<i>Time-Delay</i>
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The transform of a delayed function is simply  $e^{-st_d}$  times the transform of the undelayed function.

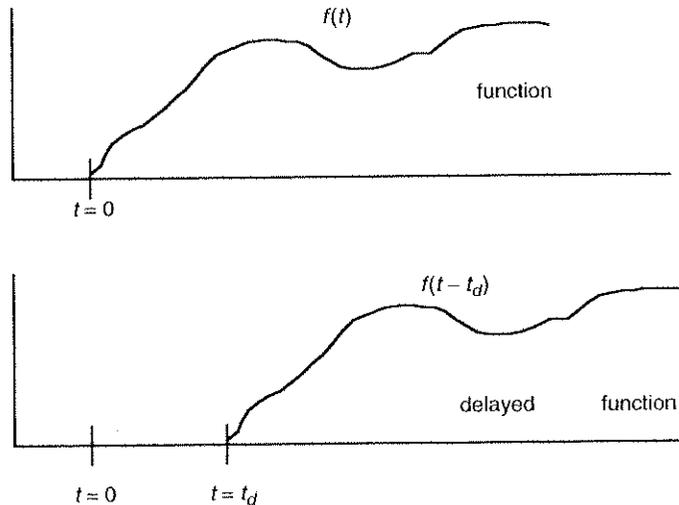


FIGURE 7.3 Delay function.

### 7.3.4 Derivatives

This will be important in transforming the derivative (accumulation) term in a dynamic equation to the Laplace domain.

$$L\left[\frac{df(t)}{dt}\right] = \int_0^{\infty} \frac{df(t)}{dt} e^{-st} dt$$

Using integration by parts ( $\int u dv = uv - \int v du$ )

Let  $u = e^{-st}$  and  $v = f(t)$

$$L\left[\frac{df(t)}{dt}\right] = \int_0^{\infty} \frac{df(t)}{dt} e^{-st} dt = [e^{-st} f(t)]_0^{\infty} + \int_0^{\infty} f(t) s e^{-st} dt$$

$$L\left[\frac{df(t)}{dt}\right] = [0 - f(0)] + s \int_0^{\infty} f(t) e^{-st} dt = sF(s) - f(0)$$

$$L\left[\frac{df(t)}{dt}\right] = sF(s) - f(0)$$

*Derivative*

$$L^{-1}[sF(s) - f(0)] = \frac{df(t)}{dt}$$

Since we often work with deviation variables,  $f(0) = 0$  in many cases.

In general, you should be able to show the following (see student exercise 1):

$$L\left[\frac{d^n f(t)}{dt^n}\right] = s^n F(s) - s^{n-1} f(0) - s^{n-2} f'(0) - \dots - s f^{(n-2)}(0) - f^{(n-1)}(0)$$

*nth Order Derivative*

$n$  initial conditions are needed  $f(0), \dots, f^{(n-1)}(0)$

### 7.3.5 Integrals

This is often used in process control, since many controllers use information about the integral of the error between the desired value (setpoint) and the measured value:

$$L\left[\int_0^t f(t) dt\right] = \int_0^{\infty} \left[\int_0^t f(t) dt\right] e^{-st} dt$$

Again, integrate by parts, using  $u = e^{-st} dt$  and  $v = \int_0^t f(t) dt$ , to find

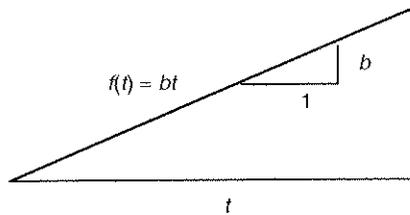


FIGURE 7.4 Ramp function.

$$L \left[ \int_0^t f(t) dt \right] = \frac{1}{s} F(s) \quad \text{Integral}$$

### 7.3.6 Ramp Function

Consider the following ramp function:

$$f(t) = bt$$

as depicted in Figure 7.4.

You should be able to show (see exercise 2) that

$$L[bt] = \frac{b}{s^2}$$

$$L^{-1}[1/s^2] = t \quad \text{Ramp}$$

### 7.3.7 Pulse

Consider the pulse function in Figure 7.5, which consists of a step from 0 to  $A$  at  $t = 0$ , and a step back to 0 at  $t = t_p$ . Find the Laplace transfer function for this pulse.

There are two ways to solve this problem.

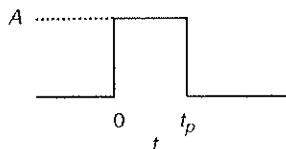


FIGURE 7.5 Pulse function.

ONE METHOD

The pulse function is defined over the following two time intervals:

$$\begin{aligned} f(t) &= A \text{ for } 0 < t < t_p \\ f(t) &= 0 \text{ for } t > t_p \end{aligned}$$

and we can write the Laplace transform as:

$$\begin{aligned} F(s) &= \int_0^{\infty} f(t) e^{-st} dt = \int_0^{t_p} f(t) e^{-st} dt + \int_{t_p}^{\infty} f(t) e^{-st} dt \\ &= \int_0^{t_p} A e^{-st} dt + \int_{t_p}^{\infty} 0 e^{-st} dt = -\frac{A}{s} [e^{-st}]_0^{t_p} \\ F(s) &= -\frac{A}{s} [e^{-t_p s} - 1] = \frac{A}{s} [1 - e^{-t_p s}] \end{aligned}$$

The use of  $A = 1$  is the unit pulse.

$$L[\text{unit pulse of duration } t_p] = \frac{1}{s} [1 - e^{-t_p s}] \quad \text{Unit Pulse}$$

A SECOND METHOD

Consider that the pulse is simply the sum of two step changes, as shown in Figure 7.6.

That is, it is the sum of a positive step change at  $t = 0$  and a negative step change at  $t = t_p$ . Let  $f_1(t)$  represent the step change at  $t = 0$ , and  $f_2(t)$  represent the negative step change at  $t = t_p$ .

$$\begin{aligned} f(t) &= f_1(t) + f_2(t) \\ F(s) &= F_1(s) + F_2(s) = L[f(t)] = L[f_1(t) + f_2(t)] \end{aligned}$$

but notice that  $f_2(t) = -f_1(t - t_p)$



FIGURE 7.6 Pulse function.

and that (from the step function):  $F_1(s) = \frac{A}{s}$

and (from the delay function):  $F_2(s) = e^{-t_p s} (-F_1(s))$   
 $= -e^{-t_p s} \frac{A}{s}$

So we can write  $F(s) = F_1(s) + F_2(s) = \frac{A}{s} [1 - e^{-t_p s}]$

which is consistent with the previous derivation.

### 7.3.8 Unit Impulse

In Figure 7.7, consider the pulse function as the pulse time is decreased, but the pulse area remains the same, as shown by the dashed lines below.

The unit impulse function is a special case of the pulse function, with zero width ( $t_p \rightarrow 0$ ) and unit pulse area (so  $A = 1/t_p$ ). Taking the limit and applying L' Hopital's rule:

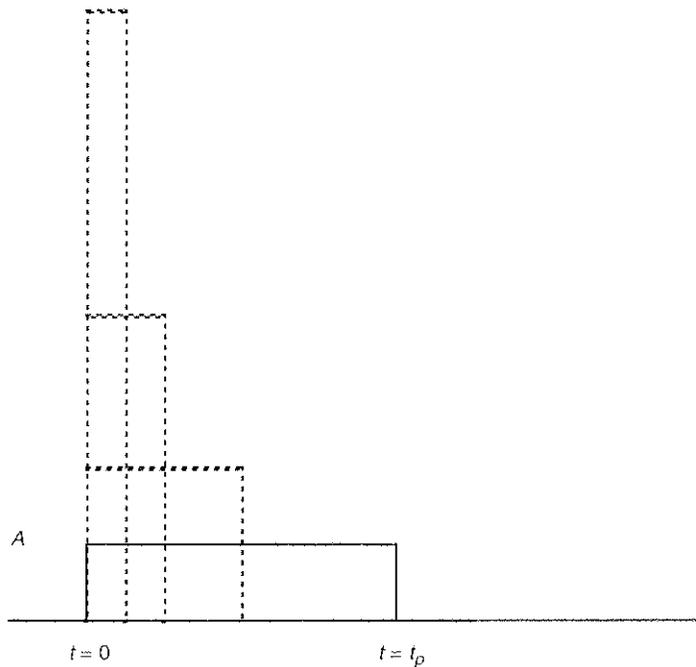


FIGURE 7.7 Impulse function.

$$L[\delta] = \lim_{t_p \rightarrow 0} \frac{1}{t_p s} [1 - e^{-t_p s}] = \lim_{t_p \rightarrow 0} \frac{-1}{s} [-s e^{-t_p s}] = 1$$

$L[\delta] = 1$	<i>Unit Impulse</i>
-----------------	---------------------

### 7.3.9 Review

Thus far we have derived the Laplace transform of a number of functions. For example, we found:

$$L[e^{-at}] = \frac{1}{s + a}$$

If we have a Laplace domain function, such as  $1/(s + a)$ , we can “invert” it to the time domain. For example,

$$L^{-1}\left[\frac{1}{s + a}\right] = e^{-at}$$

Although the student should be able to derive Laplace transforms of any time domain function, that is not our major objective. Our major objective is to use Laplace transforms as a tool to solve dynamic problems. The Laplace transforms of many time-domain functions have been derived and compiled in various tables and handbooks. Already, we can construct a table of eight (exponential, step, time-delay, derivative, integral, ramp, pulse, and impulse) time-domain functions along with their Laplace domain functions. Additional Laplace transforms are provided in Table 7.1 in Section 7.6.

## 7.4 FINAL AND INITIAL VALUE THEOREMS

The following theorems are useful for determining limiting values in dynamics studies. They will be used frequently to find the short-term and long-term behavior. The *long term* (final value) of a time domain function can be found by analyzing the Laplace domain behavior in the limit as the  $s$  variable approaches zero. The initial value of a time domain function can be found by analyzing the Laplace domain behavior in the limit as  $s$  approaches infinity.

### *Final Value Theorem*

$$\lim_{t \rightarrow \infty} f(t) = \lim_{s \rightarrow 0} [s F(s)] \quad (7.3)$$

### *Initial Value Theorem*

$$\lim_{t \rightarrow 0} f(t) = \lim_{s \rightarrow \infty} [s F(s)] \quad (7.4)$$

If we have transformed a time domain function to the  $s$  domain, we can still find out the value of the time domain function as it goes to steady-state ( $t \rightarrow \infty$ ) by finding the value of the Laplace domain function as  $s \rightarrow 0$ . An application of the final and initial value theorems is shown in Example 7.1.

**EXAMPLE 7.1 Application of Final and Initial Value Theorems to the Exponential Function**

Consider the exponential function:

$$f(t) = e^{-at}$$

which had the Laplace transform:

$$F(s) = \frac{1}{s+a}$$

*Final Value Theorem.* We first find:

$$\lim_{s \rightarrow 0} s F(s) = \lim_{s \rightarrow 0} \frac{s}{s+a} = 0$$

which checks with

$$\lim_{t \rightarrow \infty} f(t) = \lim_{t \rightarrow \infty} e^{-at} = 0$$

as long as  $a$  is positive.

*Initial Value Theorem.* We first find

$$\lim_{s \rightarrow \infty} s F(s) = \lim_{s \rightarrow \infty} \frac{s}{s+a} = 1$$

which checks with

$$\lim_{t \rightarrow 0} f(t) = \lim_{t \rightarrow 0} e^{-at} = 1$$

which is satisfied for any finite  $a$ .

One point not often made in textbooks is that the final value theorem only holds for stable systems ( $a > 0$ ).

## 7.5 APPLICATION EXAMPLES

The following is a checklist for solving dynamics problems using Laplace transforms.

- Step 1.** Start with a linear ordinary differential equation and initial conditions.
- Step 2.** Transform each of the time domain functions to the Laplace domain, generally by using a table of Laplace transforms.

**Step 3.** Use algebraic manipulations to solve for the transformed variable. The *partial fraction expansion* approach is particularly useful.

**Step 4.** “Invert” to the time domain, by using a table of Laplace transforms.

### 7.5.1 Partial Fraction Expansion

The partial fraction expansion approach is based on representing a ratio of two polynomials as a sum of simpler terms. Let  $N(s)$  and  $D(s)$  represent numerator and denominator polynomials, respectively.

$$\frac{N(s)}{D(s)} = \frac{C_1}{D_1(s)} + \frac{C_2}{D_2(s)} + \dots + \frac{C_n}{D_n(s)}$$

$C_i$  are constants and  $D_i$  are lower order (typically 1) polynomials.

The four-step procedure is used in each of the following examples. The partial fraction expansion is first used in Example 7.3.

#### EXAMPLE 7.2 Homogeneous First-order Problem

**Step 1.** Consider the simple *homogeneous* (unforced) first-order problem:

$$\frac{dx}{dt} + 2x = 0 \quad (7.5)$$

subject to the initial condition:

$$x(0) = 4 \quad (7.6)$$

**Step 2.** Recall the following transforms:

$$L\left[\frac{dx}{dt}\right] = sX(s) - x(0)$$

$$L[ax] = aL[x] = aX(s)$$

Then we can take the Laplace transform of (7.3) and (7.4) as:

$$\begin{aligned} L\left[\frac{dx}{dt}\right] + 2L[x] &= 0 \\ sX(s) - x(0) + 2X(s) &= 0 \\ sX(s) - 4 + 2X(s) &= 0 \end{aligned} \quad (7.7)$$

**Step 3.** Solving (7.7) for  $X(s)$ :

$$X(s) = \frac{4}{s+2} \quad (7.8)$$

**Step 4.** Inverting each element back to the time domain:

$$L^{-1}[X(s)] = x(t) \quad (7.9)$$

$$L^{-1}\left[\frac{4}{s+2}\right] = 4e^{-2t} \quad (7.10)$$

and the solution is

$$x(t) = 4e^{-2t} \quad (7.11)$$

Indeed, using the method in Example 7.2, we can show that the general first-order equation:

$$\frac{dx}{dt} + ax = 0$$

with initial condition  $x(0)$

has the solution

$$x(t) = x(0)e^{-at}$$

which, of course, is the same solution obtained by separating the variables and integrating. The real power of Laplace transforms is in solving heterogeneous problems, as illustrated in Example 7.3.

### EXAMPLE 7.3 Illustration of the Partial Fraction Expansion Technique

**Step 1.** Consider the simple heterogeneous first-order problem:

$$\frac{dx}{dt} + 2x = 4.5 \quad (7.12)$$

with the initial condition

$$x(0) = 4 \quad (7.13)$$

**Step 2.** Taking the Laplace transform of each element:

$$sX(s) - x(0) + 2X(s) = \frac{4.5}{s}$$

which can be written (since  $x(0) = 4$ ):

$$(s+2)X(s) = 4 + \frac{4.5}{s}$$

**Step 3.** Solving for the transformed variable

$$X(s) = \frac{4}{s+2} + \frac{4.5}{s(s+2)} \quad (7.14)$$

We would like to invert (7.14) to the time domain, however we do not know how to invert the last term  $4.5/s(s+2)$ .

We will use the approach known as a *partial fraction expansion*. That is, write:

$$\frac{4.5}{s(s+2)} = \frac{A}{s} + \frac{B}{s+2} \quad (7.15)$$

to find  $A$ , first multiply (7.15) by  $s$ :

$$\frac{4.5}{s+2} = A + \frac{Bs}{s+2}$$

then set  $s = 0$  and solve for  $A$ :

$$A = 2.25$$

To find  $B$ , first multiply (7.15) by  $s+2$ :

$$\frac{4.5}{s} = \frac{A(s+2)}{s} + B$$

and set  $s = -2$  to solve for  $B$ :

$$B = -2.25$$

which yields:

$$\frac{4.5}{s(s+2)} = \frac{2.25}{s} + \frac{-2.25}{s+2} \quad (7.16)$$

and we can write (7.15) as:

$$X(s) = \frac{4}{s+2} + \frac{2.25}{s} + \frac{-2.25}{s+2} \quad (7.17)$$

**Step 4.** Inverting element by element in (7.17) we find

$$x(t) = 4e^{-2t} + 2.25 + -2.25e^{-2t}$$

or

$$x(t) = 1.75e^{-2t} + 2.25 \quad (7.18)$$

the reader should verify that this solution satisfies the initial conditions and the differential equation.

Examples 7.4 and 7.5 provide additional illustration of the partial fraction expansion technique.

**EXAMPLE 7.4** Find the Inverse Laplace Transform of  $1/(s+a)(s+b)$

Write 
$$\frac{1}{(s+a)(s+b)} = \frac{A}{s+a} + \frac{B}{s+b} \quad (7.19)$$

Multiply (7.19) by  $s+a$ , set  $s = -a$  to find:

$$A = \frac{1}{-a + b}$$

Multiply (7.19) by  $s + b$ , set  $s = -b$  to find:

$$B = \frac{1}{a - b}$$

Therefore, 
$$\frac{1}{(s + a)(s + b)} = \left[ \frac{1}{b - a} \right] \left[ \frac{1}{s + a} \right] + \left[ \frac{1}{a - b} \right] \left[ \frac{1}{s + b} \right] \quad (7.20)$$

and we can take the inverse Laplace transform of each function on the righthand side of (7.20)

$$L^{-1} \left[ \frac{1}{(s + a)(s + b)} \right] = \left[ \frac{1}{b - a} \right] e^{-as} + \left[ \frac{1}{a - b} \right] e^{-bs} \quad (7.21)$$

Notice that this technique fails if  $a = b$ .

The method in the previous example failed if the roots of the Laplace domain function were equal. The following example shows how to perform a partial fraction expansion for *repeated roots*.

**EXAMPLE 7.5** Consider the Following Transfer Function with *Repeated Roots*

$$\frac{1}{(s + a)^2(s + b)} \quad (7.22)$$

Expand (7.22) in the following fashion:

$$\frac{1}{(s + a)^2(s + b)} = \frac{A}{s + a} + \frac{B}{(s + a)^2} + \frac{C}{s + b} \quad (7.23)$$

Here we cannot multiply by  $s + a$  and set  $s = -a$ , because we would find unbounded terms. First, multiply (7.23) by  $(s + a)^2$ :

$$\frac{1}{s + b} = A(s + a) + B + \frac{C(s + a)^2}{s + b}$$

and set  $s = -a$  to find

$$B = \frac{1}{b - a}$$

Multiply (7.23) by  $s + b$  and set  $s = -b$  to find

$$C = \frac{1}{(a - b)^2}$$

Notice that we have solved for two of the coefficients of (7.23). Now, we can solve for one equation in one unknown, by setting  $s = \text{any value}$ . For simplicity, choose  $s = 0$ . From (7.23):

$$\frac{1}{a^2b} = \frac{A}{a} + \frac{1}{(b-a)a^2} + \frac{1}{(a-b)^2b}$$

we can reduce the solution for  $A$  to  $A = \frac{-1}{(a-b)^2}$

We have solved for  $A$ ,  $B$ , and  $C$  in (7.23), so we can perform an element-by-element inversion of (7.23) to find the time domain function:

$$L^{-1} \left[ \frac{\left[ \frac{-1}{(a-b)^2} \right]}{(s+a)} + \frac{\left[ \frac{1}{(b-a)} \right]}{(s+a)^2} + \frac{\left[ \frac{1}{(a-b)^2} \right]}{(s+b)} \right] = \frac{-1}{(a-b)^2} e^{-at} + \frac{1}{b-a} t e^{-at} + \frac{1}{(a-b)^2} e^{-bt}$$

and we can write:

$$L^{-1} \left[ \frac{1}{(s+a)^2(s+b)} \right] = \frac{-1}{(a-b)^2} e^{-at} + \frac{1}{b-a} t e^{-at} + \frac{1}{(a-b)^2} e^{-bt} \quad (7.24)$$

As an alternative, we can find a common denominator for the righthand side of (7.23) and write:

$$\frac{1}{(s+a)^2(s+b)} = \frac{A(s+a)(s+b) + B(s+b) + C(s+a)^2}{(s+a)^2(s+b)} \quad (7.25)$$

then expand the numerator and solve for the coefficients  $A$ ,  $B$ , and  $C$  such that the righthand side is equal to the lefthand side. See student exercise 13.

The previous examples were for ODEs with real roots. This next example is a problem with complex roots.

#### EXAMPLE 7.6 A Second-order System with Complex Roots

**Step 1.** Consider the homogeneous problem:

$$\frac{d^2x}{dt^2} + \frac{dx}{dt} + x = 0 \quad (7.26)$$

with the initial conditions:

$$\dot{x}(0) = x(0) = 1 \quad (7.27)$$

**Step 2.** From the table of Laplace transforms:

$$L \left[ \frac{d^n x}{dt^n} \right] = s^n X(s) - s^{n-1} x(0) - s^{n-2} \dot{x}(0) - \dots - s x^{(n-2)}(0) - x^{(n-1)}(0)$$

So, for a second derivative:

$$L\left[\frac{d^2x}{dt^2}\right] = s^2 X(s) - s x(0) - \dot{x}(0)$$

and, for a first derivative:

$$L\left[\frac{dx}{dt}\right] = s X(s) - x(0)$$

We can now write the Laplace transform of (7.26) as:

$$s^2 X(s) - s x(0) - \dot{x}(0) + s X(s) - x(0) + X(s) = 0$$

**Step 3.** Attempting to isolate  $X(s)$  on the LHS:

$$(s^2 + s + 1) X(s) = s x(0) + x(0) + \dot{x}(0)$$

dividing by  $(s^2 + s + 1)$ :

$$X(s) = \frac{s x(0)}{s^2 + s + 1} + \frac{x(0) + \dot{x}(0)}{s^2 + s + 1}$$

and from the initial conditions:

$$X(s) = \frac{s}{s^2 + s + 1} + \frac{2}{s^2 + s + 1} \quad (7.28)$$

the roots of  $(s^2 + s + 1)$  are  $-1/2 \pm \sqrt{3}/2 j$  (from the quadratic formula):

$$(s^2 + s + 1) = \left(s + \frac{1}{2} + \frac{\sqrt{3}}{2} j\right) \left(s + \frac{1}{2} - \frac{\sqrt{3}}{2} j\right)$$

Notice another way that we can write  $(s^2 + s + 1)$  is:

$$(s^2 + s + 1) = \left(s + \frac{1}{2}\right)^2 + \left(\frac{\sqrt{3}}{2}\right)^2$$

which means that we can write (7.28) as:

$$X(s) = \frac{s}{\left(s + \frac{1}{2}\right)^2 + \left(\frac{\sqrt{3}}{2}\right)^2} + \frac{2}{\left(s + \frac{1}{2}\right)^2 + \left(\frac{\sqrt{3}}{2}\right)^2}$$

**Step 4.** Notice from a table of Laplace transforms that:

$$L[e^{-bt} \sin \omega t] = \frac{\omega}{(s + b)^2 + \omega^2} \quad (7.29)$$

$$L[e^{-bt} \cos \omega t] = \frac{s + b}{(s + b)^2 + \omega^2} \quad (7.30)$$

and we should maneuver (7.28) into the form of (7.29) and (7.30).

Notice that we can write (7.30) as:

$$X(s) = \frac{s + \frac{1}{2}}{\left(s + \frac{1}{2}\right)^2 + \left(\frac{\sqrt{3}}{2}\right)^2} + \frac{1.5}{\left(s + \frac{1}{2}\right)^2 + \left(\frac{\sqrt{3}}{2}\right)^2} \quad (7.31)$$

and we invert each element of the RHS of (7.31), using (7.29) and (7.30):

$$x(t) = e^{-t/2} \cos \frac{\sqrt{3}}{2} t + \frac{1.5}{\frac{\sqrt{3}}{2}} e^{-t/2} \sin \frac{\sqrt{3}}{2} t$$

$$x(t) = e^{-t/2} \cos \frac{\sqrt{3}}{2} t + \sqrt{3} e^{-t/2} \sin \frac{\sqrt{3}}{2} t$$

which has the time domain response shown in Figure 7.8. As we noticed in Chapter 6, complex roots give oscillatory responses. We see in Chapter 9 that this type of response is called under-damped.

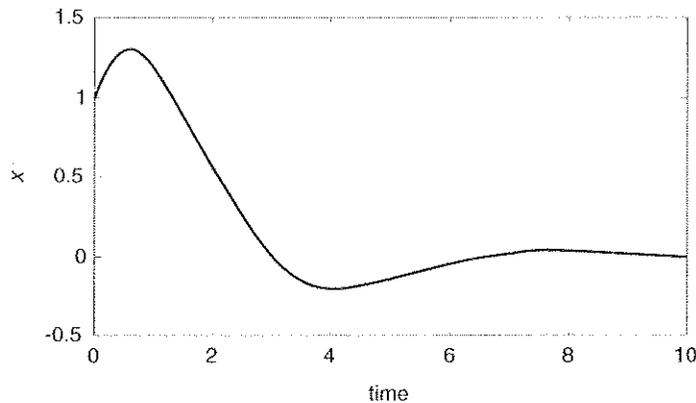


FIGURE 7.8 Oscillatory response due to complex roots.

## 7.6 TABLE OF LAPLACE TRANSFORMS

For your convenience, selected Laplace transforms are presented in Table 7.1. If you desire to transform a function from the time domain to the Laplace domain, then look for the time domain function in the first column ( $f(t)$ ) and write down the corresponding Laplace domain function in the second column ( $F(s)$ ). Similarly, if you are trying to “invert” a Laplace domain function to the time domain, then look for the Laplace domain function in the second column and write down the corresponding time domain function from the first column.

TABLE 7.1 Laplace Transforms for Selected Time-Domain Functions

$f(t)$	$F(s)$
$\delta(t)$ (unit impulse)	1
$S(t)$ (unit step) $\begin{cases} 0 & \text{for } t < 0 \\ 1 & \text{for } t > 0 \end{cases}$	$\frac{1}{s}$
$A$ (constant)	$A/s$
$f(t-\theta)$ (time delay)	$e^{-\theta s} F(s)$
$t$ (ramp)	$\frac{1}{s^2}$
$t^{n-1}$	$\frac{(n-1)!}{s^n}$
$\frac{df}{dt}$ (derivative)	$sF(s) - f(0)$
$\frac{d^n f}{dt^n}$	$s^n F(s) - s^{n-1}f(0) - s^{n-2}f'(0) - \dots - sf^{(n-2)}(0) - f^{(n-1)}(0)$
$e^{-at}$	$\frac{1}{s+a}$
$\frac{1}{a_1 - a_2} (e^{-a_2 t} - e^{-a_1 t})$	$\frac{1}{(s+a_1)(s+a_2)}$
$\frac{a_3 - a_1}{a_2 - a_1} e^{-a_1 t} + \frac{a_3 - a_2}{a_1 - a_2} e^{-a_2 t}$	$\frac{s+a_3}{(s+a_1)(s+a_2)}$
$1 - e^{-t/\tau}$	$\frac{1}{s(\tau s + 1)}$
$\sin \omega t$	$\frac{\omega}{s^2 + \omega^2}$
$\cos \omega t$	$\frac{s}{s^2 + \omega^2}$
$e^{-at} \sin \omega t$	$\frac{\omega}{(s+a)^2 + \omega^2}$
$e^{-at} \cos \omega t$	$\frac{s+a}{(s+a)^2 + \omega^2}$
$1 + \frac{1}{\tau_2 - \tau_1} (\tau_1 e^{-t/\tau_1} - \tau_2 e^{-t/\tau_2})$	$\frac{1}{s(\tau_1 s + 1)(\tau_2 s + 1)}$
$\left(1 - \frac{1}{\sqrt{1-\xi^2}} e^{-\xi t/\tau} \sin(\omega t + \Phi)\right)$	$\frac{1}{s(\tau^2 s^2 + 2\xi\tau s + 1)}$
where $\omega = \frac{\sqrt{1-\xi^2}}{\tau}$ , $\Phi = \tan^{-1} \frac{\sqrt{1-\xi^2}}{\xi}$	
$1 + \frac{\tau_3 - \tau_1}{\tau_1 - \tau_2} e^{-t/\tau_1} + \frac{\tau_3 - \tau_2}{\tau_2 - \tau_1} e^{-t/\tau_2}$	$\frac{(\tau_3 s + 1)}{s(\tau_1 s + 1)(\tau_2 s + 1)}$
$1 - \left(1 - \frac{\tau_n}{\tau_d}\right) e^{-t/\tau_d}$	$\frac{\tau_n s + 1}{s(\tau_d s + 1)}$

## SUMMARY

We have defined the Laplace transform and applied it to several functions that commonly appear in the solution of chemical process dynamics problems. Although the Laplace transform concept seems quite abstract at this point, in the chapters that follow you will find it extremely useful in solving differential equation models. The final (7.3) and initial value (7.4) theorems will be useful for checking the long-term (steady-state) behavior and the initial conditions for a particular problem.

A number of examples were provided to illustrate the power of the Laplace transform technique for solving ordinary differential equations. We noted that the technique allows us to convert the ODE problem to an algebraic problem, which is easier for us to solve. After performing algebraic manipulations in the Laplace domain, often with the use of a partial fraction expansion, we then look up inverse transforms to obtain the time domain solution.

In the chapters that follow, we use Laplace transforms to analyze the dynamic behavior of different types of linear process models.

## FURTHER READING

Many differential equations and process control textbooks provide details on Laplace transforms. Some examples are:

Boyce, W., & R. DiPrima. (1992). *Ordinary Differential Equations and Boundary Value Problems*, 5th ed. New York: Wiley.

Luyben, W.L. (1990). *Process Modeling, Simulation and Control for Chemical Engineers*, 2nd ed. New York: McGraw-Hill.

Seborg, D.E., T.F. Edgar, & D.A. Mellichamp. (1989). *Process Dynamics and Control*. New York: Wiley.

Stephanopoulos, G. (1984). *Chemical Process Control: An Introduction to Theory and Practice*. Englewood Cliffs, NJ: Prentice Hall.

## STUDENT EXERCISES

1-5. The student should derive the Laplace transform for the following functions:

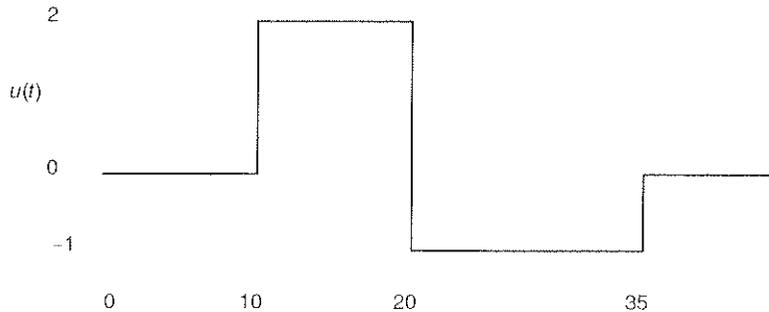
1.  $\frac{d^n f}{dt^n}$
2.  $f(t) = bt$
3.  $f(t) = t^2$

4.  $L \left[ \int_0^t f(t) dt \right]$

5.  $f(t) = \cos \omega t$

(Hint: Although you can solve question 5 using integration by parts, you may wish to use the Euler identity  $\cos \omega t = 1/2 (e^{j\omega t} + e^{-j\omega t})$ .)

6. Find the Laplace transform,  $u(s)$ , of the following input function:



7. Find the Laplace transform of the function  $y(t)$  that satisfies the differential equation and initial conditions:

$$\frac{d^3 y}{dt^3} + 4 \frac{d^2 y}{dt^2} + 5 \frac{dy}{dt} + 2y = 2$$

$$y(0) = \frac{dy(0)}{dt} = \frac{d^2 y(0)}{dt^2} = 0$$

8. Solve the differential equation:

$$\frac{dy}{dt} + 3y = 0$$

$$y(0) = 2.0$$

9. A process input has the following Laplace transform:

$$u(s) = \frac{2}{s^3} - \frac{6}{s^2} e^{-\lambda s}$$

What is the time domain input,  $u(t)$ ? Find this analytically.

Sketch the time domain input.

10. Find the time domain solution  $y(t)$  for the Laplace domain transfer function (with  $\xi < 1$ ):

$$Y(s) = \frac{1}{s(\tau^2 s^2 + 2\xi\tau s + 1)}$$

11. Derive the time domain solution  $y(t)$  for the Laplace domain transfer function:

$$Y(s) = \frac{(\tau_1 s + 1)}{s(\tau_1 s + 1)(\tau_2 s + 1)}$$

12. Derive the time domain solution  $y(t)$ , for the Laplace domain transfer function:

$$Y(s) = \frac{\tau_2 s + 1}{s(\tau_2 s + 1)}$$

13. Consider Example 7.5, involving the following transfer function with *repeated roots*:

$$\frac{1}{(s + a)^2(s + b)} = \frac{A}{s + a} + \frac{B}{(s + a)^2} + \frac{C}{s + b}$$

Find a common denominator for the righthand side:

$$\frac{1}{(s + a)^2(s + b)} = \frac{A(s + a)(s + b) + B(s + b) + C(s + a)^2}{(s + a)^2(s + b)}$$

then expand the numerator and solve for the coefficients  $A$ ,  $B$ , and  $C$  such that the righthand side is equal to the lefthand side.

# TRANSFER FUNCTION ANALYSIS OF FIRST-ORDER SYSTEMS

After studying this chapter, the reader should understand:

- The responses of first-order systems to step and impulse inputs.
- How chemical reactions change the time constant of a stirred tank.
- The behavior of an integrating process.
- How to compare the long-term behavior of a nonlinear process with that of a linear process without integrating the nonlinear modeling equations.
- The responses of first-order + time-delay models.
- How to estimate the parameters of first-order and first-order + time-delay transfer functions by applying step input changes.
- The response of a lead/lag model to a step input.

The important sections in this chapter are:

- 8.1 Perspective
- 8.2 Responses of First-Order Systems
- 8.3 Examples of Self-Regulating Processes
- 8.4 Integrating Processes
- 8.5 Lead-Lag Models

## 8.1 PERSPECTIVE

One of the powers of the Laplace transform technique is the ease with which it handles heterogeneous (forced input) problems. It is most useful when the models are separate from the type of input imposed (step, ramp, etc.). The models that are developed are called *transfer function* models and will be used frequently in control system design.

Process engineers often learn much about the behavior of a process by changing the inputs and seeing how the outputs respond. The goal of this chapter is to illustrate the typical responses of first-order models to step changes in inputs. Knowledge of these types of responses will allow an engineer to determine a good approximate model for the process, including the best parameter values, based on measured data from the process.

## 8.2 RESPONSES OF FIRST-ORDER SYSTEMS

The equation for a linear first-order process is generally written in the following form

$$\tau \frac{dy}{dt} + y = k u \quad (8.1)$$

where the parameters ( $\tau$  and  $k$ ) and variables ( $y$  and  $u$ ) have the following names:

- $\tau$  = time constant (units of time)
- $k$  = process gain (units of output/input)
- $y$  = output variable
- $u$  = input variable

The model (8.1) is sometimes derived by linearizing a nonlinear model about a given steady-state and then placing the resulting linear model in deviation variable form. For this reason, we assume that the initial conditions are  $y(0) = 0$  and  $u(0) = 0$ . The input,  $u$  and the output  $y$  are functions of time;  $u(t)$  must be specified to solve for  $y(t)$ .

In the next example, we show how a standard first-order process model arises.

### EXAMPLE 8.1 A mixing tank

Assume that a chemical compound,  $A$ , is in a feedstream entering a mixing tank. Assume that there is no reaction, and that the concentration of  $A$  has no effect on the density of the fluid (this is true for trace components in water, for example). Also assume that the flowrate is constant and the volume in the tank is constant—this implies that the outlet flowrate is equal to the inlet flowrate, as shown in Figure 8.1. The process is operating at steady-state, then the inlet concentration is suddenly changed to a new value. Find the tank outlet concentration as a function of time.

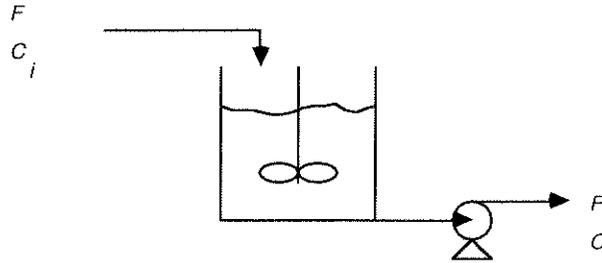


FIGURE 8.1 Mixing tank.

### Overall Material Balance

$$\frac{dV}{dt} = F - F = 0 \quad (\text{from problem statement})$$

### Component Material Balance

$$\frac{dVC}{dt} = FC_i - FC$$

since  $V$  is constant:

$$\frac{dC}{dt} = \frac{F}{V}C_i - \frac{F}{V}C \quad (8.2)$$

First of all, we can solve for the initial steady-state concentration. At steady-state,  $dC/dt = 0$ , so from (8.2) we find:

$$C_s = C_{is}$$

where  $C_s$  is the steady-state tank outlet concentration and  $C_{is}$  is the steady-state tank inlet concentration. Now, since  $-FV C_{is} + FV C_s = 0$ , we can add this to (8.2). Also, since  $C_s$  is a constant,  $dC/dt = d(C - C_s)/dt$ , and we can write:

$$\frac{d(C - C_s)}{dt} = \frac{F}{V}(C_i - C_{is}) - \frac{F}{V}(C - C_s) \quad (8.3)$$

or

$$\frac{V}{F} \frac{d(C - C_s)}{dt} + (C - C_s) = (C_i - C_{is}) \quad (8.4)$$

Equation (8.4) is identical to the first-order equation:

$$\tau \frac{dy}{dt} + y = k u \quad (8.1)$$

with  $\tau = VF$ ,  $k = 1$ ,  $y = C - C_s$ ,  $u = C_i - C_{is}$

Notice that the time constant in this case is simply the residence time of the tank, that is, the average amount of time that a molecule stays in the tank.

Notice that for linear systems, we can directly write the deviation variable model directly from the physical model, skipping several intermediate steps. Also, since deviation variables are defined on the basis of a steady-state operating condition, if the process is initially at steady-state, then  $y(0) = 0$  and  $u(0) = 0$ .

Taking the Laplace transform of (8.1) we find:

$$\begin{aligned}\tau [s Y(s) - y(0)] + Y(s) &= k U(s) \\ \tau s Y(s) + Y(s) &= k U(s) \\ (\tau s + 1) Y(s) &= k U(s)\end{aligned}\quad (8.5)$$

which is most commonly written:

$$Y(s) = \frac{k}{\tau s + 1} U(s) \quad (8.6)$$

or,

$$Y(s) = g(s) U(s) \quad (8.7)$$

where:

$$g(s) = \frac{k}{\tau s + 1} \quad (8.8)$$

The reader should become familiar with this type of representation. In general terms,  $g(s)$  is known as a *transfer function*. In this specific case,  $g(s)$  is a first-order transfer function. You will often see a *block diagram* representation of (8.7) as shown in Figure 8.2

One nice thing about (8.6) is that it holds for any first-order process (with zero initial conditions)—we have not had to use any knowledge (yet) about the input  $u$  as a function of time. Once we know  $u(t)$ , we can use Laplace transforms to find  $U(s)$  to solve the problem. We will see later that block diagrams and transfer functions are easy to work with, when we have a complex system that is composed of a number of subsystems. Before we deal with such systems, we will first understand the behavior of first-order systems to different types of inputs.

### 8.2.1 Step Inputs

The most common input forcing function is the step input. For this problem, assume a step input of magnitude  $\Delta U$  at time  $t = 0$ . We know that the Laplace transform of a step input is (from Chapter 7):

$$L[\Delta U] = \frac{\Delta U}{s} \quad (8.9)$$

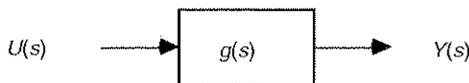
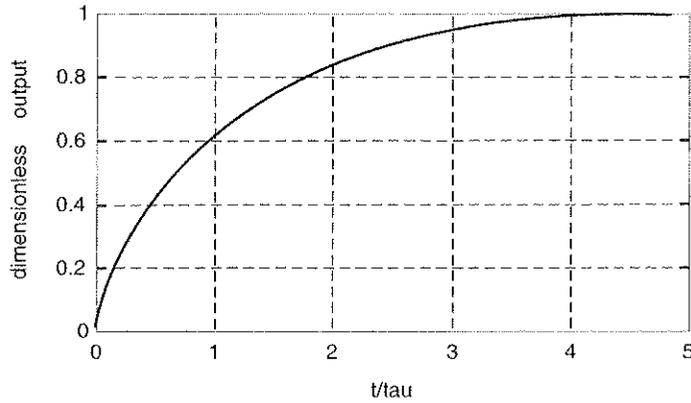


FIGURE 8.2 Block diagram.



**FIGURE 8.3** Dimensionless output step response of a first-order process.

and we can then write (8.6) as:

$$Y(s) = \frac{k \Delta U}{\tau s + 1} \frac{1}{s} \quad (8.10)$$

$$Y(s) = \frac{k \Delta U}{s(\tau s + 1)} \quad (8.11)$$

From the table of Laplace transforms in Chapter 7 (the reader should be able to derive this result, using a partial fraction expansion):

$$L^{-1} \left[ \frac{1}{s(\tau s + 1)} \right] = 1 - e^{-t/\tau} \quad (8.12)$$

and the solution to (8.11) is then:

$$y(t) = k \Delta U [1 - e^{-t/\tau}] \quad (8.13)$$

Notice that we can represent the solution of (8.13) with a single plot, by dividing (8.13) by  $k \Delta U$  to obtain the dimensionless output:

$$\frac{y(t)}{k \Delta U} = [1 - e^{-t/\tau}] \quad (8.14)$$

A plot of (8.14) is shown in Figure 8.3, where we have used  $t/\tau$  as a dimensionless time.

#### **EXAMPLE 8.1** Continued

As a numerical example, consider the case where  $V = 5 \text{ ft}^3$ ,  $F = 1 \text{ ft}^3/\text{min}$ , and the steady-state concentration (inlet and outlet) is  $1.25 \text{ lbmol}/\text{ft}^3$ . Consider a step change in inlet concentration from  $1.25 \text{ lbmol}/\text{ft}^3$  to  $1.75 \text{ lbmol}/\text{ft}^3$ . Then:

$$\begin{aligned}
 U(s) &= \frac{\Delta U}{s} = \frac{0.5}{s} & (\Delta u(t) = 1.75 - 1.25 = 0.5 \text{ lbmol/ft}^3) \\
 Y(s) &= \frac{1}{5s + 1} \frac{0.5}{s}
 \end{aligned}
 \tag{8.15}$$

which has the time domain solution:

$$y(t) = 0.5 [1 - e^{-t/5}] \tag{8.16}$$

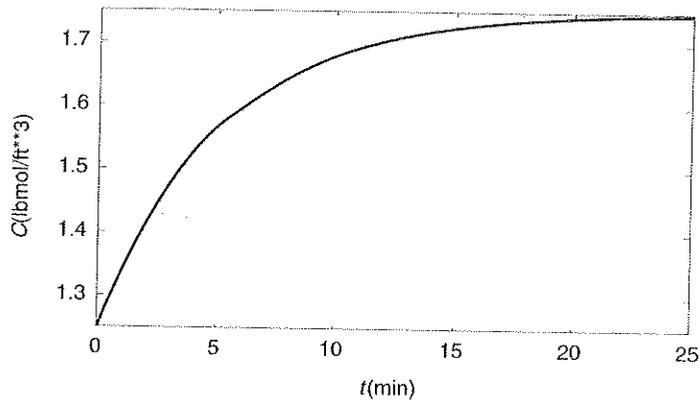
Since we desire to find the actual concentration, we can convert back to the physical variables, from the relationship:

$$y = C - C_s \Rightarrow C(t) = C_s + y(t) \tag{8.17}$$

and (8.17) can be written:

$$C(t) = 1.25 + 0.5 [1 - e^{-t/5}] \text{ lbmol/ft}^3 \tag{8.18}$$

Notice that  $C(t \rightarrow \infty) = 1.75$ , as expected. This can also be obtained by applying the Final Value Theorem to (8.16) and using (8.18). A plot of (8.18) is shown in Figure 8.4.



**FIGURE 8.4** Transient response of mixing tank.

### PARAMETER ESTIMATION FOR FIRST-ORDER PROCESSES

Returning to the general model for a first-order process, we see that there are two parameters of interest: the process gain and the process time constant.

$$y(t) = k\Delta U [1 - e^{-t/\tau}] \tag{8.13}$$

Process engineers often find process gains and time constants by performing step tests on processes.

### GAIN ESTIMATION

We see from (8.14) that after  $t \gg \tau$ , the  $e^{-t/\tau}$  term approaches 0. The value of  $k$  can be determined:

$$k = \frac{y(t) \text{ as } t \rightarrow (\text{large})}{\Delta U} = \frac{\Delta Y}{\Delta U} \quad (8.19)$$

that is, the process gain is the change in output (as it approaches a new steady-state) divided by the change in input.

### TIME CONSTANT ESTIMATION

We can find the time constant for a first-order process in the following fashion. Apply a step input to the process at  $t = 0$ . From (8.14), we see that  $y(t)$  goes to a value of  $k\Delta U$  as  $t \rightarrow \infty$ . When the time is equal to the time constant ( $t = \tau$ ), from (8.13):

$$y(t) = k\Delta U [1 - e^{-1}] = 0.632 k\Delta U$$

that is, the time constant can be determined by finding the time where the output,  $y(t)$ , is at 63.2% of the ultimate response (new steady-state). This rule is also obvious by looking at Figure 8.3: when  $t/\tau = 1$ ,  $y(t)/k\Delta U = 0.632$ .

---

You should be careful, because this is only true for first-order processes with no time-delay and a step input at  $t = 0$ . If the process is second-order or the input is not a step change, etc., this 63.2% value will not be correct.

---

*You should get in the habit of associating units with all of the variables.* Obviously, the process time constant,  $\tau$ , must have units of time because  $e^{-t/\tau}$  must be dimensionless. Also, the process gain,  $k$ , must have units of output/input to be dimensionally consistent.

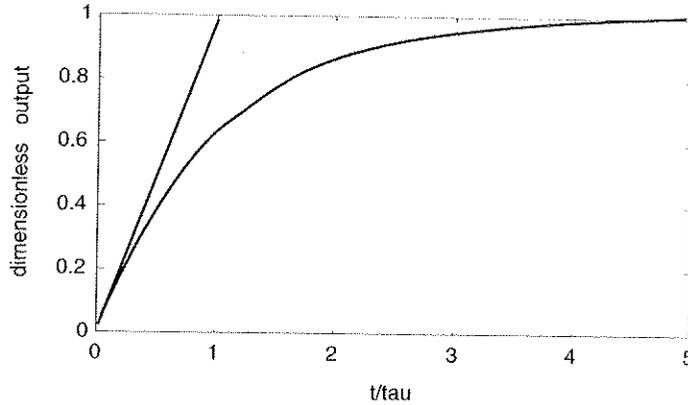
### SLOPE METHOD

An alternative method of estimating the time constant is to realize that the initial slope of the output step response for a first-order process is  $k\Delta U/\tau$ , as shown below. Taking the derivative of (8.13):

$$\frac{dy(t)}{dt} = \frac{k\Delta U}{\tau} [e^{-t/\tau}]$$

and evaluating at  $t = 0$ , we find

$$\left. \frac{dy(t)}{dt} \right|_{t=0} = \frac{k\Delta U}{\tau}$$



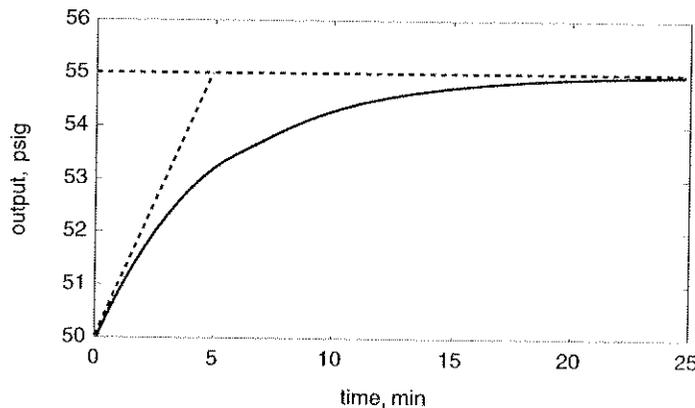
**FIGURE 8.5** Slope method for time constant estimation (dimensionless output =  $y/k\Delta u$ ).

If we extrapolate this slope to the final value of the output that is achieved, we find the time constant  $\tau$ , as shown in Figure 8.5. This is a dimensionless plot, so the intersection at  $t/\tau = 1$  indicates an intersection at  $t = \tau$  in physical time.

Parameter estimation for first-order processes using a step response is illustrated by the next example.

**EXAMPLE 8.2 Parameter Estimation of a First-Order Process**

A process operator makes a step change in an input from 20 to 17.5 gal/min (gpm) and finds that the output eventually changes from an initial value of 50 psig to 55 psig, as shown in Figure 8.6 below. Find the process gain and time constant for this system.



**FIGURE 8.6** Slope method for time constant estimation.

We can immediately calculate the process gain from  $k = \Delta y / \Delta u = 55 - 50 \text{ psig} / 17.5 - 20 \text{ gpm} = -2 \text{ psig/gpm}$ . We can calculate the time constant in a number of different ways. One way is to find the time where the output change is 63.2% of the final change. This occurs when the output is  $50 + 0.632(5) = 53.2 \text{ psig}$ . From the plot, this occurs at  $t = 5$  minutes. Another way to find the time constant is to extrapolate the initial slope of the response to the final value. This occurs at  $t = 5$  minutes, as shown. The identified process transfer function is then:

$$g(s) = \frac{-2}{5s + 1}$$

Notice that the gain ( $-2 \text{ psig/gpm}$ ) and time constant ( $5 \text{ min}$ ) have units associated with them.

### 8.2.2 Impulse Inputs

Consider a first-order process with an impulse input of magnitude  $A$ . The transform of a unit impulse ( $\delta$ ) is 1, so  $L[A\delta] = A$ . The first order Laplace domain response is:

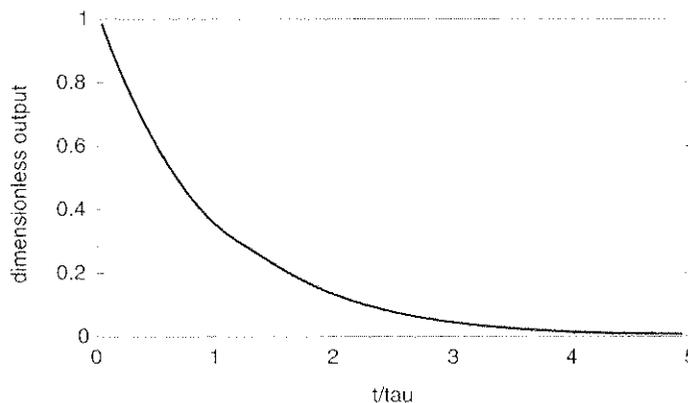
$$Y(s) = \frac{k}{\tau s + 1} \cdot U(s) = \frac{kA}{\tau s + 1} \quad (8.20)$$

the time domain response is:

$$y(t) = kA e^{-t/\tau} \quad (8.21)$$

Dividing by  $kA$ , we find the dimensionless output response shown in the Figure 8.7 below. The prime characteristic of a first-order system is that there is an immediate response to an impulse input.

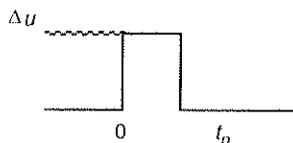
In practice it is difficult to actually implement an impulse function. A close approximation can be made by implementing a pulse input over a short period of time, as shown in the next example.



**FIGURE 8.7** Impulse Response for a first-order process. The dimensionless output is  $y(t)/kA$ .

**EXAMPLE 8.3 Comparison of Impulse and Pulse Inputs**

In the previous example an impulse of magnitude  $A$  was applied to the process. Consider a pulse input, where an input value of  $\Delta u$  is applied for  $t_p$  units of time, as shown in Figure 8.8. The total applied input is then  $A = \Delta u t_p$ .


**FIGURE 8.8** Pulse input.

From Chapter 7 we find that:

$$U(s) = \frac{\Delta u}{s} [1 - e^{-t_p s}]$$

So, the output for a first-order process with unit gain, is:

$$Y(s) = \frac{\Delta u}{s} [1 - e^{-t_p s}] \frac{1}{\tau s + 1}$$

$$Y(s) = \frac{\Delta u}{s(\tau s + 1)} - \frac{\Delta u e^{-t_p s}}{s(\tau s + 1)}$$

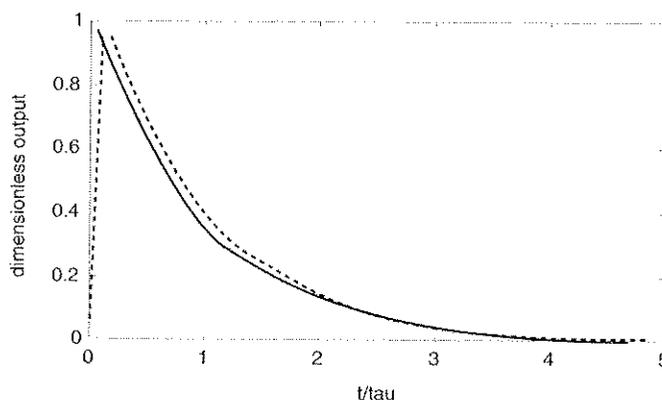
which has the time-domain solution (Chapter 7):

$$y(t) = \Delta u [1 - e^{-t/\tau}] - \Delta u [1 - e^{-(t-t_p)/\tau}] H(t - t_p) \quad (8.22)$$

where  $H(t) = 0$  for  $t < t_p$  and 1 for  $t \geq t_p$ , and the total input applied over the  $t_p$  time units is  $\Delta u t_p$ . The impulse response is:

$$y(t) = kA e^{-t/\tau} = k \Delta u t_p e^{-t/\tau} \quad (\text{impulse}) \quad (8.23)$$

The pulse and impulse responses are compared in Figure 8.9 for  $t_p = 0.1\tau$  and  $A = 1$ .


**FIGURE 8.9** Comparison of pulse (dashed,  $t_p = 0.1\tau$ ) and impulse (solid) responses.

### 8.3 EXAMPLES OF SELF-REGULATING PROCESSES

The standard first-order model presented in the previous section is a typical self-regulating process. If the input is changed to another value, the output eventually comes to a new steady-state. Contrast this with non-self-regulating systems where the output continues to change forever after a step input change. Self-regulating behavior is shown by the systems presented in the following example. One key idea to note is that a chemical reaction changes the time constant of a standard mixing tank model.

#### EXAMPLE 8.4 A CSTR with a First-Order Reaction

Now, extend the Example 8.1 to include a single decomposition reaction. The component material balance is:

$$\frac{dVC}{dt} = FC_i - FC - k_1 VC \quad (8.24)$$

where  $k_1$  is the reaction rate constant. Since  $V$  is constant:

$$\frac{dC}{dt} = -\left(\frac{F}{V} + k_1\right)C + \frac{F}{V}C_i \quad (8.25)$$

and we can calculate the steady-state concentrations from  $dC/dt = 0$

$$C_s = \frac{\frac{F}{V}C_{i0}}{\frac{F}{V} + k_1}$$

The deviation variable form of our dynamic model is

$$\frac{d(C - C_s)}{dt} = -\left(\frac{F}{V} + k_1\right)(C - C_s) + \frac{F}{V}(C_i - C_{i0}) \quad (8.26)$$

or

$$\left[ \frac{1}{\frac{F}{V} + k_1} \right] \frac{d(C - C_s)}{dt} + (C - C_s) = \left[ \frac{\frac{F}{V}}{\frac{F}{V} + k_1} \right] (C_i - C_{i0}) \quad (8.27)$$

Again, observe that this is simply a first-order ODE with:

$$\tau = \left[ \frac{1}{\frac{F}{V} + k_1} \right] = \frac{V}{F + k_1 V} \quad \text{and} \quad k = \left[ \frac{\frac{F}{V}}{\frac{F}{V} + k_1} \right] = \frac{1}{1 + \frac{V}{F}k_1}$$

$$y = C - C_s \quad \text{and} \quad u = C_i - C_{i0}$$

and therefore, we know the solution for a step change in inlet concentration at  $t = 0$ .

Notice that the gains and time constants for a stirred tank with reaction are less than those for a stirred tank without reaction. This means that an inlet composition change has a faster dynamic effect in a system with chemical reaction than in a system with just mixing.

Note that the previous examples were linear because the flowrate was constant. If the flowrate were changing (i.e., was considered an input), the models would be nonlinear (actually bilinear), because of the terms where an input multiplies a state variable. The linearization techniques developed in Chapter 5 must then be used before a Laplace transform analysis can be performed. In the following example, linearization must be used because of the second-order reaction term.

### EXAMPLE 8.5 A CSTR with a Second-Order Reaction

Here we extend the previous example to include a second-order reaction problem. We will assume that the rate of reaction (per unit volume) is proportional to the square of the concentration of the reacting component. An example would be  $A + A \rightarrow B$ . As before, we are making the simplifying assumption that the fluid density is not a function of the concentration. Again, assume that  $C_i$  is the input. The component material balance is:

$$\frac{dVC}{dt} = FC_i - FC - k_2 VC^2 \quad (8.28)$$

where  $k_2$  is the reaction rate constant. Since  $V$  is constant,

$$\frac{dC}{dt} = \frac{F}{V} C_i - \frac{F}{V} C - k_2 C^2 \quad (8.29)$$

and we can calculate the steady-state concentrations from  $dC/dt = 0$

$$k_2 C_s^2 + \frac{F}{V} C_s - \frac{F}{V} C_{i_s} = 0 \quad (8.30)$$

Notice that (8.30) is quadratic in  $C_s$ , and will always have one positive and one negative root (the reader should verify this by using the quadratic formula). Obviously, only the positive root makes physical sense.

Now, the problem with obtaining an analytical solution to (8.29) is the nonlinear term. We can use the linearization technique from Chapter 5.

$$\frac{d(C - C_s)}{dt} \approx \left. \frac{\partial f}{\partial C} \right|_{C_{i_{ss}}} (C - C_s) + \left. \frac{\partial f}{\partial C_{i_{ss}}} \right|_{C_{i_{ss}}} (C_i - C_{i_s})$$

to find that:

$$\frac{1}{\left(\frac{F}{V} + 2k_2 C_s\right)} \frac{d(C - C_s)}{dt} + (C - C_s) = \frac{\frac{F}{V}}{\left(\frac{F}{V} + 2k_2 C_s\right)} (C_i - C_{i_s}) \quad (8.31)$$

Again, we have a first-order, linear relationship, where:

$$\text{process gain} = k = \frac{\frac{F}{V}}{\left(\frac{F}{V} + 2k_2 C_s\right)} = \frac{1}{\left(1 + 2k_2 C_s \frac{V}{F}\right)}$$

$$\text{time constant} = \tau = \frac{1}{\left(\frac{F}{V} + 2k_2 C_s\right)} = \frac{\frac{V}{F}}{\left(1 + 2k_2 C_s \frac{V}{F}\right)}$$

Summarizing, the parameters for each of the previous examples are shown in Table 8.1.

TABLE 8.1 Summary of Parameters from Examples

	Ex. 8.1 Mixing Tank No Rxn	Ex. 8.4 CSTR First-Order Rxn	Ex. 8.5 CSTR Second-Order Rxn
Process Gain, $k$	1	$\frac{1}{1 + \frac{V}{F} k_1}$	$\frac{1}{1 + 2k_2 C_s \frac{V}{F}}$
Process Time Constant, $\tau$	$\frac{V}{F}$	$\frac{\frac{V}{F}}{1 + \frac{V}{F} k_1}$	$\frac{\frac{V}{F}}{1 + 2k_2 C_s \frac{V}{F}}$

**EXAMPLE 8.6 A Numerical Study of Examples 8.1, 8.4, 8.5**

Here we will perform a numerical study, using the following values:

$\frac{V}{F}$	=	5 min	All cases
$k_1$	=	0.2 min <sup>-1</sup>	CSTR with first-order Rxn
$k_2$	=	0.32 ft <sup>3</sup> lbmol <sup>-1</sup> min <sup>-1</sup>	CSTR with second-order Rxn
$C_s$	=	1.25 lbmol ft <sup>-3</sup>	All cases

Then, we can calculate the following steady-state concentrations:

$C_x$	=	1.25 lbmol ft <sup>-3</sup>	Mixing tank with no Rxn
$C_1$	=	0.625 lbmol ft <sup>-3</sup>	CSTR with first-order Rxn
$C_2$	=	0.625 lbmol ft <sup>-3</sup>	CSTR with second-order Rxn

	Mixing Tank No Rxn	CSTR First-Order Rxn	CSTR Second-Order Rxn
Process Gain, $k$	1	0.5	0.5
Process Time Constant, $\tau$ (min)	5	2.5	2.5

For all of the examples, assume that a step change in the inlet concentration occurs at  $t = 0$ . That is,  $C_i$  changes from  $1.25 \text{ lbmol ft}^{-3}$  to  $1.75 \text{ lbmol ft}^{-3}$  at  $t = 0$  minutes. In terms of deviation variables, this means that  $u$  increases from 0 to  $0.5 \text{ lbmol ft}^{-3}$  at  $t = 0$ .

Recall that the solution for a first-order system with a step input change of magnitude  $A$  is:

$$y(t) = kA [1 - e^{-t/\tau}]$$

and since

$$y(t) = C(t) - C_s$$

our solution is

$$C(t) = C_s + kA [1 - e^{-t/\tau}] \quad (8.32)$$

For the mixing tank

$$C(t) = 1.25 + 0.5 [1 - e^{-t/5}] \quad (8.33)$$

For the CSTR with first-order Rxn

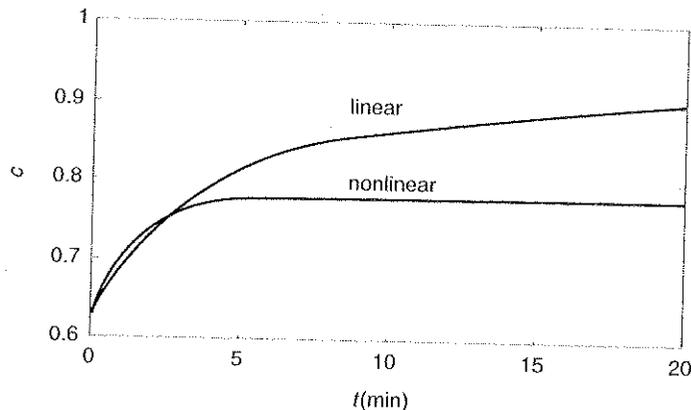
$$C(t) = 0.625 + 0.25 [1 - e^{-t/2.5}] \quad (8.34)$$

For the CSTR with second-order Rxn

$$C(t) = 0.625 + 0.25 [1 - e^{-t/2.5}] \quad (8.35)$$

Notice that solutions for the mixing tank (8.33) and the CSTR with first-order Rxn (8.34) are *exact* because these systems are inherently linear. The solution to the CSTR with second-order Rxn (8.35) is only approximate, because it is based on a linearized approximation to a nonlinear model.

The actual response of the nonlinear model (using `ode45`) is compared with the linear solution (8.35) in Figure 8.10. Notice that the initial response is similar, but the long-term re-



**FIGURE 8.10** Reactor concentration response to a step increase in inlet concentration, for a second-order reaction.

sponse of the linear model deviates significantly from the nonlinear model. Indeed, we can calculate the long-term response without doing any numerical integration, as shown below.

**Linear Model** (8.35) as  $t \rightarrow \infty$

$$C(\infty) = 0.625 + 0.25 = \mathbf{0.8750}$$

**Nonlinear Model** (8.30) as  $t \rightarrow \infty$

$$C_s^2 + \frac{F}{Vk_2} C_s - \frac{F}{Vk_2} C_{iN} = 0$$

$$C_s^2 + 0.625 C_s - 0.625(1.75) = 0$$

The solution that makes physical sense is:  $C(\infty) = \mathbf{0.7790}$

In Example 8.6 we were able to find the new steady-state for the nonlinear system by solving a single quadratic equation. For the general case, with a model composed of a set of nonlinear equations, one would need to solve a set of nonlinear algebraic equations. This would be done twice, once to find the initial steady-state, then again to find the final steady-state after a new input change.

#### EXAMPLE 8.7 First Order + Deadtime

The most common model for process control studies is known as a first-order + deadtime process model, and is written in the following form

$$\tau \frac{dy}{dt} + y = k u(t - \theta) \quad (8.36)$$

where  $\theta$  is known as the time delay. Assume that  $y(0) = 0$  and  $u(0) = 0$ . The input,  $u$  and the output  $y$  are functions of time;  $u(t)$  must be specified to solve for  $y(t)$ .

To understand how this equation might arise, see Figure 8.11.

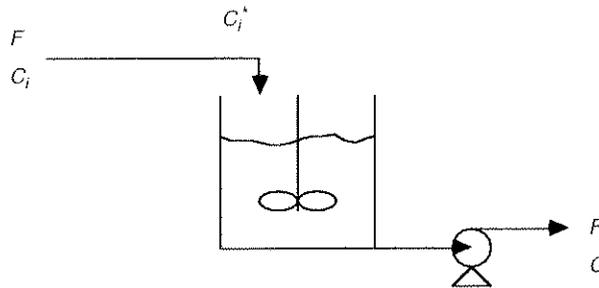


FIGURE 8.11 Mixing tank.

Notice that if the inlet pipe has a significant volume, there will be a delay between a change in the concentration at the inlet pipe and the concentration at the outlet of the pipe. The delay can be calculated as:

$$\theta = \frac{V_p}{F}$$

where  $V_p$  is the volume of the pipe. The relationship between the concentration at the exit of the pipe and the inlet of the pipe can be found by:

$$C_i^*(t) = C_i(t - \theta)$$

That is, the concentration at the exit of the pipe is equal to what the concentration at the outlet of the pipe was  $\theta$  time units in the past. The modeling equation is:

$$\frac{dC}{dt} = -\frac{F}{V}C + \frac{F}{V}C_i^*(t)$$

which can be written:

$$\frac{dC}{dt} = -\frac{F}{V}C + \frac{F}{V}C_i(t - \theta)$$

which is equivalent to (8.36) when written in deviation variable form, where:

$$u = C_i - C_{is} \quad y = C - C_s \quad \tau = \frac{V}{F}$$

Taking the Laplace transform of (8.36) we find:

$$\begin{aligned} \tau [s Y(s) - y(0)] + Y(s) &= k e^{-\theta s} U(s) \\ \tau s Y(s) + Y(s) &= k e^{-\theta s} U(s) \\ (\tau s + 1) Y(s) &= k e^{-\theta s} U(s) \end{aligned} \quad (8.37)$$

which is most commonly written:

$$Y(s) = \frac{k e^{-\theta s}}{\tau s + 1} U(s) \quad (8.38)$$

or,

$$Y(s) = g(s) U(s) \quad (8.39)$$

where:

$$g(s) = \frac{k e^{-\theta s}}{\tau s + 1} \quad (8.40)$$

Assume a step input of magnitude  $\Delta u$  at time  $t = 0$ . We know that:

$$L[\Delta u] = \frac{\Delta u}{s} \quad (8.41)$$

and we can then write (8.38) as:

$$Y(s) = \frac{k e^{-\theta s}}{\tau s + 1} \frac{\Delta u}{s} \quad (8.42)$$

$$Y(s) = \frac{k \Delta u e^{-\theta s}}{s(\tau s + 1)} \quad (8.43)$$

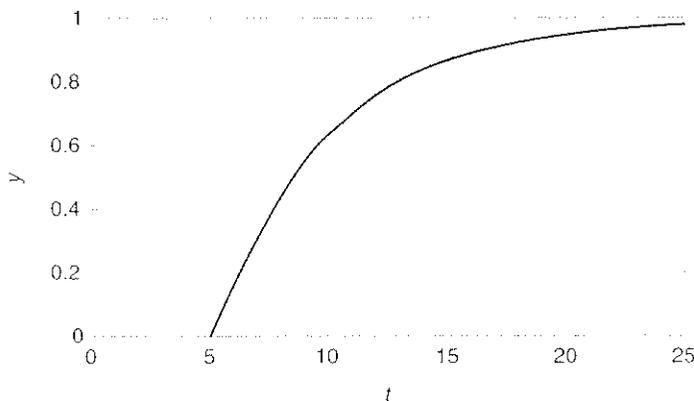
$$Y(s) = k \Delta u e^{-\theta s} \left[ \frac{1}{s} - \frac{\tau}{\tau s + 1} \right] \quad (8.44)$$

The solution to (8.44) is then (since  $L[y(t - \theta)] = e^{-\theta s}Y(s)$ ):

$$\begin{aligned} y(t) &= 0 && \text{for } 0 \leq t \leq \theta \\ y(t) &= k\Delta u [1 - e^{-k(t - \theta)}] && \text{for } t \geq \theta \end{aligned} \quad (8.45)$$

Notice that (8.45) is merely a translation of the first-order response by  $\theta$  time units.

Consider the following plot (Figure 8.12) of the response of a system to a step input change of magnitude 0.5 at time  $t = 0$ . We see immediately that the time delay is  $\theta = 5$  minutes. Since the change in output after a long period of time is  $\Delta y = 1 = k \Delta u$ , we see that  $k = 2$  (units of input/output). The process time constant can be determined from the amount of time, after the delay, that it takes for 63.2% of the change to occur. In this case, the time constant is approximately 5 minutes.



**FIGURE 8.12** Response of a first-order + deadtime (5 time units) model to a step input at  $t = 0$ .

## 8.4 INTEGRATING PROCESSES

The previous examples were for self-regulating processes. If an input changed, then the process output came to a new steady-state. Another common chemical process is the integrating process, as shown in the example below.

### EXAMPLE 8.8 An Integrating System

Consider a water storage tank with inlet and outlet streams that can be independently adjusted. The storage tank has a cross-sectional area of  $100 \text{ ft}^2$ . Initially, the flow in is equal to the flow out, which is  $5 \text{ ft}^3/\text{min}$ . The initial height of water in the tank is  $4 \text{ ft}$  and the height of the tank is  $10 \text{ ft}$ . At 1:00 pm the inlet flowrate is increased to  $6 \text{ ft}^3/\text{min}$ . When does the tank overflow? The material balance (assuming constant density) is

$$\frac{dV}{dt} = F_i - F_o \quad (8.46)$$

where  $F_i$  and  $F_o$  are the inlet and outlet flowrates, and  $V$  is the tank volume. Assuming a constant cross-sectional area:

$$\frac{dh}{dt} = \frac{1}{A} F_i - \frac{1}{A} F_o \quad (8.47)$$

To satisfy steady-state relationships  $F_{is} = F_{os}$ , so we can use the following deviation variable form:

$$\frac{d(h - h_s)}{dt} = \frac{1}{A} (F_i - F_{is}) - \frac{1}{A} (F_o - F_{os}) \quad (8.48)$$

For simplicity, let's assume that  $F_o$  is constant, then:

$$\frac{d(h - h_s)}{dt} = \frac{1}{A} (F_i - F_{is}) \quad (8.49)$$

which has the form:

$$\frac{dy}{dt} = k u \quad (8.50)$$

where  $y = h - h_s$ ,  $k = 1/A$  and  $u = F_i - F_{is}$ . Taking Laplace transforms, we find:

$$sY(s) - y(0) = k U(s) \quad (8.51)$$

where  $y(0) = h(0) - h_s$ . Assuming that we are starting from a steady-state,  $y(0) = h(0) - h_s = 0$ . So we can write (8.51) as:

$$sY(s) = k U(s)$$

or,

$$Y(s) = \frac{k}{s} U(s) \quad (8.52)$$

Using the notation  $\Delta u$  for the magnitude of the step increase:

$$U(s) = \frac{\Delta u}{s} \quad (8.53)$$

and

$$Y(s) = k \frac{\Delta u}{s^2} \quad (8.54)$$

Taking the inverse Laplace transform:

$$y(t) = L^{-1}[Y(s)] = L^{-1} \left[ \frac{k \Delta u}{s^2} \right] \quad (8.55)$$

$$y(t) = k \Delta u t \quad (8.56)$$

Substituting back for the physical variables,

$$h - h_s = \frac{1}{A} \Delta F_i t \quad (8.57)$$

or,

$$h = h_0 + \frac{1}{A} \Delta F_0 t$$

$$h = 4 \text{ ft} + \frac{(6 - 5) \text{ ft}^3/\text{min}}{100 \text{ ft}^2} t$$

Solving for  $h = 10$  ft

$$t = (10 \text{ ft} - 4 \text{ ft}) \frac{100 \text{ ft}^2}{(6 - 5) \text{ ft}^3/\text{min}} = 600 \text{ minutes}$$

$$= 10 \text{ hours}$$

Since the step change was made at 1:00 pm, the tank will overflow at 11:00 pm.

A plot of tank height versus time is shown in Figure 8.13.

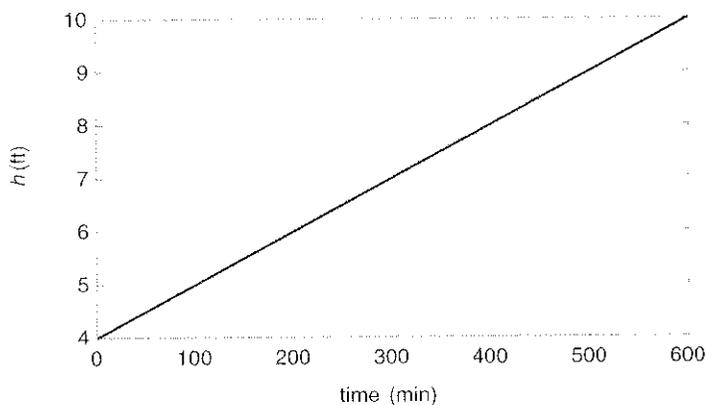


FIGURE 8.13 Integrating system.

Notice in equation (8.52) that the process transfer function has a pole at  $s = 0$ . This is a characteristic of an integrating system.

## 8.5 LEAD-LAG MODELS

Some dynamic systems, particularly involved with process control, have the following form for a transfer function model:

$$Y(s) = k \frac{\tau_n s + 1}{\tau_d s + 1} U(s) \quad (8.58)$$

Consider a step input change of magnitude  $\Delta u$

$$Y(s) = k \frac{\tau_n s + 1}{\tau_d s + 1} \frac{\Delta u}{s} \tag{8.59}$$

The reader should find that time domain response is (see student exercise 11)

$$y(t) = k \Delta u \left[ 1 - \left( 1 - \frac{\tau_n}{\tau_d} \right) e^{-t/\tau_d} \right] \tag{8.60}$$

A plot of (8.60) is shown in Figure 8.14, for  $k\Delta u = 1$ . Notice if  $\tau_n > \tau_d$  the immediate increase in the output is greater than the ultimate steady-state increase, while if  $\tau_n < \tau_d$  the immediate increase in the output is less than the ultimate steady-state increase.

### 8.5.1 Simulating Lead/Lag Transfer Functions

We have derived the step response for a lead/lag transfer function. This transfer function does not usually arise in the modeling of a physical system, but it often arises in control system design. Our desire in this section is to show how to convert a lead/lag transfer function to state-space form, so that a general simulation package can be used to integrate the corresponding ordinary differential equation.

Multiplying through by the denominator term in (8.58), we find:

$$(\tau_d s + 1) Y(s) = (\tau_n s + 1) U(s) \tag{8.61}$$

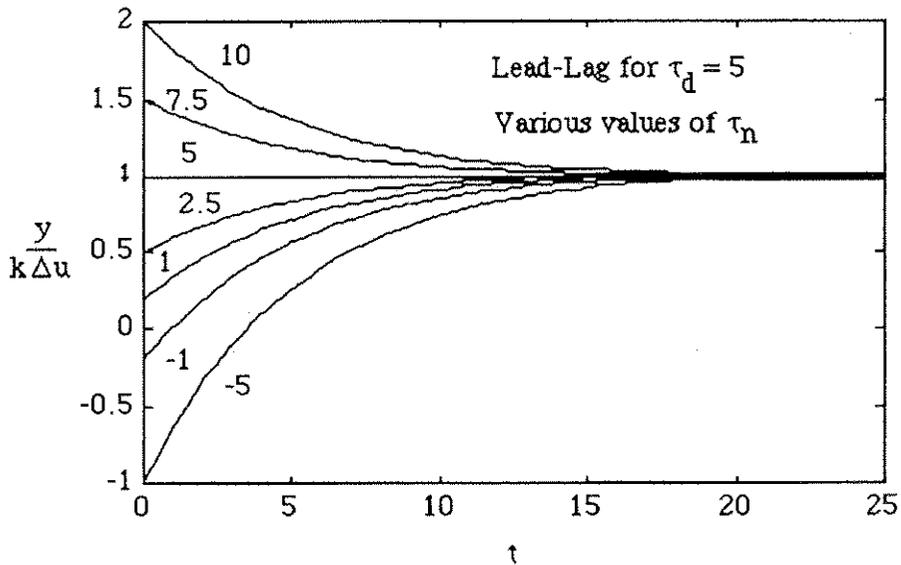


FIGURE 8.14 Lead/lag response.

Using the Laplace transform relationships,

$$\tau_d \left( \frac{dy}{dt} - y(0) \right) + y = \tau_n \left( \frac{du}{dt} - u(0) \right) + u \quad (8.62)$$

and we know that to obtain the transfer function form, the initial conditions of all variables were assumed to be zero, so:

$$\tau_d \frac{dy}{dt} + y = \tau_n \frac{du}{dt} + u \quad (8.63)$$

We cannot solve (8.63) by using a general purpose integrator, because it is not in the standard form of  $dx/dt = f(x)$ . Our goal now is to define a new variable that will allow us to use a standard integrator.

Rearrange (8.63) to find:

$$\tau_d \frac{dy}{dt} - \tau_n \frac{du}{dt} = -y + u \quad (8.64)$$

We see that we can define a new variable,  $x$ , so that:

$$x = \tau_d y - \tau_n u \quad (8.65)$$

and since  $\tau_d$  and  $\tau_n$  are constants, we can take the derivative of (8.65) with respect to time to find:

$$\frac{dx}{dt} = \tau_d \frac{dy}{dt} - \tau_n \frac{du}{dt} \quad (8.66)$$

Substituting the righthand side of (8.66) for the lefthand side of (8.64), we find:

$$\frac{dx}{dt} = -y + u \quad (8.67)$$

Now, we must solve (8.65) to find  $y$  as a function of  $x$ , to obtain:

$$y = \frac{1}{\tau_d} x + \frac{\tau_n}{\tau_d} u \quad (8.68)$$

which we substitute into (8.67) to find:

$$\frac{dx}{dt} = -\frac{1}{\tau_d} x + \left( 1 - \frac{\tau_n}{\tau_d} \right) u \quad (8.69)$$

and we see that we have the standard state-space form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}$$

except that (8.68) and (8.69) consist of scalars:

$$\frac{dx}{dt} = ax + bu \quad (8.70)$$

$$y = cx + du \quad (8.71)$$

where

$$a = -\frac{1}{\tau_d} \quad b = \left(1 - \frac{\tau_d}{\tau_n}\right)$$

$$c = \frac{1}{\tau_d} \quad d = \frac{\tau_n}{\tau_d}$$

We will see in Chapter 11 how (8.70) and (8.71) can be used within the context of a block diagram.

## SUMMARY

We have studied the response of a number of processes that have denominators of transfer function models that are first-order in the Laplace variable,  $s$ . The systems were: first-order, first-order + deadtime, integrating, and lead/lag. Most chemical processes can be represented by a cascade of these types of modes. We found that stirred tank chemical reactors are linear first-order processes, as long as they have first-order kinetics (or no reaction) and the input flowrate is not changing.

For first-order and first-order + time-delay transfer functions, we discussed how to estimate the parameters (which always have units associated with them) by applying a known step input to the process and observing the response. First-order + time-delay models are commonly used in control system design.

In the next chapter we study the transient response behavior of second- and higher-order systems.

## STUDENT EXERCISES

1. As a process engineer, you are attempting to estimate the model parameters for a process that you believe is first-order (with no deadtime). At 3:00 pm, you make a step input change to the process. At 4:00 pm, the process output has reached 80% of its final change.

What is the time constant of the process?

2. Consider a water storage tank with inlet and outlet streams that can be independently adjusted. The storage tank has a cross-sectional area of 100 ft<sup>2</sup>. Initially, the flow in is equal to the flow out, which is 5 ft<sup>3</sup>/min. The initial height of water in the tank is 4 ft and the height of the tank is 10 ft. At  $t = 0$  a ramp increase in the inlet flowrate is made, so that  $F_i(t) = 5 + 0.25t$  where the flowrate units are ft<sup>3</sup>/min.

How long does it take the tank to overflow? Solve using Laplace transforms. Obtain a general expression for systems modeled in deviation variable form by:

$$\frac{dy}{dt} = k u(t)$$

where:

$$u(t) = a t$$

3. Write a differential equation which corresponds to the following input-output transfer function relationship:

$$y(s) = k \frac{\tau_n s + 1}{\tau_d s + 1} u(s)$$

4. Consider a chemical reactor that has zero-order kinetics, that is, the rate of reaction per unit volume is a constant (a zero-order kinetic parameter) that does not depend on concentration. Compare this model with that of a stirred tank mixer, and a stirred tank reactor with first-order kinetics. Perform a numerical study, related to Example 8.5, by finding the zero-order parameter that yields the same steady-state concentration as the first-order kinetic model.
5. A process operator makes a step change on an input variable at 2:00 pm and discovers no output response is observed until after 2:10 pm. She finds that the output is 90% of the way to its final steady-state at 2:45 pm. You believe that this is a first order + deadtime process.

time	input	output
1:00 pm	200 lb/hr	100°F
1:30 pm	200 lb/hr	100°F
1:59 pm	200 lb/hr	100°F
2:00 pm	225 lb/hr	100°F
2:10 pm	225 lb/hr	100°F
2:45 pm	225 lb/hr	91°F
after 5:00 pm	225 lb/hr	90°F

- (i) What is the deadtime for this process (show units)?
- (ii) What is the time constant for this process (show units)?
- (iii) What is the process gain (show units)?
6. As the process engineer for an operating unit in a process plant, you are trying to get a "feel" for the dynamic characteristics of a particular process. You have a discussion with the operator about a process (which you feel is first-order) that uses steam flowrate as an input variable, and process temperature as a measured variable. After the steam flowrate is increased from 1000 lb/hr to 1100 lb/hr (quickly), the process fluid temperature changes from 100°F (the initial steady-state) to 110°F in 30 minutes. The temperature eventually reaches a new steady-state value of 120°F.
- (i) Find the process gain (show units).
- (ii) Find the process time constant (show units).

7. A process input is:

$$u(t) = 0 \quad \text{for } t < 0$$

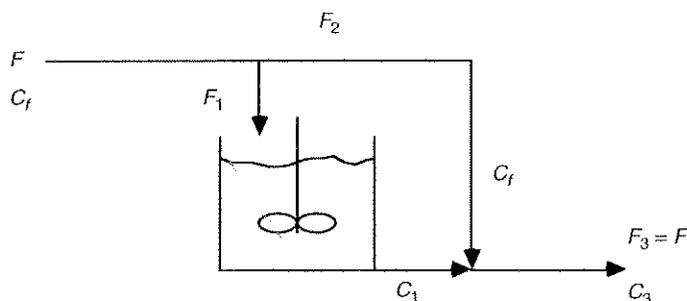
$$u(t) = 1 - e^{-t} \quad \text{for } t > 0$$

The process transfer function is:

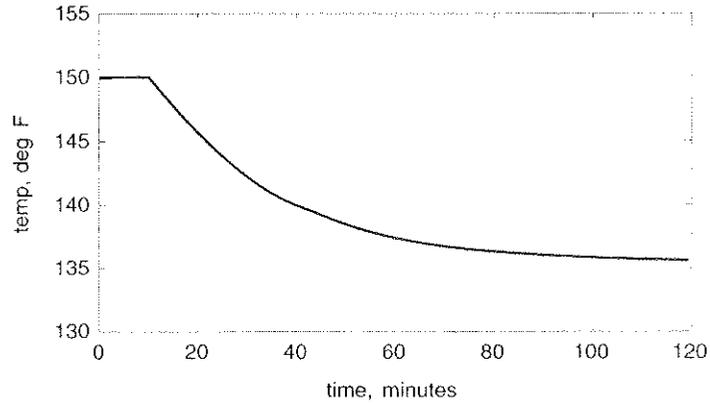
$$g(s) = \frac{2.5}{12s + 1}$$

Find the time domain output,  $y(t)$ . Plot both the input and the output.

8. Consider the mixing process shown below, where a portion of the feed stream bypasses the mixing tank.
- Show that the process has a lead/lag transfer function, if the input is  $C_f$  and the output is  $C_3$ . (*Hint:* Write a dynamic balance around the tank and a static balance around the mixing point (after the tank outlet). Use deviation variable form.)
  - Let  $F = 2 \text{ m}^3/\text{min}$ ,  $F_1 = 1 \text{ m}^3/\text{min}$ ,  $C_f = 1 \text{ kgmol/m}^3$ , and  $V = 10 \text{ m}^3$ . Find the state-space model and the transfer function representing this system.
  - Consider a step increase of  $C_f$  to  $1.5 \text{ kgmol/m}^3$ . Find the response in  $C_3$  to this change.



9. *Comparison of Impulse and Pulse Responses.* Consider a tank with constant cross-sectional area,  $A_t = 1 \text{ m}^2$ , and assume that the flow out of the tank is a linear function of the height of liquid in the tank. The steady-state values of tank height and flowrate are 1 meter and  $1 \text{ m}^3/\text{hr}$ , respectively. Find the impulse response of tank height if  $1 \text{ m}^3$  (in addition to the constant steady-state flow) is instantaneously dumped in the tank. Compare this with several pulse responses, where the additional  $1 \text{ m}^3$  is added over 0.05, 0.1, and 0.15 hour periods.
10. Consider a chemical reactor where a step change in coolant flowrate from 10 gal/min to 12 gal/min (at  $t = 0$ ) causes the change in reactor temperature shown in the figure below.



Find the gain, time constant, and time-delay for this system.

11. For step response of the lead/lag transfer function:

$$Y(s) = k \frac{\tau_u s + 1}{\tau_d s + 1} \frac{\Delta u}{s}$$

Show that time domain response is

$$y(t) = k \Delta u \left[ 1 - \left( 1 - \frac{\tau_u}{\tau_d} \right) e^{-t/\tau_d} \right]$$

# TRANSFER FUNCTION ANALYSIS OF HIGHER-ORDER SYSTEMS 9

After studying this chapter, the reader should be able to:

- Understand the dynamic behavior of second-order systems.
- Understand the effect of poles and zeros on the response for higher-order systems.
- Use the Padé approximation for time-delays.
- Understand the concept of inverse response.
- Understand how to simulate transfer function models using ODE solvers that require sets of first-order ODEs.
- Use the MATLAB routine `tf2ss` to convert from transfer function to state-space form.
- Use the MATLAB routines `step` and `impz`.

The major sections are:

- 9.1 Responses of Second-Order Systems
- 9.2 Second-Order Systems with Numerator Dynamics
- 9.3 The Effect of Pole-Zero Locations on System Step Responses
- 9.4 Padé Approximation for Deadtime
- 9.5 Converting the Transfer Function Model to State-Space Form
- 9.6 MATLAB Routines for Step and Impulse Response

The dynamic behavior of *first-order* systems was studied in Chapter 8. In this chapter, we present results for *higher-order* systems and show how to use standard numerical integration routines for time domain simulation of these models. We first study second-order systems, then generalize our results to higher-order systems.

## 9.1 RESPONSES OF SECOND-ORDER SYSTEMS

Consider a linear second-order ODE, with constant parameters:

$$a_2 \frac{d^2 y}{dt^2} + a_1 \frac{dy}{dt} + a_0 y = b u(t) \quad (9.1)$$

This is often written in the form:

$$\tau^2 \frac{d^2 y}{dt^2} + 2\zeta\tau \frac{dy}{dt} + y = k u(t) \quad (9.2)$$

where (obviously  $a_0 \neq 0$ ):

$$\tau^2 = \frac{a_2}{a_0} \quad 2\zeta\tau = \frac{a_1}{a_0} \quad k = \frac{b}{a_0}$$

where the parameters are:

- $k$  = gain (units of output/input)
- $\zeta$  = damping factor (dimensionless)
- $\tau$  = natural period (units of time)

We discussed in Chapter 6 that single  $n$ th order ODEs do not naturally arise in chemical processes. The second-order model shown in (9.1) or (9.2) generally arises by changing a set of two first-order equations (state-space model) to a single second-order equation. For a given second-order ODE, there are an infinite number of sets of two first-order (state-space) models that are equivalent.

Taking the Laplace transform of (9.2):

$$\tau^2 [s^2 Y(s) - sy(0) - \dot{y}(0)] + 2\zeta\tau [sY(s) - y(0)] + Y(s) = kU(s)$$

where  $Y(s)$  indicates the Laplace transformed variable.

Assuming initial conditions are zero, that is  $\dot{y}(0) = y(0) = 0$ , we find:

$$Y(s) = \frac{k}{\tau^2 s^2 + 2\zeta\tau s + 1} U(s) \quad (9.3)$$

which can be represented as:

$$Y(s) = g(s) U(s)$$

The *characteristic equation* of the second-order transfer function is  $\tau^2 s^2 + 2\zeta\tau s + 1$ . We can find the roots (also known as the *poles*) by using the quadratic formula:

**TABLE 9.1 Characteristic Behavior of Second-Order Transfer Functions**

Case	Damping Factor	Pole Location	Characteristic Behavior
I	$\zeta > 1$	2 real, distinct poles	overdamped
II	$\zeta = 1$	2 real, equal poles	critically damped
III	$\zeta < 1$	2 complex conjugate poles	underdamped

$$p_i = \frac{-2\zeta\tau \pm \sqrt{4\zeta^2\tau^2 - 4\tau^2}}{2\tau^2} \quad (9.4)$$

which yields the following values for the roots:

$$p_1 = -\frac{\zeta}{\tau} + \frac{\sqrt{4\tau^2(\zeta^2 - 1)}}{2\tau^2} = -\frac{\zeta}{\tau} + \frac{\sqrt{\zeta^2 - 1}}{\tau} \quad (9.5)$$

$$p_2 = -\frac{\zeta}{\tau} - \frac{\sqrt{\zeta^2 - 1}}{\tau} \quad (9.6)$$

The following analysis assumes that  $\zeta > 0$  and  $\tau > 0$ . This implies that the real portions of  $p_1$  and  $p_2$  are negative and, therefore, the system is stable. The three possible cases are shown in Table 9.1.

### 9.1.1 Step Responses

Now, we consider the dynamic response of second-order systems to step inputs ( $U(s) = \Delta u/s$ ):

$$Y(s) = \frac{k}{\tau^2 s^2 + 2\zeta\tau s + 1} \frac{\Delta u}{s} \quad (9.7)$$

where  $\Delta u$  represents the magnitude of the step change.

#### CASE 1 Overdamped ( $\zeta > 1$ )

Since  $\zeta > 1$ , we can see that the two roots will be real and distinct. Also, since we assumed that  $\tau > 0$ , the system is stable (the roots are less than zero, since we are assured that  $\sqrt{\zeta^2 - 1} < \zeta$ ). We factor the polynomial  $\tau^2 s^2 + 2\zeta\tau s + 1$  into the following form:

$$\tau^2 s^2 + 2\zeta\tau s + 1 = (\tau_1 s + 1)(\tau_2 s + 1) \quad (9.8)$$

We see immediately from (9.8) that the poles (values of  $s$  where the polynomial = 0) are:

$$p_1 = -1/\tau_1 \quad p_2 = -1/\tau_2 \quad (9.9)$$

from (9.5), (9.6) and (9.8) we find:

$$p_1 = -1/\tau_1 = -\zeta/\tau + \sqrt{(\zeta^2 - 1)}/\tau$$

which gives the following value for the first time constant:

$$\tau_1 = \frac{\tau}{\zeta - \sqrt{\zeta^2 - 1}} \quad (9.10)$$

Also, we find the second pole:

$$p_2 = -1/\tau_2 = -\zeta/\tau - \sqrt{\zeta^2 - 1}/\tau$$

which gives the following value for the second time constant:

$$\tau_2 = \frac{\tau}{\zeta + \sqrt{\zeta^2 - 1}} \quad (9.11)$$

Expanding the righthand side of (9.8),

$$\tau^2 s^2 + 2\zeta\tau s + 1 = \tau_1\tau_2 s^2 + (\tau_1 + \tau_2)s + 1 \quad (9.12)$$

we can write:

$$\tau^2 = \tau_1\tau_2 \quad \text{and} \quad 2\zeta\tau = \tau_1 + \tau_2$$

which lead to the relationships

$$\tau = \sqrt{\tau_1\tau_2} \quad (9.13)$$

$$\zeta = \frac{\tau_1 + \tau_2}{2\sqrt{\tau_1\tau_2}} \quad (9.14)$$

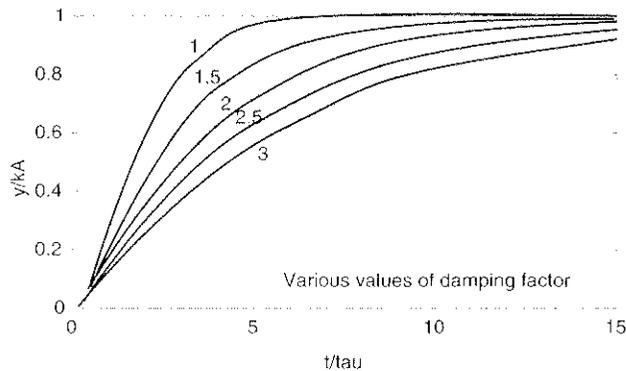
We can derive (see student exercise 1a) the following solution for step responses of overdamped systems

**Overdamped,  $\zeta > 1$**

$$y(t) = k\Delta u \left[ 1 + \frac{\tau_1 e^{-t/\tau_2} - \tau_2 e^{-t/\tau_1}}{\tau_2 - \tau_1} \right] \quad (9.15)$$

where  $\tau_1 = \frac{\tau}{\zeta - \sqrt{\zeta^2 - 1}}$  and  $\tau_2 = \frac{\tau}{\zeta + \sqrt{\zeta^2 - 1}}$

Note that, as in the case of first-order systems, we can divide by  $k\Delta u$  to develop a dimensionless output. Also, the dimensionless time is  $t/\tau$  and we can plot curves for dimensionless output as a function of  $\zeta$ . This is done in Figure 9.1, which includes the critically damped case, as discussed next. Most chemical processes exhibit overdamped behavior. The critically damped step response is also shown in Figure 9.1 (curve with  $\zeta = 1$ ).



**FIGURE 9.1** Step response of a second-order overdamped system.

**CASE 2 Critically Damped ( $\zeta = 1$ )**

The transition between overdamped and underdamped is known as critically damped. We can derive the following for the step response of a critically damped system (see student exercise 1b)

**Critically damped,  $\zeta = 1$  [Repeated poles]**

$$y(t) = k\Delta u \left( 1 - \left( 1 + \frac{t}{\tau} \right) e^{-t/\tau} \right) \quad (9.16)$$

Notice that the main difference between overdamped (or critically damped) step responses and first-order step responses is that the second-order step responses have an “S” shape with a maximum slope at an inflection point, whereas the first-order responses have their maximum slope initially.

The initial behavior for a step change is really dictated by the *relative order* of the system. The relative order is the difference between the orders of the numerator and denominator polynomials. If the relative order is 1, then output response has a non-zero slope at the time of the step input; the step response of a system with a relative order greater than 1 has a zero slope at the time of the step input.

**CASE 3 Underdamped ( $\zeta < 1$ )**

For  $\zeta < 1$ , from (9.5) and (9.6), we find that the poles are complex:

$$p = -\frac{\zeta}{\tau} \pm \frac{\sqrt{\zeta^2 - 1}}{\tau} = -\frac{\zeta}{\tau} \pm j \frac{\sqrt{1 - \zeta^2}}{\tau}$$

which is written in terms of the real and imaginary contributions:

$$p = \alpha \pm j\beta$$

where: 
$$\alpha = -\frac{\zeta}{\tau} \quad \beta = \frac{\sqrt{1 - \zeta^2}}{\tau}$$

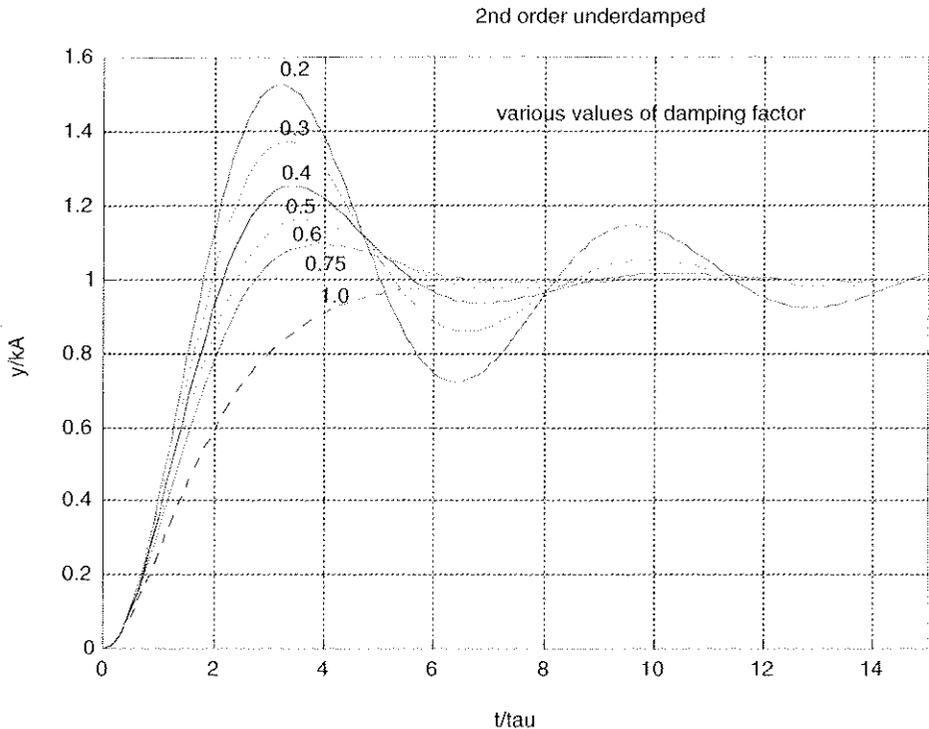
We can derive the following step response for an underdamped system (see student exercise 1):

**Underdamped, ( $\zeta < 1$ ) [Complex poles]**

$$y(t) = k\Delta u \left( 1 - \frac{1}{\sqrt{1 - \zeta^2}} e^{-\zeta t/\tau} \sin(\beta t + \phi) \right) \quad (9.17)$$

where 
$$\beta = \frac{\sqrt{1 - \zeta^2}}{\tau} \quad \phi = \tan^{-1} \frac{\sqrt{1 - \zeta^2}}{\zeta}$$

Again, dividing by  $k\Delta u$ , we can produce the plot shown in Figure 9.2.



**FIGURE 9.2** Step response of a second-order underdamped system as a function of the damping factor ( $\zeta$ ).

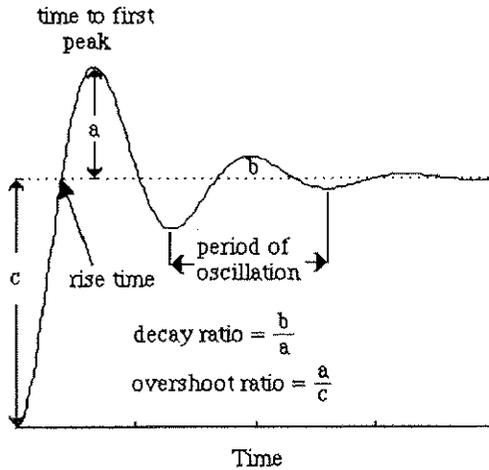
A number of insights can be obtained from Figure 9.2 and an analysis of the step response equations. Notice that the poles for the second-order system can be written:

$$p = [-\zeta \pm j\sqrt{1-\zeta^2}] \frac{1}{\tau}$$

Observe that, for smaller  $\zeta$ , the response is more oscillatory. For  $\zeta < 1$ , the ratio of the imaginary portion to the real portion of the pole is:

$$\frac{\text{imaginary}}{\text{real}} = \frac{\sqrt{1-\zeta^2}}{\zeta}$$

As the imaginary/real ratio gets larger the response becomes more oscillatory. We also notice that a decreasing  $\tau$  corresponds to a larger negative value for the real portion. As the real portion becomes larger in magnitude (more negative) the response becomes faster. We use these insights to interpret pole/zero plots in Section 9.3.



**FIGURE 9.3** Step response characteristics of underdamped second-order processes.

### 9.1.2 Underdamped Step Response Characteristics

The following common measures of underdamped second-order step responses are shown on Figure 9.3 and defined below: (1) rise time, (2) time to first peak, (3) overshoot, (4) decay ratio, (5) period of oscillation.

*Rise time.* The amount of time it takes to first reach the new steady-state value.

*Time to first peak.* The time required to reach the first peak. Notice that there are an infinite number of peaks.

*Overshoot.* The distance between the first peak and the new steady-state. Usually expressed as the overshoot ratio, as shown in the figure.

*Decay ratio.* A measure of how rapidly the oscillations are decreasing. A  $b/a$  ratio of  $1/4$  is commonly called "quarter wave damping".

*Period of oscillation.* The time between successive peaks.

The following example shows how to use Figure 9.2 to estimate these values.

#### EXAMPLE 9.1 Underdamped Second-Order System

Consider the following transfer function, subject to a unit step ( $\Delta u = 1$ ) input change (assume time units are minutes):

$$g(s) = \frac{5}{4s^2 + 0.8s + 1}$$

Find the (1) rise time, (2) time to first peak, (3) overshoot, (4) decay ratio, (5) period of oscillation, (6) value of  $y(t)$  at the peak time.

Our first step is to calculate the system parameters. We can see that:

$$\begin{aligned} k &= 5 \\ \tau^2 &= 4 \text{ so } \tau = 2 \\ 2\zeta\tau &= 0.8 \text{ so } \zeta = \frac{0.8}{2\tau} = \frac{0.8}{4} = 0.2 \end{aligned}$$

We use Figure 9.2 as the basis for the following calculations.

1. The rise time for  $\zeta = 0.2$  is  $\frac{t_r}{\tau} = 1.8$ , so  $t_r = 1.8 \tau = 3.6$  minutes
2. The time to first peak for  $\zeta = 0.2$  is  $\frac{t_p}{\tau} = 3.2$ , so  $t_p = 3.2 \tau = 6.4$  minutes
3. The overshoot ratio is  $\frac{1.53 - 1}{1} = 0.53$ .
4. The decay ratio is  $\frac{1.15 - 1}{1.53 - 1} = 0.3$
5. The period of oscillation is  $\frac{t_{osc}}{\tau} = 9.6 - 3.3$ , so  $t_{osc} = 6.3 \tau = 12.6$  minutes.
6. The value of  $y(t_p)$  is  $\frac{y}{k\Delta u} = 1.53$ , so  $y = 1.53 k\Delta u = 1.53(5) = 7.65$ .

Although equation (9.17) can be used to solve the previous example, it is often easier to use the dimensionless plot (Figure 9.2).

### 9.1.3 Impulse Responses

Now, we consider the dynamic response of second-order systems to impulse inputs.

$$Y(s) = \frac{k}{\tau^2 s^2 + 2\zeta\tau s + 1} A\delta$$

where  $A$  represents the magnitude of the impulse.

#### CASE 1 Overdamped ( $\zeta > 1$ )

The time domain solution for the overdamped case is (see student exercise 2a):

$$y(t)/kA = \frac{1}{\tau \sqrt{\zeta^2 - 1}} e^{-\zeta t/\tau} \sinh\left(\sqrt{\zeta^2 - 1} \frac{t}{\tau}\right)$$

where  $y(t)/kA$  is the dimensionless output and  $t/\tau$  is the dimensionless time.

**CASE 2 Critically Damped ( $\zeta = 1$ )**

The impulse response for the critically damped case is (see student exercise 2b):

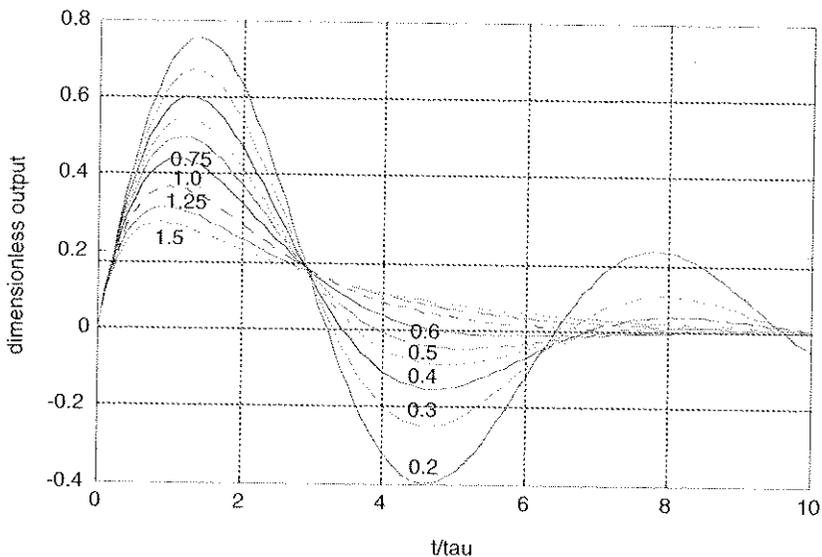
$$y(t)/kA = \frac{t}{\tau^2} e^{-t/\tau}$$

**CASE 3 Underdamped ( $\zeta < 1$ )**

The time domain solution for the underdamped case is (see student exercise 2c):

$$y(t)/kA = \frac{1}{\tau} \frac{1}{\sqrt{1-\zeta^2}} e^{-\zeta t/\tau} \sin\left(\sqrt{1-\zeta^2} \frac{t}{\tau}\right)$$

The impulse responses as a function of  $\zeta$  are shown in Figure 9.4.



**FIGURE 9.4** Impulse response as a function of  $\zeta$ .

The underdamped responses show characteristic oscillatory behavior.

### 9.1.4 Response to Sine Inputs

Consider the case where the input is a sine function, with amplitude  $A$  and frequency  $\omega$ :

$$u(t) = A \sin \omega t$$

The Laplace transform is:

$$U(s) = \frac{A\omega}{(s^2 + \omega^2)}$$

when applied to the second-order transfer function and inverted to the time domain, the response after a long period of time is the periodic function:

$$y(t) = \frac{kA}{\sqrt{(1 - \tau^2\omega^2)^2 + (2\zeta\tau\omega)^2}} \sin(\omega t + \phi) \quad (9.18)$$

where:

$$\phi = \tan^{-1} \left( \frac{-2\zeta\tau\omega}{1 - \tau^2\omega^2} \right) \quad (9.19)$$

(see student exercise 3). The amplitude of the output is:

$$\frac{kA}{\sqrt{(1 - \tau^2\omega^2)^2 + (2\zeta\tau\omega)^2}}$$

and the phase angle is  $\phi$ . Often, system behavior is discussed in terms of an amplitude ratio, which is the amplitude of the output divided by the amplitude of the input. The amplitude ratio is:

$$\frac{k}{\sqrt{(1 - \tau^2\omega^2)^2 + (2\zeta\tau\omega)^2}}$$

These relationships are used in Example 9.2.

#### EXAMPLE 9.2 Sine Forcing of Second-Order Systems

Consider the following system:

$$g(s) = \frac{1}{s^2 + 0.2s + 1}$$

A low frequency sine forcing ( $\omega = 0.1 \text{ min}^{-1}$ ) yields the input/output response shown in Figure 9.5.

Notice that the output lags slightly behind the input, and the amplitude of the output is slightly smaller than the input amplitude. Contrast this result with the following case of a high frequency input.

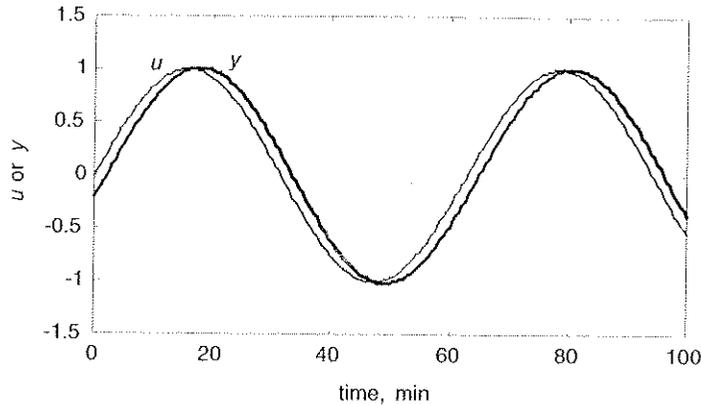


FIGURE 9.5 Low frequency sine input response.

A high frequency sine forcing ( $\omega = 5 \text{ min}^{-1}$ ) yields the input/output response shown in Figure 9.6.

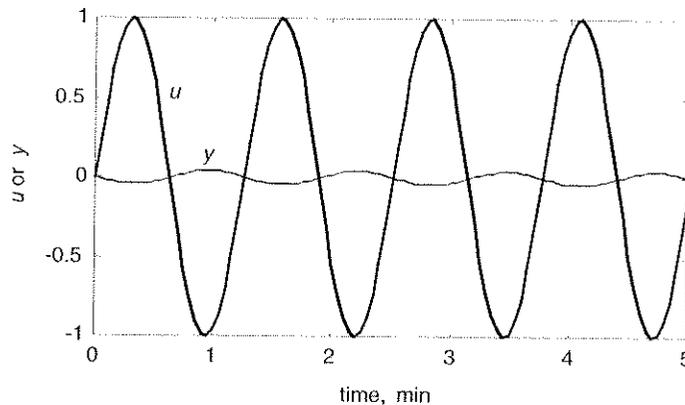
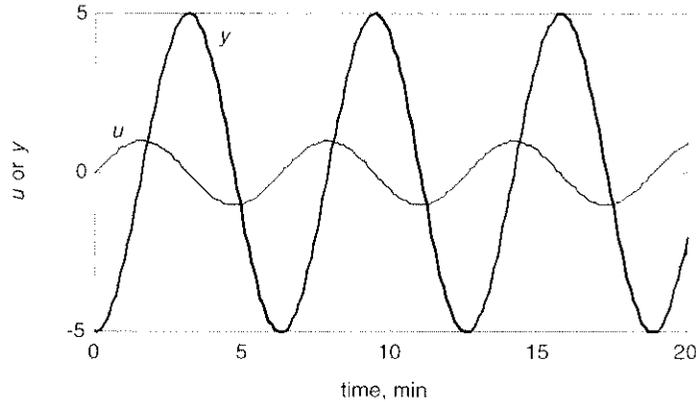


FIGURE 9.6 High frequency sine input response.

Notice that the output lags significantly behind the input, and the amplitude of the output is much smaller than the input amplitude.

A particularly interesting type of behavior that can occur with second-order underdamped systems is known as *resonance peaking*, which occurs in intermediate frequency ranges as shown in Figure 9.7, where a frequency of  $1 \text{ rad/min}$  is used.

Here the output amplitude is significantly higher than the input amplitude although the input/output gain is 1. At lower (Figure 9.5) and higher (Figure 9.6) frequencies the output had a lower amplitude than the input, while at an intermediate frequency (Figure 9.7) the output had a higher amplitude than the input. This phenomena can only happen in systems with complex roots.



**FIGURE 9.7** Resonance peaking phenomenon.

The concept of phase angle is illustrated by Figures 9.5 through 9.7. At low frequencies (Figure 9.5) the output barely lags the input, and therefore has a phase lag of almost 0 deg. At intermediate frequencies (Figure 9.7) the output lags the input by 90°, and at high frequencies (Figure 9.6) the output lags the input by almost 180°. Also note that the notion of “high,” “intermediate,” and “low” frequencies is relative (dependent on  $\tau$ ). Low, medium, and high frequencies correspond roughly to  $\omega\tau \approx 0.1$ , 1, and 10, respectively.

The method of sine-forcing a system is used in the analysis of feedback control systems and is known as frequency response analysis. Bode diagrams are used to plot the amplitude and phase angle as a function of frequency. We do not provide further analysis here, but refer the reader to any textbook on process control for more detail.

## 9.2 SECOND-ORDER SYSTEMS WITH NUMERATOR DYNAMICS

The previous discussion involved pure second-order systems. Consider now, a second-order system with numerator dynamics with the gain/time constant form:

$$y(s) = \frac{k(\tau_n s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)} u(s) \quad (9.20)$$

The pole-zero form is:

$$y(s) = \frac{k_p(s - z_1)}{(s - p_1)(s - p_2)} u(s)$$

where:

$$k_{pc} = \frac{k\tau_n}{\tau_1\tau_2} \quad p_1 = -\frac{1}{\tau_1} \quad p_2 = -\frac{1}{\tau_2}$$

The gain/time constant form has the following time domain response to a step input (see student exercise 4):

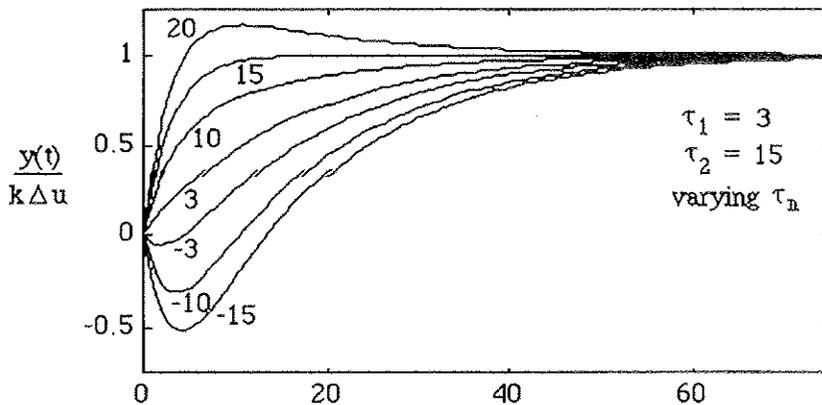
$$y(t) = k\Delta u \left[ 1 + \frac{\tau_n - \tau_1}{\tau_1 - \tau_2} e^{-t/\tau_1} - \frac{\tau_n - \tau_2}{\tau_2 - \tau_1} e^{-t/\tau_2} \right] \quad (9.21)$$

The reader should show that, if  $\tau_n = \tau_2$ , the response is the same as a first-order process.

**EXAMPLE 9.3 Consider the Following Transfer Function**

$$y(s) = \frac{k(\tau_n s + 1)}{(3s + 1)(15s + 1)} u(s) \quad (9.22)$$

The step responses are shown in Figure 9.8. Notice that negative numerator time constants yield a step response that initially decreases before increasing to the final steady-state. This type of response is known as *inverse response* and causes tough challenges for process control systems.



**FIGURE 9.8** Step responses of a second-order system with numerator dynamics.

Notice also that a numerator time constant that is greater than the denominator time constant causes overshoot before settling to the final steady-state. Also notice that the inverse response becomes “deeper” as the process zero ( $-1/\tau_n$ ) approaches a value of zero from the right.

### 9.3 THE EFFECT OF POLE-ZERO LOCATIONS ON SYSTEM STEP RESPONSES

There are a number of different ways to represent process transfer functions. The "gain-time constant" form is:

$$g(s) = \frac{k(\tau_{m1}s + 1)(\tau_{m2}s + 1)\dots(\tau_{mm}s + 1)}{(\tau_{d1}s + 1)(\tau_{d2}s + 1)\dots(\tau_{dn}s + 1)} \quad (9.23)$$

where  $\tau_{mi}$  is a numerator time constant and  $\tau_{di}$  is a denominator time constant.

The "polynomial" form is

$$g(s) = \frac{(b_m s^m + b_{m-1} s^{m-1} + \dots + b_1 s + b_0)}{a_n s^n + a_{n-1} s^{n-1} + \dots + a_1 s + a_0} \quad (9.24)$$

The values of  $s$  that cause the numerator of (9.23) or (9.24) to equal zero are known as the "zeros" of the transfer function. The values of  $s$  that cause the denominator of (9.23) or (9.24) to equal zero are known as the "poles" of the transfer function.

The "pole-zero" form is:

$$g_{pz}(s) = \frac{k_p (s - z_1)(s - z_2)\dots(s - z_m)}{(s - p_1)(s - p_2)\dots(s - p_n)} \quad (9.25)$$

where:

$$k_p = k \frac{\prod_{i=1}^n (-p_i)}{\prod_{i=1}^m (-z_i)} \quad (9.26)$$

The notation  $\prod_{i=1}^n (-p_i)$  is shorthand for  $(-p_1)(-p_2)\dots(-p_n)$ .

Notice also that the poles are

$$p_i = -\frac{1}{\tau_{di}} \quad (9.27)$$

and the zero is

$$z_i = -\frac{1}{\tau_{mi}} \quad (9.28)$$

and that complex poles (or zeros) must occur in complex conjugate pairs.

#### EXAMPLE 9.4 Comparison of Various Transfer Function Forms

Consider a transfer function with the following gain-time constant form:

$$g(s) = \frac{2(-10s + 1)}{(3s + 1)(15s + 1)}$$

The polynomial form is:

$$g(s) = \frac{-20s + 2}{45s^2 + 18s + 1}$$

The gain-polynomial form is:

$$g(s) = \frac{2(-10s + 1)}{(45s^2 + 18s + 1)}$$

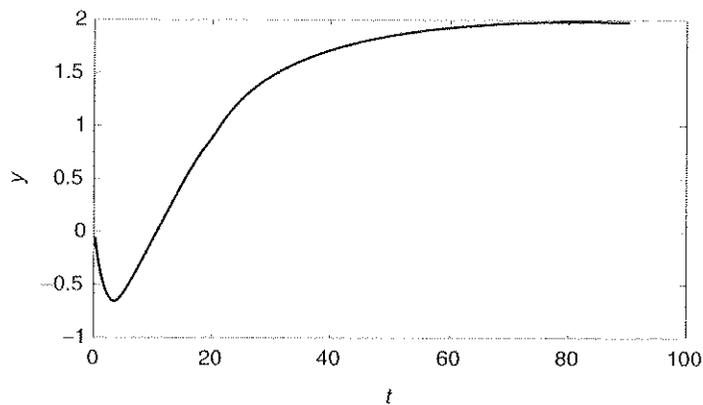
and the pole-zero form is:

$$g_{pz}(s) = \left(-\frac{4}{9}\right) \frac{\left(s - \frac{1}{10}\right)}{\left(s + \frac{1}{3}\right)\left(s + \frac{1}{15}\right)}$$

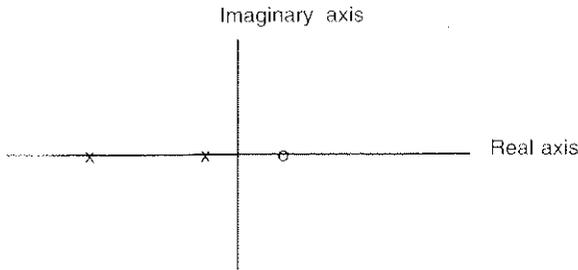
The zero is 0.1, and the poles are  $-1/3$  and  $-1/15$ .

Notice that the zero for Example 9.4 is positive. A positive zero is called a right-half-plane (RHP) zero, because it appears in the right half of the complex plane. Right-half-plane zeros have a characteristic *inverse response*, as shown in Figure 9.9.

Also notice that the poles are negative (left-half-plane), indicating a stable process. Right-half-plane poles (positive poles) are unstable. Recall that complex poles will yield an oscillatory response. A pole-zero plot of the transfer function in Example 9.4 is shown in Figure 9.10 (the pole locations are  $(-1/3, 0)$ ,  $(-1/15, 0)$  and the zero location is  $(0.1, 0)$ ; the coordinates are (real, imaginary)). For this system, there is no imaginary component and the poles and zeros lie on the real axis (Figure 9.10).



**FIGURE 9.9** Inverse response.



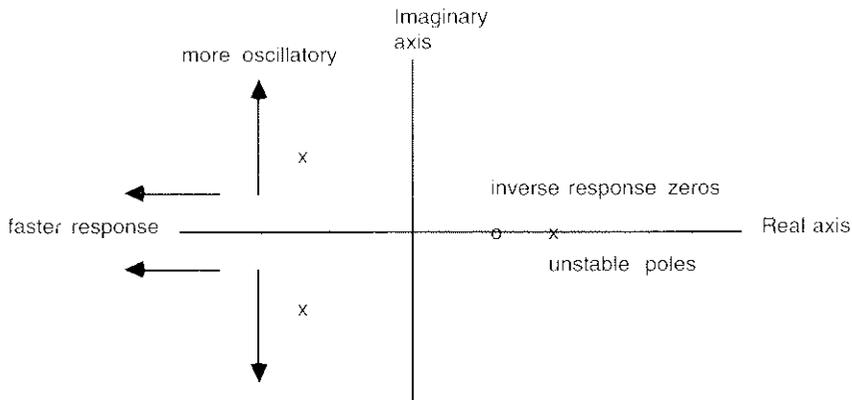
**FIGURE 9.10** Pole-zero location plot for Example 9.4 (x-poles, o-zero).

As poles move further to the left they yield a faster response, while increasing the magnitude of the imaginary portion makes the response more oscillatory. This behavior is summarized in Figure 9.11. Recall also that a process with a pole at the origin (and none in the right-half-plane) is known as an *integrating* system, that is the system never settles to a steady-state when a step input change is made.

Multiple right-half-plane zeros cause multiple “changes in direction”: for example, with two RHP zeros, the step response is initially in one direction, switches direction, then switches back to the initial direction.

#### 9.4 PADÉ APPROXIMATION FOR DEADTIME

Recall that the Laplace transfer function for a pure time-delay is  $e^{-\theta s}$  where  $\theta$  is the time-delay. This is an irrational transfer function: an approximation that is rational and often provides an adequate representation of the deadtime is known as the Padé approximation.



**FIGURE 9.11** Effect of pole-zero location on dynamic behavior (x-poles, o-zero). As poles become more negative, the response is faster. As the imaginary/real ratio increases, the response becomes more oscillatory.

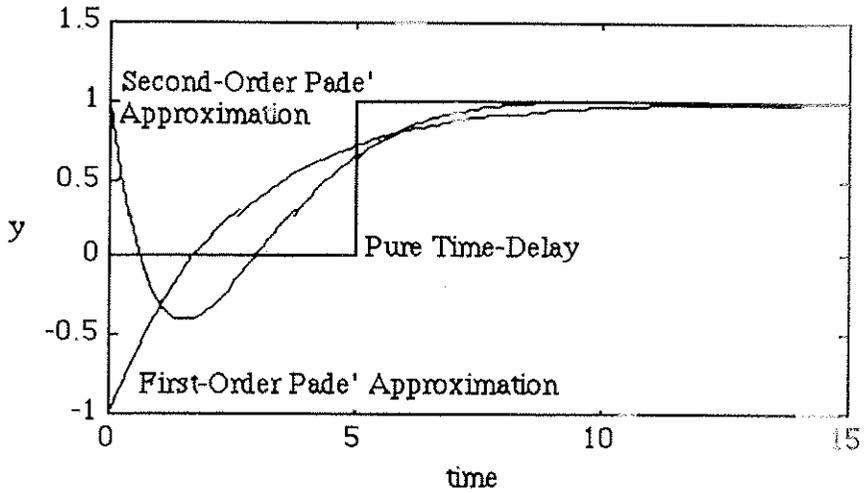


FIGURE 9.12 Comparison of step responses for pure time-delay with first-order and second-order Padé approximations. Deadtime = 5.

The first-order Padé approximation is

$$e^{-\theta s} \approx \frac{1 - \frac{\theta}{2}s}{1 + \frac{\theta}{2}s} \tag{9.29}$$

The second-order Padé approximation is

$$e^{-\theta s} \approx \frac{1 - \frac{\theta}{2}s + \frac{\theta^2}{12}s^2}{1 + \frac{\theta}{2}s + \frac{\theta^2}{12}s^2} \tag{9.30}$$

A comparison of the step responses of first and second-order Padé approximations with pure time delay are shown in Figure 9.12.

**EXAMPLE 9.5 Comparison of the Padé Approximations for Deadtime**

Consider the following first-order + deadtime transfer function

$$g(s) = \frac{e^{-5s}}{5s + 1}$$

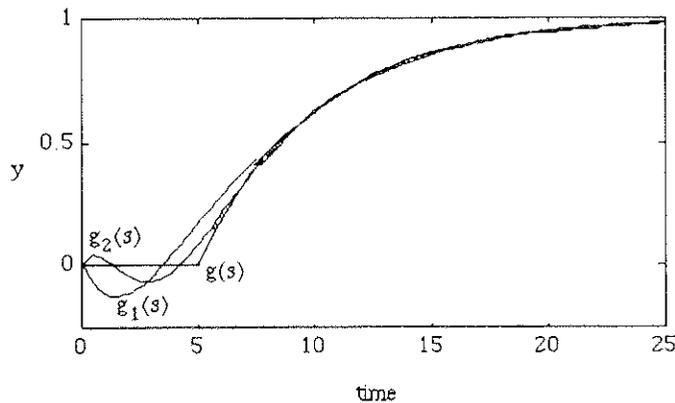
The first-order Padé approximation yields the following transfer function

$$g_1(s) = \frac{-2.5s + 1}{12.5s^2 + 7.5s + 1}$$

and the second-order Padé approximation yields

$$g_2(s) = \frac{2.0833s^2 - 2.5s + 1}{10.4167s^3 + 14.5833s^2 + 7.5s + 1}$$

a comparison of the step responses of  $g(s)$ ,  $g_1(s)$  and  $g_2(s)$  is shown in Figure 9.13. Notice that the first-order approximation has an inverse response, while the second-order approximation has a "double inverse response." The reader should find that there is a single positive zero for  $g_1(s)$  and there are two positive, complex-conjugate zeros of the numerator transfer function of  $g_2(s)$ .



**FIGURE 9.13** Comparison of first-order + deadtime response with first- and second-order Padé approximations for deadtime.

Most ordinary differential equation numerical integrators (including `ode45`) require pure differential equations (with no time-delays). If you have a system of differential equations which has time-delays, the Padé approximation can be used to convert them to delay-free differential equations, which can then be numerically integrated. See student exercise 28 as an example.

One of the many advantages to using SIMULINK is that time-delays are easily handled so that no approximation is required.

## 9.5 CONVERTING THE TRANSFER FUNCTION MODEL TO STATE-SPACE FORM

In this section we show one way to convert the input-output transfer function model to state-space form. Although the Laplace domain is used for analysis, the state-space form will normally be used for time domain simulations. Consider the transfer function relationship:

$$y(s) = \frac{k}{\tau^2 s^2 \zeta \tau + 2\zeta \tau s + 1} u(s)$$

which arises from the following equation:

$$\tau^2 \frac{d^2 y}{dt^2} + 2\zeta \tau \frac{dy}{dt} + y = k u(t) \quad (9.31)$$

Let:  $x_1 = y$  (9.32)

and:  $x_2 = \dot{x}_1$  (9.33)

so:  $\dot{y} = \dot{x}_1 = \dot{x}_2$  (9.34)

Divide (9.31) by  $\tau^2$  to obtain:

$$\frac{d^2 y}{dt^2} + \frac{2\zeta}{\tau} \frac{dy}{dt} + \frac{1}{\tau^2} y = \frac{k}{\tau^2} u(t)$$

which we can write as:

$$\frac{d^2 y}{dt^2} = -\frac{2\zeta}{\tau} \frac{dy}{dt} - \frac{1}{\tau^2} y + \frac{k}{\tau^2} u(t)$$

or,

$$\dot{x}_2 = -\frac{2\zeta}{\tau} x_2 - \frac{1}{\tau^2} x_1 + \frac{k}{\tau^2} u(t)$$

and since:

$$\dot{x}_1 = x_2$$

and we can write in the state-space form

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{1}{\tau^2} & -\frac{2\zeta}{\tau} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{k}{\tau^2} \end{bmatrix} [u] \quad (9.35)$$

$$y = [1 \quad 0] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (9.36)$$

The student should show that defining  $y = x_2$  leads to the following state-space model:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -\frac{2\zeta}{\tau} & -\frac{1}{\tau^2} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \frac{k}{\tau^2} \\ 0 \end{bmatrix} [u] \quad (9.37)$$

$$y = [0 \quad 1] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (9.38)$$

MATLAB has routines for converting from transfer function form to state-space form (`tf2ss`) and vice versa (`ss2tf`). `tf2ss` is used in Example 9.5.

#### EXAMPLE 9.5 MATLAB Routine `tf2ss`

Consider the following second-order system:

$$y(s) = \frac{3}{2s^2 + 0.7071s + 1} u(s)$$

First, define the numerator and denominator arrays by:

$$\begin{aligned} \text{num} &= [ 3 ] \\ \text{den} &= [ 2 \quad 0.7071 \quad 1 ] \end{aligned}$$

and enter the command:

$$[a, b, c, d] = \text{tf2ss}(\text{num}, \text{den})$$

MATLAB returns the state-space matrices:

$$\begin{aligned} a &= \begin{bmatrix} -0.3535 & -0.5000 \\ 1.0000 & 0 \end{bmatrix} \\ b &= \begin{bmatrix} 1 \\ 0 \end{bmatrix} \\ c &= \begin{bmatrix} 0 & 1.5000 \end{bmatrix} \\ d &= \begin{bmatrix} 0 \end{bmatrix} \end{aligned}$$

Notice that the state space models in Example 9.5 are different than the matrices that are obtained from (9.35) and (9.36) or (9.37) and (9.38), but the different forms would all yield the same results for the output variable via simulation. Remember that a transfer function relates inputs to outputs but does not represent the actual states of the system. There are an infinite number of state-space models that will yield the same input/output model.

After finding the state-space form for a transfer function, we can use any available numerical integrator to solve problems. MATLAB routines of interest include `ode45`, `initial`, and `step`.

## 9.6 MATLAB ROUTINES FOR STEP AND IMPULSE RESPONSE

MATLAB has routines for step and impulse response of either transfer function models or state-space models. In the following, we show how these routines are used for transfer function models.

### 9.6.1 `step`

A quick way to generate step responses is to use the MATLAB function `step`. This can be used with either a state-space or a Laplace domain model.

Consider the following Laplace domain model:

$$g(s) = \frac{2(10s + 1)}{50s^2 + 15s + 3}$$

which can be written:

$$g(s) = \frac{20s + 2}{50s^2 + 15s + 3}$$

The following MATLAB commands are used to generate the response shown in Figure 9.14.

```
num = [20 2];
den = [50 15 3];
[y, x, t] = step(num, den)
plot(t, y)
```

Notice that a time vector is automatically generated, with a length close to the *settling time* of the process.

The same plot could be generated from the state-space form by using:

```
[y, x, t] = step(A, B, C, D, 1)
plot(t, y)
```

where  $A$ ,  $B$ ,  $C$ , and  $D$  are the state-space matrices and '1' indicates the first input. Although state variables are calculated, only the output variables are of interest.

We could supply an equally spaced time vector and use:

```
[y, x] = step(num, den, t)
```

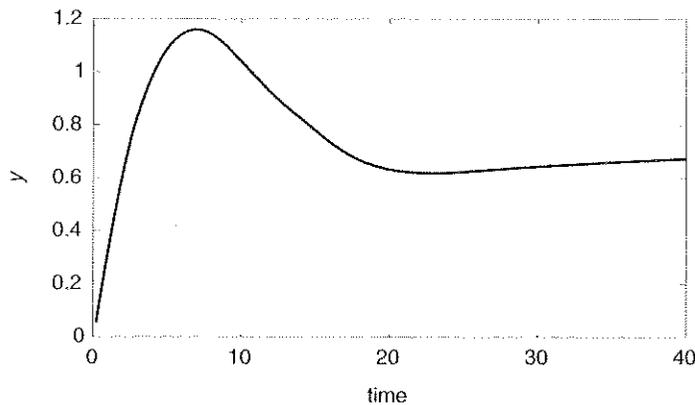
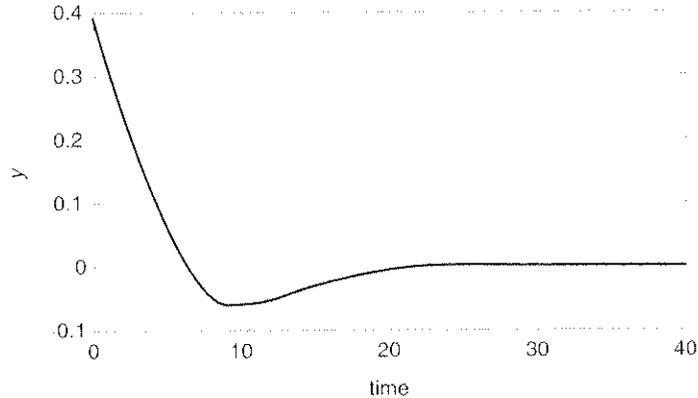


FIGURE 9.14 Step response for the example system.



**FIGURE 9.15** Impulse response for the example system.

for the step response of a transfer function model. The number of arguments determines whether a transfer function or state space model is used by the step function, and whether the time vector has been specified or not.

### 9.6.2 `impulse`

The output and time vectors are generated using:

```
[y, x, t] = impulse(num, den);
```

the plot is obtained from

```
plot(t, y)
```

The plot is shown in Figure 9.15 above. Notice that an impulse has an immediate (discontinuous) effect on the output, because this is a relative order one system.

We could also supply an equally spaced time vector and use:

```
[y, x] = impulse(num, den, t);
```

## SUMMARY

The step responses of the classical second order system (overdamped, critically damped, and underdamped) were presented. In addition, we showed the effect of numerator dynamics (and particularly right-half-plane zeros) on the response of a second-order system. The Padé approximations for deadtime were presented. You should understand the effect of the location of poles and zeros on the speed and quality of response of a transfer function model. The process gain is simply the ultimate change in output divided by the change in input.

The MATLAB routines used were

`tf2ss`: transfer function to state space  
`step`: step response  
`impulse`: impulse response

Critical concepts from this chapter include:

damping factor  
 natural period  
 numerator dynamics  
 Padé approximation for time-delay  
 relative order

## STUDENT EXERCISES

1. Derive the *step* responses for the following second-order systems.
  - a. Overdamped
  - b. Critically damped
  - c. Underdamped
2. Derive the *impulse* responses for the following second-order systems.
  - a. Overdamped
  - b. Critically damped
  - c. Underdamped
3. Consider a sine input with magnitude  $A$  and frequency  $\omega$ . Solve for the time domain value of the output for the following second-order systems.
  - a. Overdamped
  - b. Critically damped
  - c. Underdamped
4. For a second-order system with numerator dynamics, find the step response for the following.
  - a. Overdamped.
  - b. Underdamped.
  - c. Critically damped.
5. A second-order system has the following Laplace transfer function form:

$$Y(s) = \frac{2.5}{25s^2 + 5s + 1} U(s)$$

where the time unit is hours. The initial steady-state value for the output is 20 psig and the input is 4 gpm.

At  $t = 0$ , a step input decrease is made, from 4 gpm to 3 gpm.

- a. What is the final value of the output?
  - b. When does the output first reach this final value?
  - c. What is the minimum value of the output?
  - d. When does the output hit this minimum value?
  - e. Plot the response.
6. Consider the following second-order ODE:

$$\tau_1 \tau_2 \frac{d^2 y}{dt^2} + (\tau_1 + \tau_2) \frac{dy}{dt} + y = k \tau_n \frac{du}{dt} + k u$$

with the initial conditions  $y'(0) = y(0) = u'(0) = u(0) = 0$

- a. Find the Laplace transform of the differential equation. Write this expression in the form of  $y(s) = g(s) u(s)$
  - b. Now, assume that a step change of magnitude  $A$  in the variable  $u$  occurs at time = 0. Find the time domain result,  $y(t)$ .
  - c. Now, assume that a step change of magnitude  $A$  in the variable  $u$  occurs at time = 0. Find the time domain result,  $y(t)$ , by using a partial fraction expansion and solving for the inverse Laplace transform by hand.
  - d. Plot the time domain response,  $y(t)$  from part c. using the following parameter values  $k = 1$ ,  $\tau_1 = 3$ ,  $\tau_2 = 10$ , and try several plots, varying  $\tau_n$  from 3 to 10.
  - e. Plot the time domain response,  $y(t)$  from part c. using the following parameter values  $k = 1$ ,  $\tau_1 = 3$ ,  $\tau_2 = 10$ , and try several plots, varying  $\tau_n$  from -10 to 0.
7. Consider the following two first-order ODEs:

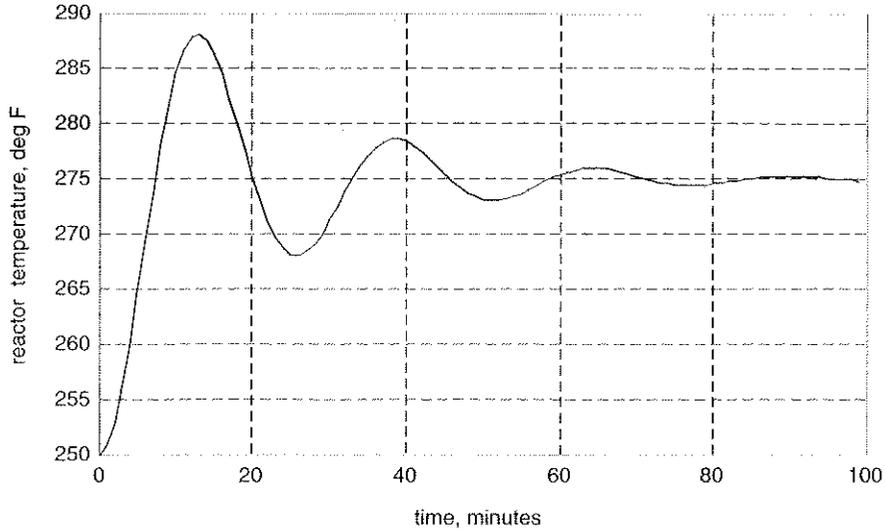
$$\tau_1 \frac{dx_1}{dt} + x_1 = k_1 u$$

$$\tau_2 \frac{dx_2}{dt} + x_2 = k_2 u$$

and the static relationship  $y = x_1 + x_2$

where  $x_1$  and  $x_2$  are two state variables,  $y$  is the output variable, and  $u$  is an input variable.

- a. Show that the two equations can be combined to yield a single ODE in the form of problem 6. Find  $k$  and  $\tau_n$  as a function of  $k_1$ ,  $k_2$ ,  $\tau_1$ ,  $\tau_2$ .
  - b. Now, assume that a step change of magnitude  $\Delta u$  in the variable  $u$  occurs at time = 0. Find the time domain result,  $y(t)$ , by using a partial fraction expansion and solving for the inverse Laplace transform by hand.
  - c. Plot  $x_1(t)$ ,  $x_2(t)$  and  $y(t)$  if  $\Delta u = 1$ ,  $k_1 = -1$ ,  $k_2 = 2$ ,  $\tau_1 = 3$ , and  $\tau_2 = 10$ .
8. As a process engineer with the Complex Pole Corporation, you are assigned a unit with an exothermic chemical reactor. In order to learn more about the dynamics of the process, you decide to make a step change in the input variable, which is coolant temperature, from 10°C to 15°C. Assume that the reactor was initially at a steady-state. You obtain the following plot for the output variable, which is reactor temperature (notice that the reactor temperature is in °F).



- What is the value of the process gain? (show units)
  - What is the value of  $\tau$ ? (show units)
  - What is the value of  $\zeta$ ? (show units)
  - What is the decay ratio?
  - What is the period of oscillation? (show units)
  - Write the second-order transfer function.
9. A process is described by the following linear ordinary differential equation:

$$4 \frac{d^2y}{dt^2} + 1.2 \frac{dy}{dt} + y = 2.5 \frac{d^2u}{dt^2}$$

where  $y$  is the output and  $u$  is the input. Assume that:

$$\frac{dy(0)}{dt} = y(0) = \frac{du(0)}{dt} = 0$$

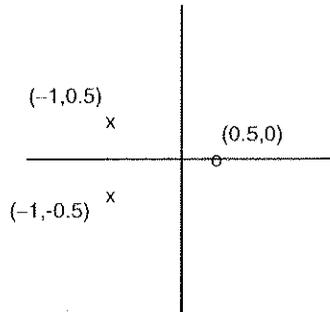
also, assume that at time  $t = 0$ , the input begins to increase with the following relationship

$$u(t) = \frac{1}{2} t^2$$

The units for time are minutes.

- What are the values of the poles of this process (give units)?
  - When does the output of the process reach a maximum value?
  - What is the maximum value of the process output?
10. A process has two poles and one zero. The poles are located at  $-1 \pm 0.5j$  and the zero is located at 0.5. Sketch the type of response that you expect to a step change in

input. Explain. Find the transfer function and verify these results assuming a gain of one.

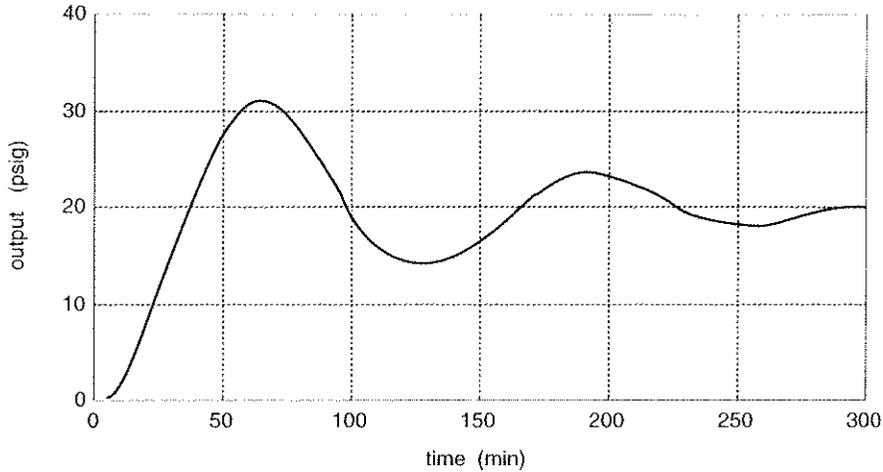


11. Consider the following state-space model (from Module 7):

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -2.405 & 0 \\ 0.833 & -2.238 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 7 \\ -1.117 \end{bmatrix} u$$

$$y = [0 \quad 1] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

- a. Find the transfer function  $g(s)$  where  $y(s) = g(s) u(s)$ .
  - b. Find the poles and zeros.
  - c. Plot the response to a unit step input.
  - d. Plot the response to a unit impulse input.
12. A process engineer responsible for the operation of a complex chemical reactor has the process operator make a step change in the coolant flowrate from 10 gpm to 15 gpm to the reactor at 2:00 pm. The reactor temperature is initially 150°F at 2:00 pm and drops to a low of 115°F at 2:10 pm. Eventually the reactor temperature comes to a final steady-state temperature of 125°F. Assuming that the response is second-order ( $k/\tau^2 s^2 + 2\zeta\tau s + 1$ ), find  $k$ ,  $\zeta$ ,  $\tau$  (show units).
13. The output of a second-order, underdamped system has a rise time of 1 hour, and a maximum value of 15°F (in deviation variables), after a step change at time  $t = 0$ . After a long period of time, the output is 12°F (again in deviation variables).
- a. What is the value of  $\tau$ ?
  - b. What is the value of  $\zeta$ ?
  - c. What are the poles? (also, show their location in the complex plane)
14. A step change of magnitude 2 lb/min is applied to the input of a process. The resulting output response, in deviation variables, is shown in the figure below.



Step response of a physical system, in deviation variables.

- a. Find the period of oscillation, rise time, and time to first peak, for this system. Show your work.
  - b. Find parameters (show the units) in the transfer function,  $g(s) = k/(\tau^2 s^2 + 2\zeta\tau s + 1)$ , by using the dimensionless plot, Figure 9.2. Show your work.
15. Consider the following third-order transfer function, where  $\beta$  is a parameter. Find the conditions on the parameter  $\beta$  that will give an inverse response.

$$g(s) = \frac{(2s^2 + s + \beta)}{(5s + 1)(3s + 1)(2s + 1)}$$

Show your work and explain your answer.

16. Consider the following transfer function:

$$g(s) = \frac{s^2 + s - 2}{s^2 + 4s + 3}$$

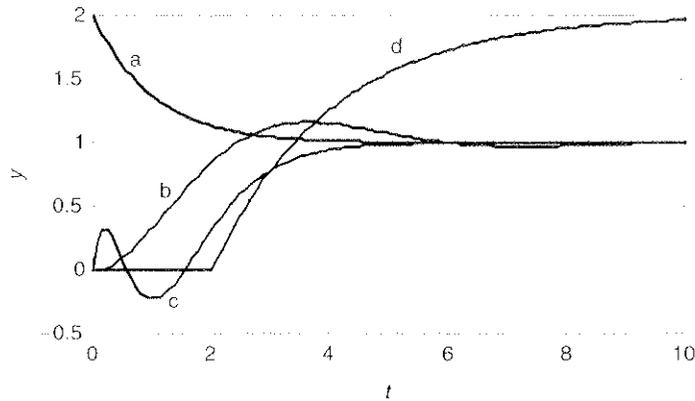
- a. Find the poles and zeros for this transfer function.
  - b. A unit step change is made at  $t = 0$ . Find the value of the output, using the final and initial value theorems:
    - i. After a long time.
    - ii. Immediately after the step change.
  - c. Verify your results in **b** by finding (analytically) the time domain solution.
  - d. Verify the results in **b** using the MATLAB function `step`.
17. Consider the following state-space model:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -6.5 & 2.5 \\ 4 & -6.5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0.00155 \\ 0.00248 \end{bmatrix} u$$

Find the transfer functions relating the input to each output. Find the step response of each output.

18. A unit step change in input is made on a number of processes (I–IV). The resulting outputs are shown in the plot below. Associate each process with a response curve.

Process	Transfer Function	Curve (letter) from Plot
I.	$g(s) = \frac{2e^{-2s}}{2s + 1}$	
II.	$g(s) = \frac{1}{s^2 + s + 1}$	
III.	$g(s) = \frac{2s - 1}{s + 1}$	
IV.	$g(s) = \frac{4(s^2 - 2s + 2)}{(s - 2)^2}$	



19. Consider a second-order transfer function with numerator dynamics:

$$y(s) = \frac{k(\tau_n s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)} u(s)$$

let  $\tau_1$  represent the smaller denominator time constant. Assume a step change in input. Show that a maximum in  $y(t)/k\Delta u$  occurs if  $\tau_n > \tau_2$  and that a minimum (indicating inverse response) occurs if  $\tau_n < 0$ . Also show that there is no extrema in the step response if  $0 < \tau_n < \tau_2$ . (*Hint:* Realize that a maximum or minimum occurs at  $\dot{y}/\Delta u = 0$ .)

20. Consider the transfer function  $g_p(s) = \frac{12s + 2}{3s^2 + 4s + 1}$

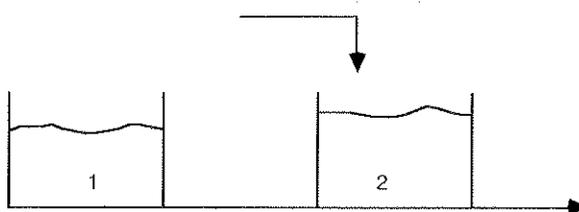
- a. Write the gain-polynomial form  $g_p(s) = \frac{k(\tau_p s + 1)}{\tau^2 s^2 + 2\zeta\tau s + 1}$
- b. Write the gain-time constant form  $g_p(s) = \frac{k(\tau_p s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)}$
- c. Write the gain-pole-zero form  $g_p(s) = \frac{k_1(s - z)}{(s - p_1)(s - p_2)}$

21. The reader should show how the first- and second-order Padé approximations relate to a Taylor series expansion. The Taylor series approximation to a time-delay in the Laplace domain is

$$e^{-\theta s} \approx 1 - \theta s + \frac{\theta^2 s^2}{2!} - \frac{\theta^3 s^3}{3!} + \frac{\theta^4 s^4}{4!} - \frac{\theta^5 s^5}{5!} + \frac{\theta^6 s^6}{6!} - \dots$$

Use long division of the first- and second-order Padé approximations and comment on the number of terms that are consistent with the Taylor series expression.

22. Consider the following interacting tank problem. Assume that the flow between tanks 2 and 1 is linearly proportional ( $\beta_1$ ) to the difference in tank heights and that the outlet flow from tank 2 is proportional ( $\beta_2$ ) to tank height 2. Develop the transfer function models relating the inlet flowrate to both tank heights.



23. Consider an exothermic chemical reactor that has the following transfer function relationship between the inlet flowrate (input) and the reactor temperature (output).

$$g(s) = \frac{2(-2.5s + 1)}{9s^2 + 3s + 1}$$

The units of the input are liter/min and the output is in deg C.

- a. Find the values of the zeros and poles. Is this system underdamped or overdamped?
- b. For a step input change of +3 liter/min, find how the output changes with time. How much does the temperature decrease before increasing? Compare plots of your analytical solution with those obtained using the MATLAB function `step`.
- c. What is the ultimate change in temperature after a long period of time?
- d. If the steady-state input and output values (in physical terms) are 10 liter/min and 75°C respectively, what are the physical values of the results in **b** and **c**?

- e. If a step decrease in the input of  $-3$  liter/min is made, what would be the results in **b**, **c**, and **d**?
24. Consider a CSTR with a first-order irreversible reaction  $A \rightarrow B$ . The modeling equations are:

$$\frac{dC_A}{dt} = -\left(\frac{F}{V} + k\right)C_A + \frac{F}{V}C_{Af}$$

$$\frac{dC_B}{dt} = kC_A - \frac{F}{V}C_B$$

The following parameters and steady-state input values characterize this system:

$$\frac{F}{V} = 0.2 \text{ min}^{-1}$$

$$k = 0.2 \text{ min}^{-1}$$

$$C_{Af} = 1.0 \frac{\text{gmol}}{\text{liter}}$$

The input is  $C_{Af}$  and the output is  $C_B$ . You should be able to show that the steady-state values of  $C_A$  and  $C_B$  are  $0.5$  gmol/liter.

- a. Show that the transfer function relating the feed concentration of  $A$  to the concentration of  $B$  is:

$$y(s) = \frac{0.5}{(5s + 1)(2.5s + 1)}$$

where the gain is  $\frac{\text{gmol B/liter}}{\text{gmol A/liter}}$ , and the time unit is minutes.

- b. At time  $t = 0$ , the input begins to vary in a sinusoidal fashion with amplitude  $0.25$  and frequency  $0.5 \text{ min}^{-1}$ ; that is,

$$u(t) = 0.25 \sin(0.5 t)$$

Using Laplace transforms, find how the output varies with time.

- c. Compare your results in **b** with the integration of the modeling equations using the MATLAB integration routine `ode45`. Remember to use the correct initial conditions. Also, remember that the transfer function results are in deviation variable form and must be converted back to physical variable values.
- d. Discuss how the amplitude of the output changes if the input frequency is changed to  $5 \text{ min}^{-1}$ .
25. Often higher-order process transfer functions are approximated by lower-order transfer functions. Consider the following second-order transfer function:

$$g(s) = \frac{1}{(2s + 1)(s + 1)}$$

Find the value of  $\tau$  in a first-order transfer function,  $1/(\tau s + 1)$ , which best approximates the step response of this second-order transfer function, in a least-squares sense.

(Hint: Define an error as a function of time as  $e(t) = y_2(t) - y_1(t)$ , where  $y_2$  and  $y_1$  are the step responses of the second- and first-order responses respectively. Find  $t$  which minimizes  $e^2(t)$  when  $t \rightarrow \infty$ .)

26. Consider a critically damped second-order system:

$$g(s) = \frac{1}{(\tau s + 1)(\tau s + 1)}$$

- For a unit step input change ( $\Delta u = 1$ ), find the time at which the rate of change of the output is greatest (i.e., find the inflection point).
- Compare this rate of change with a unit step response of a first-order system with the following transfer function:

$$g(s) = \frac{1}{(2\tau s + 1)}$$

- Plot the step responses for *a* and *b*, for  $\tau = 1$ . Compare and contrast the responses.
27. Pharmacokinetics is the study of how drugs infused to the body are distributed to other parts of the body. The concept of a compartmental model is often used, where it is assumed that the drug is injected into compartment 1. Some of the drug is eliminated (reacted) in compartment 1, and some of it diffuses into compartment 2 (the rest accumulates in compartment 1). Similarly, some of the drug that diffuses into compartment 2 diffuses back into compartment 1, while some is eliminated by reaction and the rest accumulates in compartment 2. Assuming that the rates of diffusion and reaction are directly proportional to the concentration of drug in the compartment of interest, the following balance equations arise:

$$\frac{dx_1}{dt} = -(k_{10} + k_{12})x_1 + k_{21}x_2 + u$$

$$\frac{dx_2}{dt} = k_{12}x_1 - (k_{20} + k_{21})x_2$$

where  $x_1$  and  $x_2$  = drug concentrations in compartments 1 and 2 ( $\mu\text{g}/\text{kg}$  patient weight), and  $u$  = rate of drug input to compartment 1 (scaled by the patient weight,  $\mu\text{g}/\text{kg min}$ ).

Experimental studies (of the response of the compartment 1 concentration to various drug infusions) have led to the following parameter values for the drug atracurium, which is a muscle relaxant:

$$(k_{10} + k_{12}) = 0.26 \text{ min}^{-1}$$

$$(k_{20} + k_{21}) = 0.094 \text{ min}^{-1}$$

$$k_{12}k_{21} = 0.015 \text{ min}^{-1}$$

- a. Find the poles and zeros of the transfer function that relate the input,  $u$ , to the output,  $x_1$ .
  - b. Find the response of the concentration in compartment 1,  $x_1$ , to a *step* input of  $1 \mu\text{g}/\text{kg min}$ . What is the value at 10 minutes? What is the value after a long period of time?
  - c. Find the response of the concentration in compartment 1,  $x_1$ , to an *impulse* input of  $10 \mu\text{g}/\text{kg}$ . What is the value at  $t = 0$ ? What is the value at 10 minutes?
28. Consider the following delay-differential equations:

$$\frac{dx_1}{dt} = -x_2(t - \theta) + u(t)$$

$$\frac{dx_2}{dt} = -2x_1$$

using the first-order Padé approximation for deadtime, write the corresponding (approximate) pure differential equations. (*Hint*: define a new variable  $x_3 = x_2(t - \theta)$ .)

Solve the equations using `ode45`, for an initial condition of 0 in all states, and a value of 1 for the input.

# MATRIX TRANSFER FUNCTIONS

# 10

Chapter 6 presented simple examples for transforming a state-space model to a single  $n$ th order differential equation. Once the single differential equation was obtained, the methods of characteristics and undetermined coefficients (Chapter 6) or Laplace transforms (Chapters 7–9) could be used to obtain a solution. A general method for converting a state-space model directly to the Laplace domain is presented in this chapter. With the transfer function representation, one can easily obtain the corresponding single  $n$ th order differential equation. After studying this chapter, the reader should be able to:

- Convert a state-space model to a transfer function model analytically.
- Convert a state-space model to a transfer function model using the MATLAB routine `ss2tf`.
- Discuss interesting effects from pole-zero cancellation.

The major sections are:

- 10.1 A Second-Order Example
- 10.2 The General Method
- 10.3 MATLAB Function `ss2tf`

The goal of this chapter is to take a general state-space model:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}$$

and convert it to the matrix transfer function form:

$$\mathbf{Y}(s) = \mathbf{G}(s) \mathbf{U}(s)$$

and use this model to solve for the responses of each output to each input. We will also use this technique to easily find the  $n$ th order differential equation corresponding to each output variable.

## 10.1 A SECOND-ORDER EXAMPLE

Consider the following two-state, single-input, single-output model:

$$\frac{dx_1}{dt} = a_{11}x_1 + a_{12}x_2 + b_{11}u \quad (10.1)$$

$$\frac{dx_2}{dt} = a_{21}x_1 + a_{22}x_2 + b_{21}u \quad (10.2)$$

$$y = c_{11}x_1 + c_{12}x_2 + d_{11}u \quad (10.3)$$

Taking Laplace transforms of (10.1) through (10.3), we find:

$$sX_1(s) - x_1(0) = a_{11}X_1(s) + a_{12}X_2(s) + b_{11}U(s) \quad (10.4)$$

$$sX_2(s) - x_2(0) = a_{21}X_1(s) + a_{22}X_2(s) + b_{21}U(s) \quad (10.5)$$

$$Y(s) = c_{11}X_1(s) + c_{12}X_2(s) + d_{11}U(s) \quad (10.6)$$

Assuming  $x_1(0) = x_2(0) = 0$ , and rearranging:

$$(s - a_{11})X_1(s) - a_{12}X_2(s) = b_{11}U(s) \quad (10.7)$$

$$(s - a_{22})X_2(s) - a_{21}X_1(s) = b_{21}U(s) \quad (10.8)$$

In order to generalize this procedure later, we write (10.7) and (10.8) in matrix form:

$$\begin{Bmatrix} s & 0 \\ 0 & s \end{Bmatrix} - \begin{Bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{Bmatrix} \begin{Bmatrix} X_1(s) \\ X_2(s) \end{Bmatrix} = \begin{Bmatrix} b_{11} \\ b_{21} \end{Bmatrix} U(s)$$

or,

$$\begin{Bmatrix} s & 1 \\ s & 1 \end{Bmatrix} - \begin{Bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{Bmatrix} \begin{Bmatrix} X_1(s) \\ X_2(s) \end{Bmatrix} = \begin{Bmatrix} b_{11} \\ b_{21} \end{Bmatrix} U(s) \quad (10.9)$$

and (10.6) is written in matrix form:

$$Y(s) = [c_{11} \quad c_{12}] \begin{bmatrix} X_1(s) \\ X_2(s) \end{bmatrix} + d_{11} U(s) \quad (10.10)$$

We see (10.9) is of the form:

$$(s\mathbf{I} - \mathbf{A}) \mathbf{X}(s) = \mathbf{B} U(s) \quad (10.11)$$

with the solution for  $\mathbf{X}(s)$ :

$$\mathbf{X}(s) = (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} U(s) \quad (10.12)$$

and writing (10.10) as:

$$Y(s) = \mathbf{C} \mathbf{X}(s) + \mathbf{D} U(s) \quad (10.13)$$

combining (10.12) and (10.13):

$$Y(s) = [\mathbf{C} (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + \mathbf{D}] U(s) \quad (10.14)$$

recall that often  $\mathbf{D} = \mathbf{0}$ , in which case (10.15) is written:

$$Y(s) = [\mathbf{C} (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}] U(s) \quad (10.15)$$

or,

$$Y(s) = \mathbf{G}(s) U(s) \quad (10.16)$$

In this example, since there is a single input and a single output,  $\mathbf{G}(s)$  is a single transfer function, which we call  $g(s)$ . The transfer function is the ratio of a numerator and a denominator polynomial:

$$g(s) = \frac{N(s)}{D(s)} \quad (10.17)$$

The reader should show that the polynomials in (10.17), based on (10.15) are (see student exercise 4):

$$N(s) = n_1 s + n_0 \quad (10.18a)$$

$$D(s) = s^2 + d_1 s + d_0 \quad (10.18b)$$

where the polynomial coefficients, in terms of the matrix coefficients, are:

$$n_1 = c_{11} b_{11} + c_{12} b_{21} \quad (10.19a)$$

$$n_0 = c_{11} [a_{12} b_{21} - a_{22} b_{11}] + c_{12} [a_{21} b_{11} - a_{11} b_{21}] \quad (10.19b)$$

$$d_1 = a_{11} + a_{22} \quad (10.19c)$$

$$d_0 = a_{11} a_{22} - a_{12} a_{21} \quad (10.19d)$$

Since the input-output relationship is written:

$$\mathbf{Y}(s) = \frac{N(s)}{D(s)} \mathbf{U}(s)$$

We can further write:

$$D(s) \mathbf{Y}(s) = N(s) \mathbf{U}(s)$$

or,

$$[s^2 + d_1 s + d_0] \mathbf{Y}(s) = [n_1 s + n_0] \mathbf{U}(s)$$

The corresponding differential equation is:

$$\frac{d^2 y}{dt^2} + d_1 \frac{dy}{dt} + d_0 y = n_1 \frac{du}{dt} + n_0 u$$

We now have an automated procedure to find the transfer function for a single-input, single-output, two-state system. An example is shown below.

#### Example 10.1 Linear Bioreactor Model

Consider a linearized model of a bioreactor, with the second-state variable (substrate concentration) measured and with dilution rate ( $F/V$ ) as the input variable.

The state-space matrices are

$$\mathbf{A} = \begin{bmatrix} 0 & 0.9056 \\ -0.7500 & -2.5640 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} -1.5302 \\ 3.8255 \end{bmatrix}$$

$$\mathbf{C} = [0 \quad 1]$$

$$\mathbf{D} = 0$$

Using the following steps to find  $\mathbf{G}(s) = \mathbf{C} (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}$ :

$$(s\mathbf{I} - \mathbf{A}) = \begin{bmatrix} s & -0.9056 \\ 0.7500 & s + 2.5640 \end{bmatrix}$$

Recalling the simple method for inverting a  $2 \times 2$  matrix, we find:

$$(s\mathbf{I} - \mathbf{A})^{-1} = \begin{bmatrix} s + 2.5640 & 0.9056 \\ -0.7500 & s \end{bmatrix} \frac{1}{s^2 + 2.5640s + 0.67920}$$

$$\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} = [-0.7500 \quad s] \frac{1}{s^2 + 2.5640s + 0.67920}$$

$$\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} = [-0.7500 \quad s] \begin{bmatrix} -1.5302 \\ 3.8255 \end{bmatrix} \frac{1}{s^2 + 2.5640s + 0.67920}$$

$$C(s\mathbf{I} - \mathbf{A})^{-1}B = \frac{3.8255s + 1.14765}{s^2 + 2.5640s + 0.67920}$$

so,

$$Y(s) = \frac{3.8255s + 1.14765}{s^2 + 2.5640s + 0.67920} U(s)$$

and we easily find that

$$\frac{d^2y}{dt^2} + 2.5640 \frac{dy}{dt} + 0.67920 y = 3.8255 \frac{du}{dt} + 1.14765 u$$

We generalize this procedure in Section 10.2.

### 10.2 THE GENERAL METHOD

Consider a general state-space model with  $n$  states,  $m$  inputs, and  $r$  outputs (see Chapter 5):

$$\begin{aligned} \frac{dx_1}{dt} &= a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n + b_{11}u_1 + \dots + b_{1m}u_m \\ &\vdots \\ \frac{dx_n}{dt} &= a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nm}x_n + b_{n1}u_1 + \dots + b_{nm}u_m \\ y_1 &= c_{11}x_1 + c_{12}x_2 + \dots + a_{1n}x_n + d_{11}u_1 + \dots + b_{1m}u_m \\ &\vdots \\ y_r &= c_{r1}x_1 + c_{r2}x_2 + \dots + c_{rn}x_n + d_{r1}u_1 + \dots + b_{rm}u_m \end{aligned} \tag{10.20}$$

which can be written in matrix form as:

$$\begin{aligned} \begin{bmatrix} \dot{x}_1 \\ \vdots \\ \dot{x}_n \end{bmatrix} &= \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & \dots & b_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ b_{n1} & b_{n2} & \dots & b_{nm} \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} \\ \begin{bmatrix} y_1 \\ \vdots \\ y_r \end{bmatrix} &= \begin{bmatrix} c_{11} & c_{12} & \dots & c_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{r1} & c_{r2} & \dots & c_{rn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} d_{11} & d_{12} & \dots & d_{1m} \\ \vdots & \vdots & \ddots & \vdots \\ d_{r1} & d_{r2} & \dots & d_{rm} \end{bmatrix} \begin{bmatrix} u_1 \\ \vdots \\ u_m \end{bmatrix} \end{aligned} \tag{10.21}$$

which has the form:

$$\begin{aligned}\dot{\mathbf{x}} &= \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \\ \mathbf{y} &= \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}\end{aligned}\tag{10.22}$$

where the dot over a state variable indicates the derivative with respect to time. Recall from Chapter 5 that the eigenvalues of the Jacobian matrix ( $\mathbf{A}$ ) determine the stability of the system of equations and the "speed" of response. Now, taking the Laplace transform of (10.22):

$$\begin{aligned}\mathbf{X}(s) &= (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} \mathbf{U}(s) \\ \mathbf{Y}(s) &= [\mathbf{C} (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + \mathbf{D}] \mathbf{U}(s)\end{aligned}$$

If  $\mathbf{D} = \mathbf{0}$  we can write:

$$\mathbf{Y}(s) = \mathbf{G}(s) \mathbf{U}(s)$$

where:

$$\mathbf{G}(s) = \mathbf{C} (s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B}$$

$(r \times m) \quad (r \times n) \quad (n \times n) \quad (n \times m)$

The transfer function matrix,  $\mathbf{G}(s)$ , is:

$$\mathbf{G}(s) = \begin{bmatrix} g_{11}(s) & g_{12}(s) & \cdot & \cdot & g_{1m}(s) \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ g_{r1}(s) & g_{r2}(s) & \cdot & \cdot & g_{rm}(s) \end{bmatrix}$$

Notice that  $\mathbf{G}(s)$  is square if  $r = m$  (number of outputs = number of inputs).

### 10.3 MATLAB ROUTINE `ss2tf`

The routine `ss2tf` can be used to convert a state-space model to a transfer function model. After entering the  $\mathbf{A}$ ,  $\mathbf{B}$ ,  $\mathbf{C}$ , and  $\mathbf{D}$  matrices, the command:

$$[\text{num}, \text{den}] = \text{ss2tf}(\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}, m)$$

will generate the numerator and denominator Laplace domain polynomials for the transfer function between input number  $m$  and the outputs, in descending order of  $s$ .

#### EXAMPLE 10.2 Example 10.1 Using MATLAB `ss2tf`

Here we consider the linearized bioreactor model, with two inputs. The first input is dilution rate, the same input used above. The second input is the substrate feed concentration. We will also consider both state 1 and state 2 to be outputs, and modify the  $\mathbf{C}$  and  $\mathbf{D}$  matrices so that `ss2tf` provides the transfer functions between the input and both outputs.

```

> A = [0,0.9056;-0.75,-2.5640]
A =
      0  0.9056
 -0.7500 -2.5640
> B = [-1.5302,0;3.8255,0.3]
B =
 -1.5302      0
  3.8255  0.3000
> C = [1,0;0,1]
C =
  1  0
  0  1
> D = [0,0;0,0]
D =
  0  0
  0  0

```

### Input 1

The numerator and denominator polynomials relating the first input to the two outputs are found using the following command:

```

> [num,den]=ss2tf(A,B,C,D,1)
num =
      0  -1.5302  -0.4591
      0   3.8255   1.1476
den =
  1.0000  2.5640  0.6792

```

where the first row of the num matrix is the coefficients of  $s$  in the  $g_{11}(s)$  polynomial, in decreasing order from left to right. Similarly, the second row of the num matrix is the coefficients of  $s$  in the  $g_{21}(s)$  polynomial, in decreasing order from left to right:

$$y_1(s) = g_{11}(s) u_1(s) = \frac{-1.5302s - 0.4591}{s^2 + 2.5640s + 0.6792} u_1(s)$$

$$y_2(s) = g_{21}(s) u_1(s) = \frac{3.8255s + 1.1476}{s^2 + 2.5640s + 0.6792} u_1(s)$$

We realize that the eigenvalues of the **A** matrix and the poles of the transfer functions will be the same. This is verified by the `roots` and `eig` commands

```

> roots(den)

ans =
    -2.2640
    -0.3000

> eig(a)

ans =
    -0.3000
    -2.2640

```

We can also write the transfer functions in pole-zero form:

$$y_1(s) = \frac{-1.5302 (s + 0.3)}{(s + 2.2640)(s + 0.3)} u_1(s)$$

$$y_2(s) = \frac{3.8255 (s + 0.3)}{(s + 2.2640)(s + 0.3)} u_1(s)$$

where we have the interesting result that the zero cancels one of the poles to yield first-order systems

$$y_1(s) = \frac{-1.5302}{(s + 2.2640)} u_1(s)$$

$$y_2(s) = \frac{3.8255}{(s + 2.2640)} u_1(s)$$

which we are more used to seeing in gain-time constant form:

$$y_1(s) = \frac{-0.6759}{0.4417 s + 1} u_1(s)$$

$$y_2(s) = \frac{1.6897}{0.4417 s + 1} u_1(s)$$

We would notice the zero-pole cancellation if we also used the `roots` command to find the roots of the numerator polynomial

```

>roots(num(1,:))

ans =
    -0.3000

>roots(num(2,:))

ans =
    -0.3000

```

and we see that the root of the numerator polynomial is the same as one of the roots of the denominator polynomial.

**Input 2**

The numerator and denominator polynomials relating the second input to the two outputs are found using the following command:

```
> [num, den] = ss2tf(a, b, c, d, 2)

num =
      0      0    0.2717
      0    0.3000      0

den =
  1.0000    2.5640    0.6792
```

and we have the result that:

$$y_1(s) = g_{12}(s) u_2(s) = \frac{0.2717}{s^2 + 2.5640s + 0.6792} u_2(s)$$

$$y_2(s) = g_{22}(s) u_2(s) = \frac{0.3s}{s^2 + 2.5640s + 0.6792} u_2(s)$$

The relationship between the second input and the second output is particularly interesting. The second input has no steady-state effect on the second output, as can be seen from the final value theorem. Assume a step change of magnitude  $\Delta u_2$  in input 2.

$$y(t \rightarrow \infty) = s Y(s \rightarrow 0) = \frac{0.3s}{s^2 + 2.5640s + 0.6792} \frac{\Delta u_2}{s} = 0$$

**10.3.1 Discussion of the Results from Example 10.2****THE FIRST INPUT**

We noticed that the transfer functions with respect to the first input had pole-zero cancellation. This created an input-output relationship where the step response is faster than would be expected, because the slow pole was canceled by the process zero

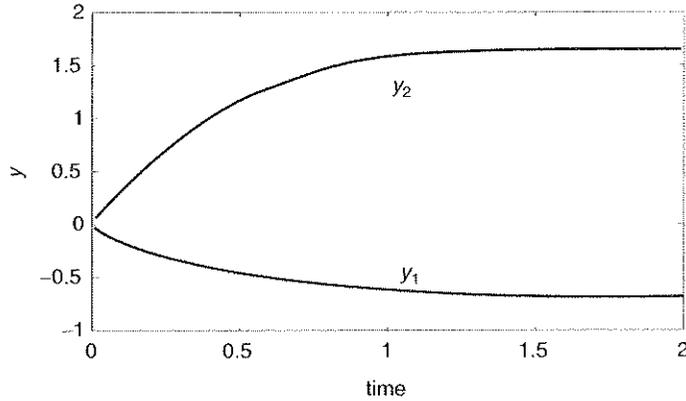
$$y_1(s) = \frac{-1.5302(s + 0.3)}{(s + 2.2640)(s + 0.3)} u_1(s)$$

$$y_2(s) = \frac{3.8255(s + 0.3)}{(s + 2.2640)(s + 0.3)} u_1(s)$$

This can also be seen using the gain-time constant form:

$$y_1(s) = \frac{-0.6759(3.3333s + 1)}{(0.4417s + 1)(3.3333s + 1)} u_1(s)$$

$$y_2(s) = \frac{1.6897(3.3333s + 1)}{(0.4417s + 1)(3.3333s + 1)} u_1(s)$$



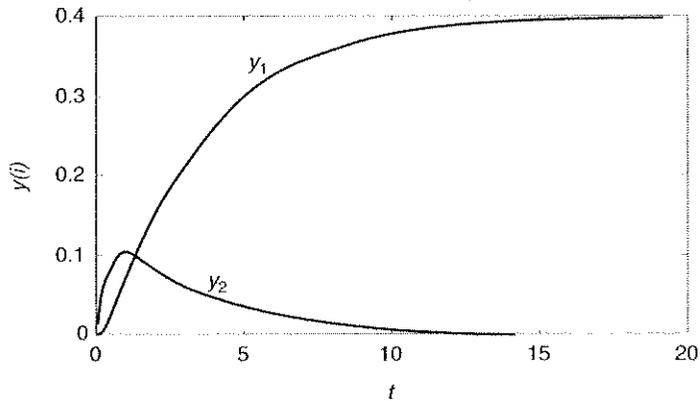
**FIGURE 10.1** Unit step change in input 1.

or,

$$y_1(s) = \frac{-0.6759}{0.4417s + 1} u_1(s)$$

$$y_2(s) = \frac{1.6897}{0.4417s + 1} u_1(s)$$

The step responses for a unit step input change are shown in Figure 10.1.



**FIGURE 10.2** Unit step change in input 2. Notice that the steady-state value of  $y_2$  does not change.

## THE SECOND INPUT

Notice that input 2 does not have a steady-state effect on output 2, only a dynamic effect. This can be seen by using the MATLAB `step` function, then plotting the results (see Figure 10.2).

```
num =
      0      0    0.2717
      0    0.3000      0

den =
  1.0000  2.5640  0.6792

>[y, x, t]=step(num, den)

plot(t, y)
```

## SUMMARY

We have shown how to convert a state-space model to a transfer function model, for multiple inputs and outputs. We have also seen some interesting results regarding pole-zero cancellation. One has to be particularly careful with pole-zero cancellation if a pole is unstable (positive), as will be shown in Section 11.3.

The following MATLAB routines were used:

```
ss2tf:  converts state space to transfer function form
eig:    matrix eigenvalues
roots:  roots of a polynomial
```

## STUDENT EXERCISES

1. Compare the step responses of the following three transfer functions:

$$\text{a. } g_1(s) = \frac{1}{(0.4417s + 1)(3.3333s + 1)}$$

$$\text{b. } g_2(s) = \frac{1}{0.4417s + 1}$$

$$\text{c. } g_3(s) = \frac{1}{3.3333s + 1}$$

Which has a faster step response? Why?

2. Consider the following state-space model (a 5-stage absorption column)

$$\mathbf{A} = \begin{bmatrix} -0.325 & 0.125 & 0 & 0 & 0 \\ 0.2 & -0.325 & 0.125 & 0 & 0 \\ 0 & 0.2 & -0.325 & 0.125 & 0 \\ 0 & 0 & 0.2 & -0.325 & 0.125 \\ 0 & 0 & 0 & 0.2 & -0.325 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 0.2 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0.25 \end{bmatrix}$$

- a. Convert this model to transfer function form, assuming that all of the states are outputs, using `ss2tf`.
  - b. Find the response of all of the states to a unit step in input 1. Use the function `step`.
  - c. Find the response of all of the states to a unit step in input 2. Use the function `step`.
  - d. Compare and contrast the curves from **b** and **c**.
3. Consider the following model for an isothermal CSTR with a single irreversible reaction (see Module 7). Find the transfer function matrix relating both inputs to both states.

$$\begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \end{bmatrix} = \begin{bmatrix} -0.4 & 0 \\ 0.2 & -0.2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0.5 & 0.2 \\ -0.5 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix}$$

4. For a 2-state, single-input, single-output process, derive the relationships shown in (10.18) and (10.19).
5. For the following state-space model, find the transfer function matrix relating all four inputs to both outputs.

$$\mathbf{A} = \begin{bmatrix} -0.4 & 0.3 \\ 3 & -4.5 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 0 & -7.5 & 0.1 & 0 \\ 50 & 0 & 0 & 1.5 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

6. Consider the following state-space model:

$$\begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{1}{5} & 0 \\ -\frac{1}{10} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \frac{7}{5} \\ \frac{2}{25} \end{bmatrix} u$$

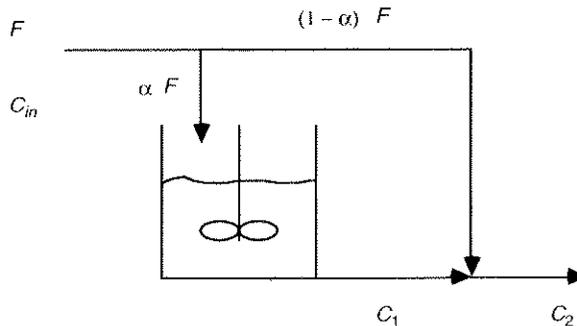
$$y = x_2$$

Show that the eigenvalues of the  $\mathbf{A}$  matrix are  $-1/5$  and  $1/2$ , so the system is unstable. Also, plot the step response. Derive the transfer function relating  $u(s)$  to  $y(s)$  and show that the unstable pole is cancelled by the positive zero. This problem will be analyzed in more detail in Chapter 11.

7. Consider a chemical reactor with bypass, as shown below. Assume that the reaction rate (per unit volume) is first-order ( $r = kC_1$ ) and  $C_1$  is the concentration in the reactor (the reactor is perfectly mixed). Assume that the volume in the reactor ( $V$ ) and the feed flowrate ( $F$ ) remain constant. The fraction of feed bypassing the reactor is  $(1 - \alpha)F$  and that entering the reactor is  $\alpha F$ . Assume that the fraction bypassing the reactor does not change. The inlet concentration ( $C_{in}$ ) is the input variable and the mixed outlet stream composition ( $C_2$ ) is the output variable. Write this model in state-space form, using deviation variables.

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u}$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u}$$

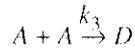
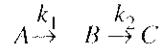


Find the transfer function relating  $u$  to  $y$ .

For the following parameters, simulate a unit step response.

$$F = 10 \text{ l/min}, V = 100 \text{ l}, C_{in} = 1 \text{ gmol/l}, \alpha = 0.5, k = 0.1 \text{ min}^{-1}.$$

8. Consider the following set of series and parallel reactions (from Module 7)



Material balances on components  $A$  and  $B$  yield the following two equations:

$$\frac{dC_A}{dt} = \frac{F}{V} (C_{Af} - C_A) + (-k_1 C_A - k_3 C_A^2)$$

$$\frac{dC_B}{dt} = \frac{F}{V} (-C_B) + (k_1 C_A - k_2 C_B)$$

where the rate constants are:

$$k_1 = \frac{5}{6} \text{ min}^{-1} \quad k_2 = \frac{5}{3} \text{ min}^{-1} \quad k_3 = \frac{1}{6} \frac{\text{liters}}{\text{mol min}}$$

and the steady-state feed and reactor concentration of component  $A$  are:

$$C_{Af} = 10 \frac{\text{mol}}{\text{liter}} \quad C_{As} = 3 \frac{\text{mol}}{\text{liter}}$$

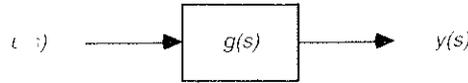
- Find the steady-state dilution rate ( $F/V$ ) and concentration of  $B$  (show all units).
- Linearize and put in state-space form (find the numerical values of the  $A$ ,  $B$ , and  $C$  matrices), assuming that the manipulated variables are dilution rate ( $F/V$ ) and feed concentration and that both states are outputs.
- Find the eigenvalues (show units).
- Find the transfer functions relating each output to each input. Find the poles and zeros for each transfer function and make plots of the responses to unit step changes in each input. Comment on your results.

The objective of this chapter is to introduce block diagram analysis. After studying this chapter, you should be able to:

- Analyze the stability of a block diagram system.
- Understand how inverse response processes can arise.
- Understand potential problems with pole-zero cancellation.
- Write a set of differential equations to simulate systems modeled by transfer functions in series.
- Use the MATLAB routines `series`, `parallel`, `feedback`, `conv`, and `roots`.
- Use SIMULINK for block diagram simulation.

Major sections of this chapter are:

- 11.1 Introduction to Block Diagrams
- 11.2 Block Diagrams of Systems in Series
- 11.3 Pole-Zero Cancellation
- 11.4 Systems in Series
- 11.5 Blocks in Parallel
- 11.6 Feedback and Recycle Systems
- 11.7 Routh Stability Criterion Applied to Transfer Functions
- 11.8 SIMULINK



**FIGURE 11.1** Block diagram representation.

We have shown how Laplace transforms are used to reduce differential equations to algebraic relationships. Algebraic equations are much easier to manipulate than differential equations. Similarly, block diagrams allow us to easily manipulate complex models that are composed of subsets of simple models.

## 11.1 INTRODUCTION TO BLOCK DIAGRAMS

Consider a standard first-order process model:

$$\tau \frac{dy(t)}{dt} + y(t) = k u(t) \quad (11.1)$$

which has the transfer function form:

$$y(s) = g(s) u(s) \quad (11.2)$$

where:

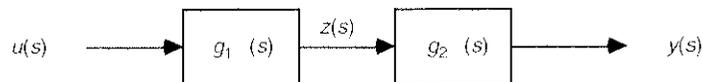
$$g(s) = \frac{k}{\tau s + 1} \quad (11.3)$$

Process engineers usually try and solve problems by sketching diagrams to understand input-output relationships. Process control engineers usually use block diagrams to understand the input-output relationships in a dynamic system. A block diagram representation of (11.2) is shown in Figure 11.1.

We can see that  $u(s)$  is the input to the transfer function block and  $y(s)$  is the output from the transfer function block. Block diagrams will be particularly useful when analyzing complex dynamic systems, which may be represented as blocks in series or parallel and with feedback. They are particularly useful for feedback control system design and analysis.

## 11.2 BLOCK DIAGRAMS OF SYSTEMS IN SERIES

Consider now the block diagram representation of two processes in series as shown in Figure 11.2.



**FIGURE 11.2** Block diagram of two processes in series.

The input/output transfer function of Figure 11.2 is:

$$y(s) = g_2(s) z(s) = g_2(s) g_1(s) u(s) \quad (11.4)$$

or,

$$y(s) = g(s) u(s) \quad (11.5)$$

where:

$$g(s) = g_2(s) g_1(s) \quad (11.6)$$

If the two transfer functions are first-order:

$$g_1(s) = \frac{k_1}{\tau_1 s + 1} \quad (11.7)$$

and

$$g_2(s) = \frac{k_2}{\tau_2 s + 1} \quad (11.8)$$

then the overall process is second order:

$$g(s) = \frac{k}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (11.9)$$

where:

$$k = k_1 k_2$$

The same idea can be continued for any number of transfer functions in series. The student should notice that the poles of a system composed of many transfer functions in series are simply the poles of each transfer function. This leads to the following conclusion about the *stability of systems with transfer functions in series*:

---

*If a system is composed of transfer functions in series, and if all of those transfer functions are stable, then the overall system is stable.*

---

Also, the zeros of a system of transfer functions in series are simply the zeros of the individual transfer functions.

### 11.3 POLE-ZERO CANCELLATION

Again, in this section we consider two blocks in series, as shown in Figure 11.2:

$$y(s) = g_2(s) z(s) = g_2(s) g_1(s) u(s) \quad (11.10)$$

If we are not careful, we can overlook possible problems with systems in series, if we look only at the overall input/output relationship. In the next example we show problems with *pole-zero cancellation*.

### EXAMPLE 11.1 Lead/Lag in Series with Unstable First-Order System

Consider the following lead/lag in series with an unstable first-order system:

$$g_1(s) = \frac{-2s + 1}{5s + 1} \quad (11.11)$$

$$g_2(s) = \frac{1}{-2s + 1} \quad (11.12)$$

We find that the zeros of  $g_1(s)$  cancel the poles of  $g_2(s)$ :

$$y(s) = g_2(s) g_1(s) u(s) = \left( \frac{-2s + 1}{5s + 1} \right) \left( \frac{1}{-2s + 1} \right) u(s)$$

yielding the transfer function relationship:

$$y(s) = g(s) u(s) = \frac{1}{5s + 1} u(s) \quad (11.13)$$

We must realize that these transfer functions ultimately represent a physical process. In practice, physical parameters cannot be known perfectly. What this means is that generally the numerator of  $g_1(s)$  will not exactly cancel the denominator of  $g_2(s)$ , in practice.

Consider a realistic case, where  $g_2(s)$  has a slight error in the value of the pole

$$g_2(s) = \frac{1}{-2.0001s + 1} \quad (11.14)$$

then we find that

$$\begin{aligned} y(s) &= g_2(s) g_1(s) u(s) = \left( \frac{-2s + 1}{5s + 1} \right) \left( \frac{1}{-2.0001s + 1} \right) u(s) \\ y(s) &= g(s) u(s) = \frac{-2s + 1}{-10.0005s^2 + 2.9999s + 1} u(s) \end{aligned} \quad (11.15)$$

Notice that when we do not have perfect pole/zero cancellation, there is an unstable pole in the input/output relationship,  $y(s) = g(s) u(s)$ . Our goal now is to compare the responses of the two models (11.13) and (11.15). Let  $y_1(s)$  represent the output in (11.13) and  $y_2(s)$  represent the output in (11.15). Assuming a unit step input,  $u(s) = 1/s$ ,

$$y_1(s) = \frac{1}{s(5s + 1)} \quad (11.16)$$

which has the time domain solution (Chapter 8):

$$y_1(t) = 1 - e^{-t/5} \quad (11.17)$$

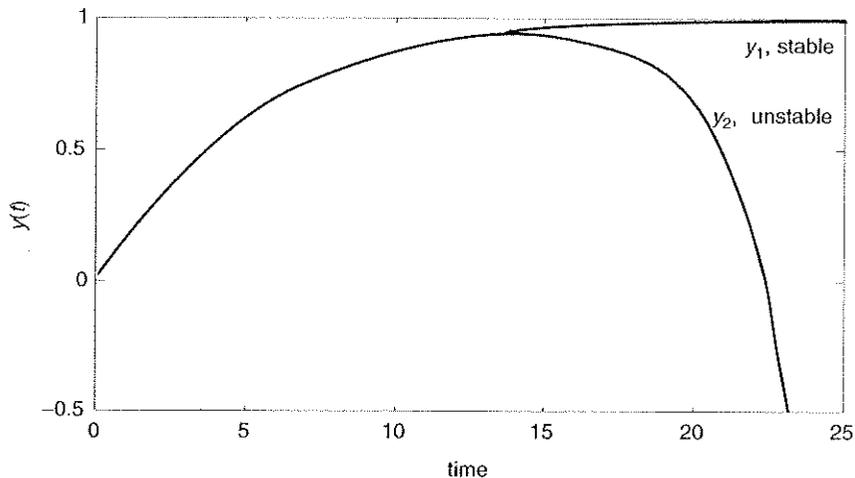
Also,

$$y_2(s) = \frac{-2s + 1}{s(-10.0005s^2 + 2.9999s + 1)} \quad (11.18)$$

which has the time domain solution (Chapter 9):

$$y_2(t) = 1 - \frac{7}{7.0001} e^{-t/5} - \frac{0.0001}{7.0001} e^{t/2.0001} \quad (11.19)$$

and we can see that, at low  $t$ , (11.19) is almost identical to (11.17). As time increases, however, the unstable exponential term in (11.19) begins to dominate. This is shown clearly in Figure 11.3.



**FIGURE 11.3** Comparison of (11.17) and (11.19).

Note that if we had used the state-space form for the model represented by equations (11.10) through (11.12), we would have discovered the instability, even for the perfect parameter case. The following example analyzes the state-space form of Example 11.1.

#### **EXAMPLE 11.1** Continued State-Space Analysis

Refer to  $z(s)$  as the output of the lead/lag block. From Chapter 8 we find the following state-space realization of the lead/lag:

$$\begin{aligned} \frac{dx}{dt} &= -\frac{1}{\tau_d} x + \left(1 - \frac{\tau_n}{\tau_d}\right) u \\ z &= \frac{1}{\tau_d} x + \frac{\tau_n}{\tau_d} u \end{aligned}$$

in our case,  $g_1(s) = \frac{\tau_a s + 1}{\tau_a s + 1} = \frac{-2s + 1}{5s + 1}$ , so:

$$\frac{dx}{dt} = -\frac{1}{5}x + \frac{7}{5}u \quad (11.20)$$

$$z = \frac{1}{5}x - \frac{2}{5}u \quad (11.21)$$

and the state space realization of the unstable lag is:

$$\frac{dy}{dt} = \frac{1}{2}y - \frac{1}{2}z \quad (11.22)$$

Substituting (11.21) into (11.22), we find

$$\frac{dy}{dt} = \frac{1}{2}y - \frac{1}{10}x + \frac{1}{5}u \quad (11.23)$$

If we use notation

$$x_1 = x$$

$$x_2 = y$$

we can write (11.20) and (11.23) in the following form:

$$\frac{dx_1}{dt} = -\frac{1}{5}x_1 + \frac{7}{5}u \quad (11.24)$$

$$\frac{dx_2}{dt} = \frac{1}{2}x_2 - \frac{1}{10}x_1 + \frac{1}{5}u \quad (11.25)$$

Using the usual state-space notation:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} u$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} u$$

we write

$$\begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{1}{5} & 0 \\ -\frac{1}{10} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} \frac{7}{5} \\ \frac{1}{5} \end{bmatrix} u \quad (11.26)$$

$$y = x_2$$

We easily find that the eigenvalues of the  $A$  matrix are  $-1/5$  and  $1/2$ . The positive eigenvalue indicates that this system is unstable.

The previous example illustrates the importance of not cancelling an unstable pole with a right-half-plane zero. It also shows how state-space analysis can always be used to address the stability of a system.

## 11.4 SYSTEMS IN SERIES

The dynamic behavior of chemical processes can often be represented as a series of simple models, such as first-order transfer functions. As an example, consider the following process, which is characterized as  $n$  first-order processes with a gain of 1 and a time constant of 5:

$$g(s) = \frac{1}{(5s + 1)^n} \quad (11.27)$$

The step responses for  $n = 1$  to 5 are shown in Figure 11.4. Notice the characteristic S-shape for all orders greater than 1 and the additional lag associated with each higher order.

### 11.4.1 Simulating Systems in Series

Although we analyze processes using transfer functions, to obtain time domain responses we must use a numerical integration package. Consider a system of  $n$  first-order processes in series, as shown in Figure 11.5.

Here we write the set of ordinary differential equations that describe this process. The ODE describing the first process is:

$$\frac{dx_1}{dt} = -\frac{1}{\tau_1} x_1 + \frac{k_1}{\tau_1} u \quad (11.28)$$

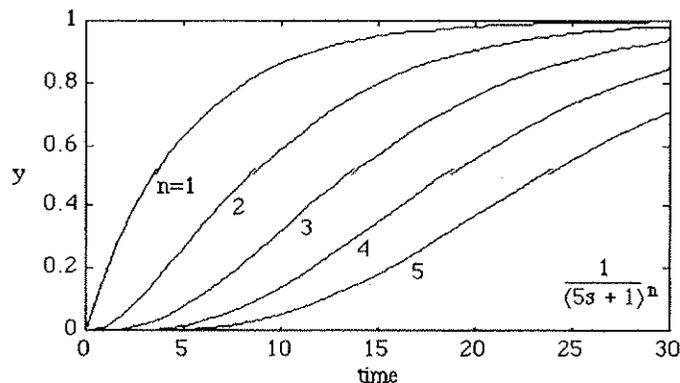
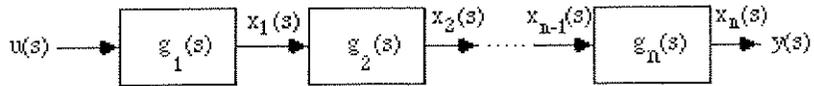


FIGURE 11.4. Step responses of first-order systems in series.

FIGURE 11.5  $n$  processes in series.

Notice that we can think of the output of the first process as the input to the second process:

$$\frac{dx_2}{dt} = -\frac{1}{\tau_2}x_2 + \frac{k_2}{\tau_2}x_1 \quad (11.29)$$

and so on through the  $n$ th process:

$$\frac{dx_n}{dt} = -\frac{1}{\tau_n}x_n + \frac{k_n}{\tau_n}x_{n-1} \quad (11.30)$$

To solve (11.28) through (11.30) we can use the numerical integration techniques developed in Chapter 4 or the analytical expressions developed in Chapter 6.

We can also write (11.28) through (11.30) in the following state-space form:

$$\begin{bmatrix} \frac{dx_1}{dt} \\ \frac{dx_2}{dt} \\ \vdots \\ \frac{dx_{n-1}}{dt} \\ \frac{dx_n}{dt} \end{bmatrix} = \begin{bmatrix} -\frac{1}{\tau_1} & 0 & \cdots & 0 & 0 \\ \frac{k_2}{\tau_2} & -\frac{1}{\tau_2} & \cdots & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdots & -\frac{1}{\tau_{n-1}} & 0 \\ 0 & 0 & \cdots & \frac{k_n}{\tau_n} & -\frac{1}{\tau_n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_{n-1} \\ x_n \end{bmatrix} + \begin{bmatrix} \frac{k_1}{\tau_1} \\ 0 \\ \cdot \\ \cdot \\ 0 \\ 0 \end{bmatrix} u \quad (11.26)$$

In Example 11.2 we show how to use the MATLAB routines `series` and `conv` to find a transfer function that represents two blocks in series.

### EXAMPLE 11.2 Two Transfer Functions in Series

Consider two processes,  $g_1(s)$  and  $g_2(s)$ , in series, where:

$$g_1(s) = \frac{1.5}{2s + 1}$$

$$g_2(s) = \frac{3}{4s + 1}$$

$$g(s) = g_1(s) g_2(s)$$

We use the following MATLAB commands to enter the numerator and denominator polynomials for each transfer function:

```
> num1 = [1.5];
> den1 = [2 1];
> num2 = [3];
> den2 = [4 1];
```

the `series` command generates the numerator and denominator polynomials for the transfer function  $g(s)$ :

```
> [num,den] = series(num1,den1,num2,den2)
num =
    0 0 4.5000
den =
    8 6 1
```

which indicates that

$$g(s) = \frac{4.5}{8s^2 + 6s + 1}$$

`conv`

`conv` is used to multiply two polynomials. Using the previous example, we multiply the numerator polynomials to find:

```
> num = conv(num1,num2)
num =
    4.5000
```

and the denominator polynomials to find:

```
> den = conv(den1,den2)
den =
    8 6 1
```

## 11.5 BLOCKS IN PARALLEL

Sometimes the behavior of a chemical process can be modeled by transfer functions in parallel as shown in Figure 11.6.

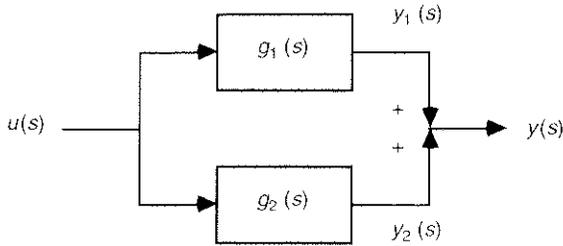


FIGURE 11.6 Systems in parallel.

For this system we can write the total output,  $y(s)$ , as the sum of two outputs,  $y_1(s) + y_2(s)$ .

$$y(s) = y_1(s) + y_2(s) \quad (11.31)$$

$$y(s) = [g_1(s) + g_2(s)] u(s) \quad (11.32)$$

or,

$$y(s) = g(s) u(s) \quad (11.33)$$

where:

$$g(s) = g_1(s) + g_2(s) \quad (11.34)$$

Consider the case where  $g_1(s)$  and  $g_2(s)$  are first-order transfer functions:

$$g_1(s) = \frac{k_1}{\tau_1 s + 1} \quad (11.35)$$

$$g_2(s) = \frac{k_2}{\tau_2 s + 1} \quad (11.36)$$

so

$$g(s) = \frac{k_1}{\tau_1 s + 1} + \frac{k_2}{\tau_2 s + 1} \quad (11.37)$$

Developing a common denominator, we find:

$$g(s) = \frac{(k_1 + k_2) \left[ \left( \frac{k_1 \tau_2 + k_2 \tau_1}{k_1 + k_2} \right) s + 1 \right]}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (11.38)$$

Notice that (11.38) has the form (see Chapter 9):

$$g(s) = \frac{k(\tau_n s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1)} \quad (11.39)$$

where:

$$k = k_1 + k_2 \quad (11.40)$$

$$\tau_n = \frac{k_1 \tau_2 + k_2 \tau_1}{k_1 + k_2} \quad (11.41)$$

We will assume that the transfer functions  $g_1(s)$  and  $g_2(s)$  are stable, so  $\tau_1$  and  $\tau_2 > 0$ . The goal of this section is to show a system where inverse response (discussed in Chapter 9 and Example 9.3) behavior can occur.

### 11.5.1 Conditions for Inverse Response

Recall that a transfer function will have inverse response only if there is a right-half-plane (positive) zero. Since the zero is  $-1/\tau_n$ , this system will have inverse response only if  $\tau_n < 0$ . We find that  $\tau_n < 0$  only if  $k_1$  and  $k_2$  are of opposite sign. We can arbitrarily assume that  $k_1 > 0$ , which means that  $k_2 < 0$  is necessary for inverse response. For inverse response, the condition:

$$\tau_n < 0 \quad \text{means that} \quad \frac{k_1 \tau_2 + k_2 \tau_1}{k_1 + k_2} < 0$$

or,

$$\frac{k_1 \tau_2}{k_1 + k_2} < \frac{-k_2 \tau_1}{k_1 + k_2}$$

which yields the following conditions for inverse response.

1. If  $k_1 + k_2 > 0$ , then  $k_1 \tau_2 < -k_2 \tau_1$ , which implies that  $\tau_2/\tau_1$  must be  $< -k_2/k_1$  for inverse response.
2. If  $k_1 + k_2 < 0$ , then  $k_1 \tau_2 > -k_2 \tau_1$ , which implies that  $\tau_2/\tau_1$  must be  $> -k_2/k_1$  for inverse response.

Physical examples of systems with inverse response include: steam drum level, reboilers in distillation columns, chemical and biochemical reactors. A reason that inverse response behavior is important is that it creates tremendous challenges for tight process control.

We can use the MATLAB routine `parallel` to simulate two systems in parallel, as shown by the next example.

#### EXAMPLE 11.3 Two systems in parallel

Consider the following system of two first-order processes in parallel (Figure 11.7):

$$g_1(s) = \frac{2}{5s + 1}$$

$$g_2(s) = \frac{-1}{1s + 1}$$

$$g(s) = \frac{2}{5s + 1} + \frac{-1}{1s + 1}$$

```

> num1 = [2];
> den1 = [5 1];
> num2 = [-1];
> den2 = [1 1];

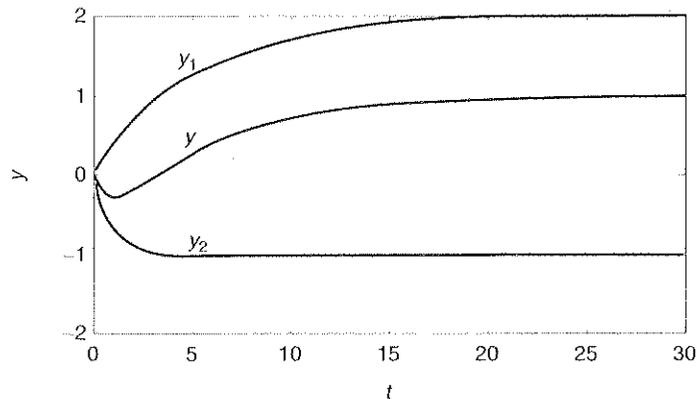
```

The following command is used to find the new transfer function:

```

> [num,den] = parallel(num1,den1,num2,den2)
num =
    0 -3 1
den =
    5 6 1
> [y,x,t] = step(num,den);
> [y1,x1] = step(num1,den1,t);
> [y2,x2] = step(num2,den2,t);
> plot(t,y,t,y1,t,y2)

```



**FIGURE 11.7** Two systems in parallel that have an inverse response when added together.

This previous example has shown that inverse response occurs in systems where the gain of the “slow process” (larger time constant) is larger in magnitude (but opposite in sign) than the “fast process” (smaller time constant).

## 11.6 FEEDBACK AND RECYCLE SYSTEMS

Feedback systems are common in engineering. Examples include chemical and biochemical reactors, where a certain portion of the product stream may be recycled to the feedstream. Feedback naturally occurs in most “self-regulating” models where, for example, the rate of change of a state variable (say, concentration of A) is a function of the same or another state variable (say, concentration of B).

The entire field of process control is based on the concept and theory of feedback systems. Our goal with this section is to introduce feedback analysis and, in particular, stability analysis of feedback systems. A block diagram of a feedback system is shown in Figure 11.8.

In this figure, the input to the feedback system is  $r(s)$  and the output is  $y(s)$ . Here we develop the relationship between  $r(s)$  and  $y(s)$ .

$$y(s) = g_1(s) u(s) \quad (11.44)$$

but 
$$u(s) = r(s) + z(s) \quad (11.45)$$

and 
$$z(s) = g_2(s) y(s) \quad (11.46)$$

So we can write (11.44) as:

$$y(s) = g_1(s) (r(s) + g_2(s)y(s)) \quad (11.47)$$

Solving for  $y(s)$  we find:

$$y(s) = \frac{g_1(s)}{1 - g_1(s)g_2(s)} r(s) \quad (11.48)$$

Notice that we can view this as:

$$y(s) = g_{cl}(s) r(s) \quad (11.49)$$

where 
$$g_{cl}(s) = \frac{g_1(s)}{1 - g_1(s)g_2(s)} \quad (11.50)$$

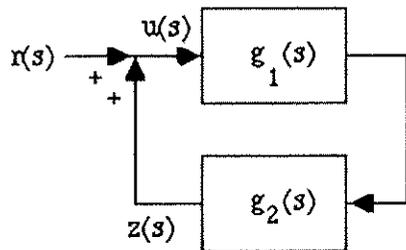


FIGURE 11.8 Feedback diagram.

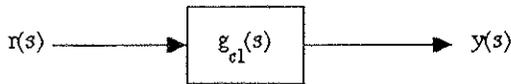
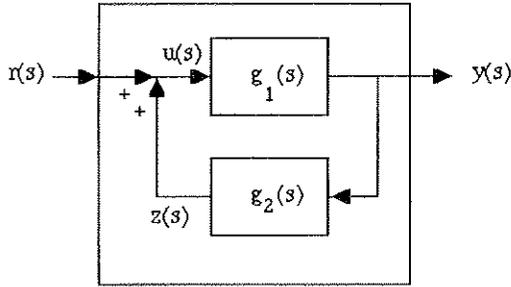


FIGURE 11.9 Equivalent block diagrams.

and we know that if the poles of  $g_{e1}(s)$  are stable, then the feedback system is stable. We realize that the two block diagrams shown in Figure 11.9 are equivalent.

#### EXAMPLE 11.4 Feedback system

Consider two first-order process transfer functions:

$$g_1(s) = \frac{k_1}{\tau_1 s + 1} \quad (11.51)$$

$$g_2(s) = \frac{k_2}{\tau_2 s + 1} \quad (11.52)$$

$$\begin{aligned} g_{e1}(s) &= \frac{g_1(s)}{1 - g_1(s)g_2(s)} = \frac{\frac{k_1}{\tau_1 s + 1}}{1 - \left(\frac{k_1}{\tau_1 s + 1}\right)\left(\frac{k_2}{\tau_2 s + 1}\right)} \\ &= \frac{k_1(\tau_2 s + 1)}{(\tau_1 s + 1)(\tau_2 s + 1) - k_1 k_2} \\ g_{e1}(s) &= \frac{k_1(\tau_2 s + 1)}{(\tau_1 \tau_2 s^2 + (\tau_1 + \tau_2)s + 1 - k_1 k_2)} \end{aligned} \quad (11.53)$$

and  $g_{e1}(s)$  is stable if the roots of  $\tau_1 \tau_2 s^2 + (\tau_1 + \tau_2)s + 1 - k_1 k_2$  are stable. We recall from the Routh stability criterion that all of the roots of a quadratic polynomial are negative if the coefficients of the polynomial are positive. If we assume that  $\tau_1$  and  $\tau_2$  are positive, then (11.53) will be stable if  $1 - k_1 k_2$  is positive. For stability, then,  $k_1 k_2$  must be less than 1. Let's consider the following numerical example:

$$g_1(s) = \frac{2}{5s + 1}$$

$$g_2(s) = \frac{k_2}{10s + 1}$$

Since  $k_1 = 2$ , then  $k_2$  must be less than 0.5 for stability.

As a numerical check, let  $k_2 = -1$ . Solving for the roots of:

$$\tau_1 \tau_2 s^2 + (\tau_1 + \tau_2)s + 1 - k_1 k_2 = 0$$

we find

$$50s^2 + 15s + 3 = 0$$

which has the roots (using the quadratic formula)

$$-0.15 \pm 0.1936j$$

(we can verify this result using the MATLAB routine `roots`)

Since the real part of the roots is negative, the system is stable. This is verified in the MATLAB simulation presented in Figure 11.10, where the response of the output to a unit step change in  $r$  is presented.

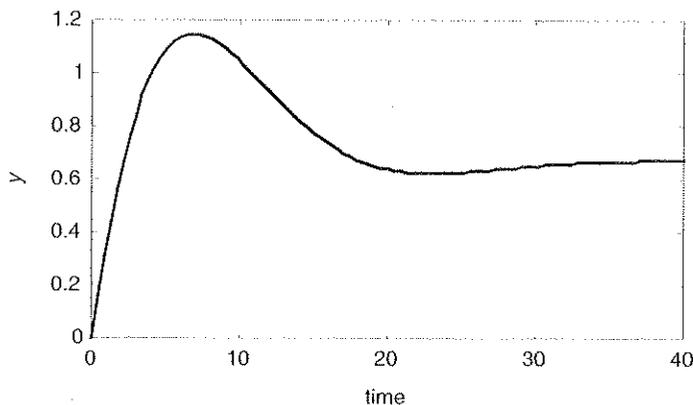


FIGURE 11.10 Step response for the example feedback system.

We can also use the MATLAB `feedback` function to obtain the closed-loop transfer function, as shown below.

$$g_1(s) = \frac{2}{5s + 1}$$

$$g_2(s) = \frac{-1}{10s + 1}$$

```

>> num1 = [2];
>> num2 = [-1];
>> den1 = [5 1];
>> den2 = [10 1];

```

and, using the routine `feedback`

```

>> [num, den] = feedback(num1, den1, num2, den2, 1)
num =
    0 20 2
den =
    50 15 3

```

We use the routine `step` to find the step response:

```
[y, x, t] = step(num, den)
```

which gives the plot shown in Figure 11.10.

## 11.7 ROUTH STABILITY CRITERION APPLIED TO TRANSFER FUNCTIONS

Recall from Chapter 6 that the purpose of the Routh stability criterion is to determine if a polynomial with the following form has any positive roots:

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \dots + a_1 \lambda + a_0 = 0 \quad (11.54)$$

Since transfer functions that have denominator polynomials in the Laplace transform variable ( $s$ ) are of the same form as (11.54), we can use Routh analysis to determine the stability of transfer functions. As before, assume that  $a_n > 0$ . If  $a_n < 0$ , then multiply (11.54) by  $-1$ . A *necessary* condition for stability is that all of the coefficients in (11.54) must be positive. If any of the coefficients are negative or zero, then at least one pole (root of the characteristic equation) is positive or zero, indicating that the equation is unstable. Even if all of the coefficients are positive, we cannot state that the system is stable. What is needed is a *sufficient* condition for stability. To determine that the system is stable, we must construct the Routh array and use the Routh stability criterion, which provides necessary and sufficient conditions for stability.

Sometimes we simply wish to determine if a particular system is stable or not, without actually evaluating the eigenvalues. This is particularly true if we wish to determine values of system parameters that will cause a system to lose stability. This approach will be useful in performing a bifurcation analysis in later chapters (14 and 15), and in tuning control systems for chemical processes.

**11.7.1 Routh Array**

If all of the coefficients of the characteristic equation (11.54) are positive, then develop the following Routh array:

Row				
1	$a_n$	$a_{n-2}$	$a_{n-4}$	...
2	$a_{n-1}$	$a_{n-3}$	$a_{n-5}$	...
3	$b_1$	$b_2$	$b_3$	...
4	$c_1$	$c_2$	...	
...				
$n+1$				

where  $n$  is the order of the polynomial. Notice that the first two rows consist of the coefficients of the polynomial. The elements of the third row are calculated in the following fashion:

$$b_1 = \frac{a_{n-1}a_{n-2} - a_n a_{n-3}}{a_{n-1}} \quad b_2 = \frac{a_{n-1}a_{n-4} - a_n a_{n-5}}{a_{n-1}}$$

and so on. Elements of the fourth and larger rows are calculated in a similar fashion:

$$c_1 = \frac{b_1 a_{n-3} - a_{n-1} b_2}{b_1} \quad c_2 = \frac{b_1 a_{n-5} - a_{n-1} b_3}{b_1}$$

and so on.

A sufficient condition for all roots of the characteristic polynomial to have negative real parts is that all of the elements in the first column of the Routh array are positive.

**EXAMPLE 11.5 Routh Array to Determine Closed-Loop Stability**

Consider the block diagram of Figure 11.9.

$$y(s) = \frac{g_1(s)}{1 - g_1(s)g_2(s)} r(s)$$

or,

$$y(s) = g_{cl}(s) r(s)$$

where:

$$g_{cl}(s) = \frac{g_1(s)}{1 - g_1(s)g_2(s)}$$

And the transfer functions are:

$$g_1(s) = \frac{2}{(5s + 1)(3s + 1)}$$

$$g_2(s) = \frac{k_2}{10s + 1}$$

Our goal is to find  $k_2$  to assure stability of the closed-loop system.

We easily find the transfer function,  $g(s)$ :

$$g(s) = \frac{2(10s + 1)}{(150s^3 + 95s^2 + 18s + 1 - 2k_2)}$$

which has the characteristic polynomial

$$150s^3 + 95s^2 + 18s + 1 - 2k_2$$

which is of the form

$$a_3s^3 + a_2s^2 + a_1s + a_0$$

The Routh array is:

Row

1	150	18
2	95	$1 - 2k_2$
3	$b_1$	0
4	$c_1$	

The *necessary* condition is that all  $a_i > 0$ , which is satisfied if  $1 - 2k_2 > 0$ , or  $k_2 < 0.5$ .

The *sufficient* condition is satisfied if all of the coefficients in the first column of the Routh array are positive.

$$b_1 = \frac{a_2a_1 - a_3a_0}{a_2} = 18 - \frac{150}{90}(1 - 2k_2) > 0$$

$$c_1 = \frac{b_1a_0 - a_2b_2}{b_1} = a_0 = 1 - 2k_2 > 0$$

The  $b_1$  condition is satisfied if  $k_2 > -5.2$ , while the  $c_1$  condition is the same as the necessary condition. We then have the following restriction on  $k_2$  for stability:

$$-5.2 < k_2 < 0.5$$

## 11.8 SIMULINK

In the previous sections we have shown how MATLAB routines can be used for block diagram analysis and simulation. The objective of this section is to use the block diagram simulation features of SIMULINK.

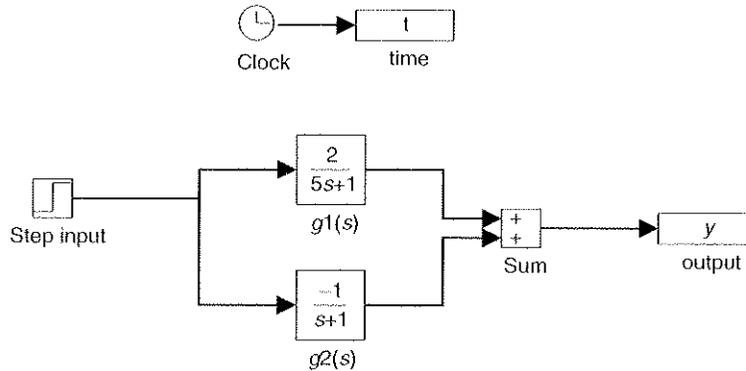


FIGURE 11.11 SIMULINK block diagram for two blocks in parallel.

Consider the block diagram system from Example 11.3. A SIMULINK block diagram is shown in Figure 11.11. Notice the use of step, transfer function, sum, workspace and clock blocks to generate the necessary input and output information.

The parameters menu is used to specify the integration type (LINSIM), final time (30), and minimum (0.01) and maximum (1) step sizes. The results are the same as shown in Figure 11.7. More information on SIMULINK is provided in Module 4 in the final section of the text.

## SUMMARY

Block diagram analysis is important because it allows us to think about a system of processes in terms of a combination of the individual processes. We have shown how to analyze the stability of a block diagram system, particularly if there are recycle or feedback processes. We have shown how inverse response processes can arise from systems in parallel. We have also shown potential problems with pole-zero cancellation when analyzing transfer functions in series.

The following MATLAB routines were used:

- `series`: two models in series (either transfer function or state space)
- `conv`: multiplies two polynomials
- `parallel`: two models in parallel (either transfer function or state space)
- `feedback`: two models in feedback form (either transfer function or state space, and either positive or negative feedback)
- `roots`: find the roots (zeros) of a polynomial

SIMULINK has also been used for block diagram simulation.

## STUDENT EXERCISES

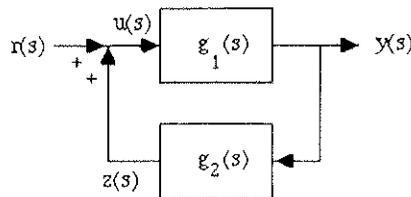
1. Consider a first-order process that has a positive pole (negative time constant), indicating that the process is open-loop unstable.

$$g_1(s) = \frac{1}{-5s + 1}$$

It is desirable to design a feedback compensator  $g_2(s)$ , so that the feedback system is stable. Assume that  $g_2(s)$  is simply a gain:

$$g_2(s) = k_2$$

Find the range of gains that will make the following feedback system stable.

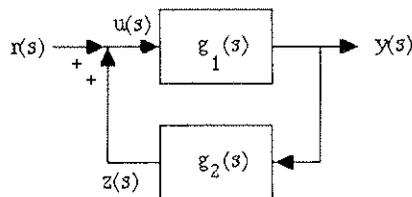


2. Consider the recycle system shown below, where:

$$g_1(s) = \frac{1}{(s-1)(s+0.5)}$$

$$g_2(s) = k$$

Find the values of  $k$  (if any) that will ensure stability of the system. Show your work and explain your reasoning.



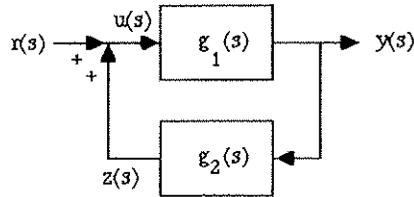
3. Find the analytical solution for a unit step applied to the following process:

$$g(s) = \frac{1}{(5s+1)^3}$$

4. Consider the recycle system shown below, where:

$$g_1(s) = \frac{1}{(s + 1)}$$

$$g_2(s) = \frac{k_2}{(\tau_2 s + 1)}$$



Discuss how the values of  $k_2$  and  $\tau_2$  effect the dynamic behavior of  $y$  with respect to a unit step input change in  $r$ . Use SIMULINK and show compare plots for various values of  $k_2$  and  $\tau_2$  to illustrate your points.

One purpose of this chapter is to summarize the techniques that have been developed in Chapters 5 through 11 to solve linear ordinary differential equations. Since the focus has been on initial value problems, we also introduce techniques to solve boundary value ODE problems. Also, since the emphasis has been on continuous (differential equation-based) models, another objective is to introduce discrete models. After studying this chapter, the student should be able to:

- Use the characteristic equation method to solve boundary value linear ODE problems
- Select an appropriate technique to solve a particular linear initial value problem
- Formulate linear discrete-time models
- Estimate parameters for linear discrete-time models

The major sections of this chapter are:

- 12.1 Background
- 12.2 Linear Boundary Value Problems
- 12.3 Review of Methods for Linear Initial Value Problems
- 12.4 Introduction to Discrete-Time Models
- 12.5 Parameter Estimation of Discrete Linear Systems

## 12.1 BACKGROUND

Thus far in this text, all of the problems that we have solved have been initial value ordinary differential equations. To solve these problems we simply need to know the initial values of the state variables, and how the inputs change with time. The models are then integrated to find how the states change with time. Ordinary differential equation models may be constrained to satisfy boundary conditions. Boundary value problems often arise when solving for the steady-state behavior of a dynamic system modeled by a partial differential equation. Typically, a boundary value problem has distance as the independent variable and the boundary conditions that must be satisfied are the values of the state variables at different locations (typically at each “end” of the system).

Recall that in Chapter 11 we required  $n$  initial conditions to solve an  $n$ th order initial value ODE. Similarly, we require  $n$  boundary conditions to solve an  $n$ th order boundary value ODE. Most chemical processes that can be modeled as second-order boundary value problems (e.g., the reaction-diffusion equation) are two-point boundary value problems. A second-order split boundary value problem has a boundary condition at one end and another boundary condition at the other end. If both boundary conditions were at the front end, then our problem would be an initial value problem. If both boundary conditions were at the rear end, then we would have an initial value problem by simply redefining the independent variable and forming an initial value problem in the opposite direction.

In this chapter, we first cover linear boundary value problems in Section 12.2 and review methods to solve linear initial value problems in Section 12.3. We provide an introduction to discrete-time models in Section 12.4 and show how to estimate parameters for discrete-time models in Section 12.5.

## 12.2 LINEAR BOUNDARY VALUE PROBLEMS

An analytical solution to boundary value ordinary conditions can be obtained using the method of characteristics when the ODE and the boundary conditions are linear. Consider the following second order ODE

$$a_2 \frac{d^2x}{dz^2} + a_1 \frac{dx}{dz} + a_0 x = 0 \quad (12.1)$$

where  $a_0$ ,  $a_1$  and  $a_2$  are constant coefficients,  $x$  is the state variable (dependent) and  $z$  is the independent variable (often distance). The solution to (12.1) will have the form

$$x = c_1 e^{\lambda_1 z} + c_2 e^{\lambda_2 z} \quad (12.2)$$

where  $\lambda_1$  and  $\lambda_2$  are obtained by rewriting (12.1) as

$$a_2 \lambda^2 + a_1 \lambda + a_0 = 0 \quad (12.3)$$

using the method discussed in Chapter 6. The constant coefficients ( $c_1$  and  $c_2$ ) are obtained from the boundary conditions.

### EXAMPLE 12.1 Second-order Boundary Value Problem

Consider the following second-order equation:

$$\frac{d^2x}{dz^2} + 4\frac{dx}{dz} + \frac{7}{4}x = 0 \quad (12.4)$$

subject to the boundary conditions at each end:

$$x(z = 0) = 2 \quad (12.5)$$

$$x(z = 1) = 1 \quad (12.6)$$

We solve for the eigenvalues by using the characteristic equation:

$$\lambda^2 + 4\lambda + \frac{7}{4} = 0 \quad (12.7)$$

which yields (from the quadratic formula):

$$\lambda_1 = -3.5 \quad (12.8)$$

$$\lambda_2 = -0.5 \quad (12.9)$$

and the solution is:

$$x = c_1 e^{-3.5z} + c_2 e^{-0.5z} \quad (12.10)$$

Substituting the boundary conditions results in two equations and two unknowns:

$$2 = c_1 + c_2 \quad (12.11)$$

$$1 = c_1 e^{-3.5} + c_2 e^{-0.5} \quad (12.12)$$

which yields:

$$c_1 = 0.36968$$

$$c_2 = 1.63032$$

A plot of the solution,  $x = 0.36968 e^{-3.5z} + 1.63032 e^{-0.5z}$ , is shown in Figure 12.1.

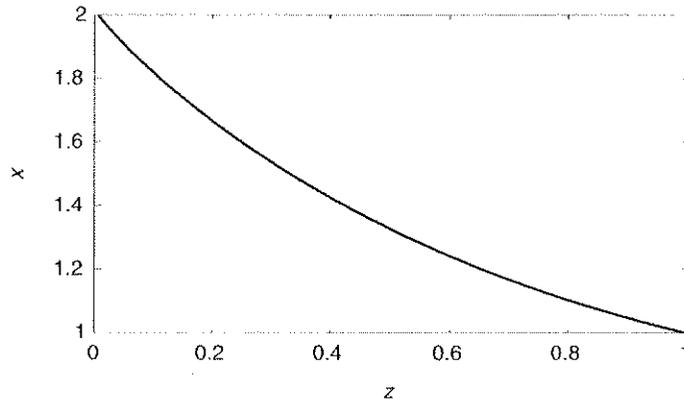


FIGURE 12.1 Solution to Example 12.1.

More generally, the boundary conditions may consist of some function of the state variable and its derivative. The more general linear boundary condition is the form:

$$b_1 \frac{dx}{dz} + b_0 x = d$$

### EXAMPLE 12.2 Second-Order Boundary Value Problem

Consider the second-order problem from the previous example:

$$\frac{d^2x}{dz^2} + 4 \frac{dx}{dz} + \frac{7}{4}x = 0 \quad (12.4)$$

subject to the new boundary conditions,

$$\frac{dx}{dz} + x = 1 \quad \text{at } z = 0 \quad (12.13)$$

$$\frac{dx}{dz} = 0 \quad \text{at } z = 1 \quad (12.14)$$

Since the solution is:

$$x = c_1 e^{-3.5z} + c_2 e^{-0.5z} \quad (12.15)$$

then the first derivative with respect to  $z$  is:

$$\frac{dx}{dz} = -3.5 c_1 e^{-3.5z} - 0.5 c_2 e^{-0.5z} \quad (12.16)$$

and boundary condition (12.13) yields:

$$-3.5 c_1 - 0.5 c_2 + c_1 + c_2 = 1 \quad (12.17)$$

while boundary condition (12.14) yields:

$$-3.5 c_1 e^{-3.5} - 0.5 c_2 e^{-0.5} = 0 \quad (12.18)$$

Solving these two equations for  $c_1$  and  $c_2$ , we obtain the solution:

$$x = -0.37394 e^{-3.5z} + 0.13032 e^{-0.5z} \quad (12.19)$$

which is shown in Figure 12.2.

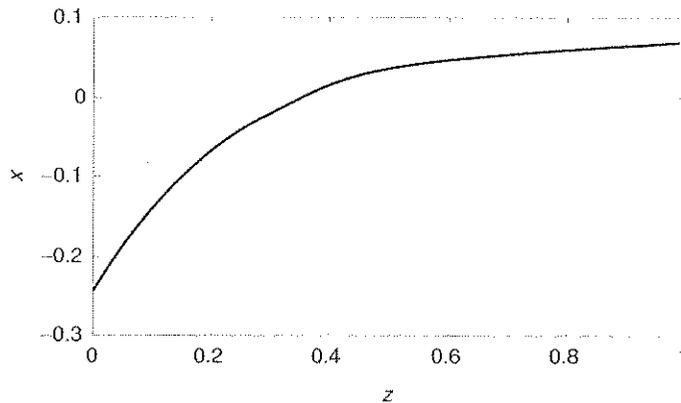


FIGURE 12.2 Solution to Example 12.2.

We have illustrated how the method of characteristics is used to solve linear boundary value problems. The solution to nonlinear boundary value problems generally involves iterative methods. For example, consider a single second-order nonlinear problem with boundary conditions at each end. We know that the second-order equation can be converted to two first-order equations. Typically, one boundary condition will fix an “initial condition” for one of the states. A second initial condition can be iteratively guessed (using a Quasi-Newton method, for example) until the equations, when integrated, yield the correct value for the end boundary condition. This approach is shown in Example 12.3 for the linear system considered in Example 12.1.

### EXAMPLE 12.3 Formulating a Boundary Value Problem as an Iterative Initial Value Problem

Consider the second-order boundary value problem:

$$\frac{d^2x}{dz^2} + 4\frac{dx}{dz} + \frac{7}{4}x = 0 \quad (12.4)$$

with the boundary conditions:

$$x(z = 0) = 2 \quad (12.5)$$

$$x(z = 1) = 1 \quad (12.6)$$

It can be shown that (see student exercise 1), by defining  $x_1 = x$  and  $x_2 = dx/dz$ , the following equations are obtained:

$$dx_1/dz = x_2 \quad (12.20)$$

$$dx_2/dz = -\frac{7}{4}x_1 - 4x_2 \quad (12.21)$$

and that one of the initial conditions is

$$x_1(z = 0) = 2 \quad (12.22)$$

We see that  $x_2(z = 0)$  must be "guessed," then the two equations can be integrated from  $z = 0$  to  $z = 1$ . The value of  $x_1$  at  $z = 1$  is then checked; if  $x_1(z = 1)$  is not equal to 1 (within an acceptable tolerance) then values of  $x_2(z = 0)$  are iteratively guessed until the final value is satisfied. This method is known as the "shooting method." The reader is encouraged to use this approach to solve exercise 1.

## 12.3 REVIEW OF METHODS FOR LINEAR INITIAL VALUE PROBLEMS

In Chapters 5 through 11 we presented a number of techniques for solving linear initial value ordinary differential equations. In Chapter 5 we noted that dynamic chemical process models are often formulated as a set of first-order, nonlinear differential equations, where the initial values are known. These equations have the general form:

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \quad (12.23)$$

$$\mathbf{y} = \mathbf{g}(\mathbf{x}, \mathbf{u}) \quad (12.24)$$

where  $\mathbf{x}$  is a vector of  $n$  state variables,  $\mathbf{u}$  is a vector of  $m$  input variables, and  $\mathbf{y}$  is a vector of  $r$  output variables:

$$\begin{aligned} \dot{x}_1 &= f_1(x_1, \dots, x_n, u_1, \dots, u_m) \\ &\vdots \\ \dot{x}_n &= f_n(x_1, \dots, x_n, u_1, \dots, u_m) \\ y_1 &= g_1(x_1, \dots, x_n, u_1, \dots, u_m) \\ &\vdots \\ y_r &= g_r(x_1, \dots, x_n, u_1, \dots, u_m) \end{aligned}$$

### 12.3.1 Linearization

Elements of the linearization matrices are defined in the following fashion:

$$\mathbf{A}_{ij} = \left. \frac{\partial f_i}{\partial x_j} \right|_{\mathbf{x}_s, \mathbf{u}_s}, \quad \mathbf{B}_{ij} = \left. \frac{\partial f_i}{\partial u_j} \right|_{\mathbf{x}_s, \mathbf{u}_s},$$

$$\mathbf{C}_{ij} = \left. \frac{\partial g_i}{\partial x_j} \right|_{\mathbf{x}_s, \mathbf{u}_s}, \quad \mathbf{D}_{ij} = \left. \frac{\partial g_i}{\partial u_j} \right|_{\mathbf{x}_s, \mathbf{u}_s},$$

where  $\mathbf{x}_s$ ,  $\mathbf{u}_s$ , and  $\mathbf{y}_s$  represent the steady-state values of the states, inputs, and outputs, which solve:

$$\mathbf{0} = \mathbf{f}(\mathbf{x}_s, \mathbf{u}_s) \quad (12.25)$$

$$\mathbf{y}_s = \mathbf{g}(\mathbf{x}_s, \mathbf{u}_s) \quad (12.26)$$

After linearization, we have the state space form:

$$\dot{\mathbf{x}}' = \mathbf{A} \mathbf{x}' + \mathbf{B} \mathbf{u}' \quad (12.27)$$

$$\mathbf{y}' = \mathbf{C} \mathbf{x}' + \mathbf{D} \mathbf{u}' \quad (12.28)$$

where the deviation variable vectors are:

$$\mathbf{x}' = \mathbf{x} - \mathbf{x}_s \quad (12.29)$$

$$\mathbf{u}' = \mathbf{u} - \mathbf{u}_s \quad (12.30)$$

Generally, the (') notation is dropped and it is understood that the model is in deviation variable form:

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \quad (12.31)$$

$$\mathbf{y} = \mathbf{C} \mathbf{x} + \mathbf{D} \mathbf{u} \quad (12.32)$$

Once the model is in this form, a number of techniques can be used.

### 12.3.2 Direction Solution Techniques

- a. Solve the zero-input (perturbation in initial conditions) form (Chapter 5):

$$\mathbf{x}(t) = e^{\mathbf{A}t} \mathbf{x}(0) \quad (12.33)$$

One way the matrix exponential can be solved is

$$e^{\mathbf{A}t} = \mathbf{V} e^{\Lambda t} \mathbf{V}^{-1} \quad (12.34)$$

The MATLAB function for matrix exponential is `expm`.

- b. For a constant step input at time zero (Chapter 5):

$$\mathbf{x}(t) = e^{\mathbf{A}t} \mathbf{x}(0) + (e^{\mathbf{A}t} - \mathbf{I}) \mathbf{A}^{-1} \mathbf{B} \mathbf{u}(0) \quad (12.35)$$

- c. For inputs that are constant over each time step (from  $t$  to  $t + \Delta t$ ) (Chapter 5):

$$\mathbf{x}(t + \Delta t) = e^{\mathbf{A}\Delta t} \mathbf{x}(t) + (e^{\mathbf{A}\Delta t} - \mathbf{I}) \mathbf{A}^{-1} \mathbf{B} \mathbf{u}(t) \quad (12.36)$$

which is often written as:

$$\mathbf{x}(k+1) = e^{A\Delta t} \mathbf{x}(k) + (e^{A\Delta t} - \mathbf{I}) \mathbf{A}^{-1} \mathbf{B} \mathbf{u}(k) \quad (12.37)$$

where  $k$  represents the  $k$ th time step. This represents a discrete-time model, which is discussed in more detail in Section 12.4.

### 12.3.3 Rewrite the State-Space Model as a Single $n$ th Order Ordinary Differential Equation

- a. Solve the homogeneous problem (Chapter 6):

$$a_n \frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = 0 \quad (12.38)$$

by first writing the characteristic equation:

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \dots + a_1 \lambda + a_0 = 0 \quad (12.39)$$

and solving for the roots (eigenvalues) of the  $n$ th order polynomial. If the roots are distinct, the solution is of the form:

$$x(t) = c_1 e^{\lambda_1 t} + c_2 e^{\lambda_2 t} + \dots + c_n e^{\lambda_n t} \quad (12.40)$$

where the coefficients are found using the  $n$  initial conditions.

- b. Solve the nonhomogeneous problem using the method of undetermined coefficients (Chapter 6):

$$a_n \frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = f(u(t)) \quad (12.41)$$

using a three-step procedure.

- i. Solve the *homogeneous* problem to find:

$$x_H(t) \quad (12.42)$$

- ii. Solve for the particular solution by determining the coefficients of a trial function (see Table 6.1, Chapter 6) that satisfy the *nonhomogeneous* equation:

$$x_P(t) \quad (12.43)$$

- iii. Combine the two solutions for:

$$x(t) = x_H(t) + x_P(t) \quad (12.44)$$

- c. Use Laplace transforms to solve the  $n$ th order equation (most useful for nonhomogeneous equations) (Chapters 7–11):

$$x(s) = \frac{1}{a_n s^n + a_{n-1} s^{n-1} + \dots + a_1 s + a_0} u(s) \quad (12.45)$$

which corresponds to the differential equation:

$$a_n \frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x = u(t) \quad (12.46)$$

The more general case is:

$$x(s) = \frac{b_n s^n + b_{n-1} s^{n-1} + \dots + b_1 s + b_0}{a_n s^n + a_{n-1} s^{n-1} + \dots + a_1 s + a_0} u(s) \quad (12.47)$$

which corresponds to the differential equation:

$$\begin{aligned} a_n \frac{d^n x}{dt^n} + a_{n-1} \frac{d^{n-1} x}{dt^{n-1}} + \dots + a_1 \frac{dx}{dt} + a_0 x \\ = b_n \frac{d^n u}{dt^n} + b_{n-1} \frac{d^{n-1} u}{dt^{n-1}} + \dots + b_1 \frac{du}{dt} + b_0 u \end{aligned} \quad (12.48)$$

For physically realizable systems,  $b_n = 0$ . Often many of the leading  $b_i$  terms are zero. If the leading  $r$  terms in the  $b$  polynomial are zero, then the system is referred to as relative order  $r$ .

### 12.3.4 Use Laplace Transforms Directly on the State-Space Model

Previously we have assumed that the state-space model has already been converted to a single  $n$ th order differential equation. We can also transform the set of  $n$  first-order linear state space equations directly using:

$$\mathbf{Y}(s) = [\mathbf{C}(s\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + \mathbf{D}] \mathbf{U}(s) \quad (12.49)$$

Generally, the Laplace transforms technique is used for nonhomogeneous problems, that is, systems that have an input forcing function (such as a step).

## 12.4 INTRODUCTION TO DISCRETE-TIME MODELS

Consider the general linear state space model:

$$\begin{bmatrix} \dot{x}_1 \\ \vdots \\ \dot{x}_n \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdot & a_{1n} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ a_{n1} & a_{n2} & \cdot & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} & \cdot & b_{1m} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ b_{n1} & b_{n2} & \cdot & b_{nm} \end{bmatrix} \begin{bmatrix} u_1 \\ \cdot \\ \cdot \\ u_m \end{bmatrix}$$

or,

$$\dot{\mathbf{x}} = \mathbf{A} \mathbf{x} + \mathbf{B} \mathbf{u} \quad (12.31)$$

Recall that the single variable equation:

$$\dot{x} = ax + bu \quad (12.50)$$

has the solution:

$$x(t) = e^{at} x(0) + (e^{at} - 1) \frac{b}{a} u(0) \quad (12.51)$$

when  $u(t) = \text{constant} = u(0)$ .

In a similar fashion, the solution to (12.31), for a constant input ( $\mathbf{u}(t) = \mathbf{u}(0)$ ) from  $t = 0$  to  $t$  is:

$$\mathbf{x}(t) = \Phi \mathbf{x}(0) + \Gamma \mathbf{u}(0) \quad (12.52)$$

where:

$$\Phi = e^{At} \quad (12.53)$$

and

$$G = (\Phi - \mathbf{I}) \mathbf{A}^{-1} \mathbf{B} \quad (12.54)$$

Equation (12.52) can be used to solve for a system where the inputs change from time step to time step ( $t$  to  $t+\Delta t$ ) by using:

$$\mathbf{x}(t + \Delta t) = \Phi \mathbf{x}(t) + \Gamma \mathbf{u}(t) \quad (12.55)$$

More often this is written as:

$$\mathbf{x}(k + 1) = \Phi \mathbf{x}(k) + \Gamma \mathbf{u}(k) \quad (12.56)$$

where  $k$  represents the  $k$ th time step. The output at time step  $k$  is written:

$$\mathbf{y}(k) = \mathbf{C} \mathbf{x}(k) + \mathbf{D} \mathbf{u}(k) \quad (12.57)$$

The stability of the discrete state-space model is determined by finding the eigenvalues of  $\Phi$ . If the magnitude of all of the eigenvalues is less than 1, then the system is stable.

### 12.4.1 Discrete Transfer Function Models

Continuous time models transfer function models are characterized by the Laplace transform variable,  $s$ . Similarly, for discrete transfer function models, a discrete transform variable,  $z$ , is used:

$$\mathbf{Y}(z) = \mathbf{G}(z) \mathbf{U}(z) \quad (12.58)$$

where:

$$\mathbf{G}(z) = [\mathbf{C} (z\mathbf{I} - \mathbf{A})^{-1} \mathbf{B} + \mathbf{D}] \quad (12.59)$$

For the case of a single input-single output system,  $\mathbf{G}(z)$  consists of a numerator and denominator polynomial of the form:

$$\mathbf{g}(z) = \frac{b_n z^n + b_{n-1} z^{n-1} + \dots + b_1 z + b_0}{a_n z^n + a_{n-1} z^{n-1} + \dots + a_1 z + a_0} \quad (12.60)$$

The transfer function is normally written in terms of the *backwards shift operator*,  $z^{-1}$ . Multiplying the transfer function by  $z^{-n}/z^{-n}$ , we find:

$$\mathbf{g}(z) = \frac{b_n + b_{n-1}z^{-1} + \dots + b_1z^{-n+1} + b_0z^{-n}}{a_n + a_{n-1}z^{-1} + \dots + a_1z^{-n+1} + a_0z^{-n}} \quad (12.61)$$

The backwards shift operator is defined as:

$$y(k-1) = z^{-1}y(z) \quad (12.62)$$

so  $y(k-2) = z^{-2}y(z)$ , etc. The discrete transfer function notation:

$$y(z) = \frac{b_n + b_{n-1}z^{-1} + \dots + b_1z^{-n+1} + b_0z^{-n}}{a_n + a_{n-1}z^{-1} + \dots + a_1z^{-n+1} + a_0z^{-n}} u(z) \quad (12.63)$$

then represents:

$$\begin{aligned} &(a_n + a_{n-1}z^{-1} + \dots + a_1z^{-n+1} + a_0z^{-n})y(z) \\ &= (b_n + b_{n-1}z^{-1} + \dots + b_1z^{-n+1} + b_0z^{-n})u(z) \end{aligned} \quad (12.64)$$

which corresponds to the discrete input/output model:

$$\begin{aligned} &a_n y(k) + a_{n-1} y(k-1) + \dots + a_1 y(k-n) + a_0 y(k-n-1) \\ &= b_n u(k) + b_{n-1} u(k-1) + \dots + b_1 u(k-n) + b_0 u(k-n-1) \end{aligned} \quad (12.65)$$

Usually we are solving for  $y(k+1)$ , and without loss of generality we can assume  $a_n = 1$ .

$$\begin{aligned} &y(k+1) + a_{n-1} y(k) + \dots + a_1 y(k-n+1) + a_0 y(k-n) \\ &= b_n u(k+1) + b_{n-1} u(k) + \dots + b_1 u(k-n-1) + b_0 u(k-n) \end{aligned} \quad (12.66)$$

Also, for most systems there is not an immediate effect of the input on the output, so  $b_n = 0$ .

The most common discrete-time model is first-order:

$$y(k+1) + a_0 y(k) = b_0 u(k) \quad (12.67)$$

or,

$$y(k+1) = -a_0 y(k) + b_0 u(k)$$

which has the transfer function relationship:

$$y(z) = \frac{b_0 z^{-1}}{1 + a_0 z^{-1}} \quad (12.68)$$

Physically realizable systems will always have at least a  $z^{-1}$  factor (unit time delay) in the numerator.

A first-order discrete system with  $N$  additional units of time-delay is written

$$y(k+1) + a_0 y(k) = b_0 u(k-N) \quad (12.69)$$

or,

$$y(k+1) = -a_0 y(k) + b_0 u(k-N)$$

which has the transfer function relationship:

$$y(z) = \frac{b_0 z^{-N-1}}{1 + a_0 z^{-1}} \quad (12.70)$$

#### EXAMPLE 12.4 Linear Van de Vusse Reactor Model

Consider a state-space model from the isothermal chemical reactor module (specifically, the Van de Vusse reaction):

$$\mathbf{A} = \begin{bmatrix} -2.4048 & 0 \\ 0.8333 & -2.2381 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 7.0000 \\ -1.1170 \end{bmatrix}$$

$$\mathbf{C} = [0 \quad 1]$$

$$\mathbf{D} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

For a sample time of 0.1 the discrete state-space model is (using (12.52)–(12.54), or the MATLAB `c2d` function):

$$\Phi = \begin{bmatrix} 0.7863 & 0 \\ 0.0661 & 0.7995 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} 0.6222 \\ -0.0849 \end{bmatrix}$$

and the discrete input-output model is (using (12.59), or the MATLAB `ss2tf` function)

$$\mathbf{g}(z) = \frac{-0.0751z^{-1} + 0.1001z^{-2}}{1 - 1.5857z^{-1} + 0.6286z^{-2}}$$

which has poles of 0.7995 and 0.7863 (which have a magnitude less than 1, so the system is stable). The zero of the numerator polynomial is 1.3339.

The step responses of the continuous and discrete systems are compared in Figure 12.3.

For a sample time of 0.75, the discrete state-space model is (using (12.52)–(12.54), or the MATLAB `c2d` function):

$$\Phi = \begin{bmatrix} 0.1647 & 0 \\ 0.1096 & 0.1866 \end{bmatrix}$$

$$\Gamma = \begin{bmatrix} 2.4314 \\ 0.1164 \end{bmatrix}$$

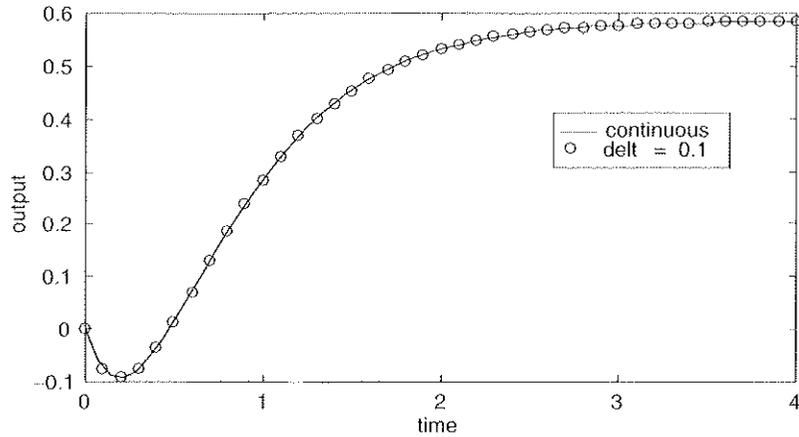


FIGURE 12.3 Step response of continuous and discrete ( $\Delta t = 0.1$ ) models.

and the discrete input-output model is (using (12.59), or the MATLAB `ss2tf` function):

$$g(z) = \frac{0.1564z^{-1} + 0.2408z^{-2}}{1 - 0.3513z^{-1} + 0.0307z^{-2}}$$

which has poles at 0.1866 and 0.1647, indicating stability. The zero of the numerator polynomial is  $-1.5399$ .

A comparison of the step responses of the continuous and discrete models is shown in Figure 12.4. Notice that the discrete sample time is too large to capture the “inverse response” behavior of the continuous system.

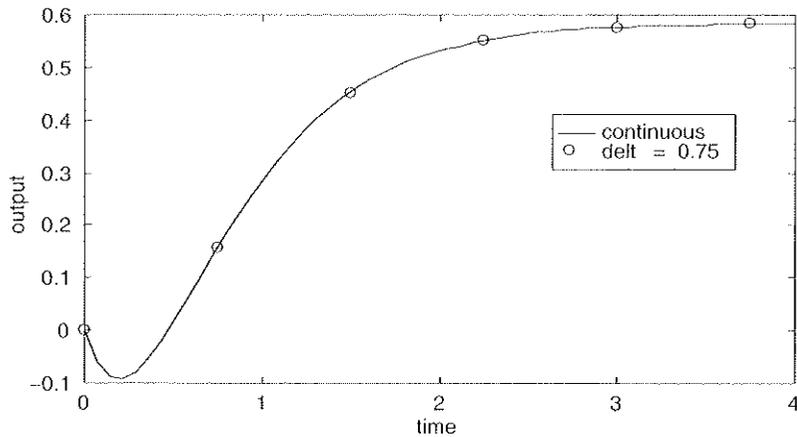


FIGURE 12.4 Step response of continuous and discrete ( $\Delta t = 0.75$ ) models.

## 12.5 PARAMETER ESTIMATION OF DISCRETE LINEAR SYSTEMS

Often when discrete linear models are developed, they are based on experimental system responses rather than converting a continuous model to a discrete model. The estimation of parameters for discrete dynamic models is no different than the linear regression analysis presented in Module 3. Please review Module 3 to understand the notation and ideas behind linear regression.

The measured inputs and outputs are the independent variables, and the dependent variables are the outputs. For simplicity, consider the following single input-single output model:

$$y(k) = -a_1 y(k-1) - a_0 y(k-2) + b_1 u(k-1) + b_0 u(k-2) \quad (12.71)$$

Now, for the system of  $N$  data points we can write:

$$\mathbf{Y} = \Phi \theta \quad (12.72)$$

where,

$$\mathbf{Y} = \begin{bmatrix} y(1) \\ \vdots \\ y(N) \end{bmatrix} \quad \Phi = \begin{bmatrix} \varphi(1)^T \\ \vdots \\ \varphi(N)^T \end{bmatrix} \quad \theta = \begin{bmatrix} -a_1 \\ -a_0 \\ b_1 \\ b_0 \end{bmatrix} \quad (12.73)$$

$$\varphi(k)^T = [y(k-1) \quad y(k-2) \quad u(k-1) \quad u(k-2)] \quad (12.74)$$

The solution to this problem is:

$$\theta = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{Y} \quad (12.75)$$

### EXAMPLE 12.5 Parameter Estimation

A unit step input is made to a system at time  $t = 0$  ( $k = 0$ ). The sample time is  $\Delta t = 0.75$ . The step response data are shown below and plotted in Figure 12.5.

$k$	$y(k)$
0	0
1	0.1564
2	0.4522
3	0.5513
4	0.5770
5	0.5830

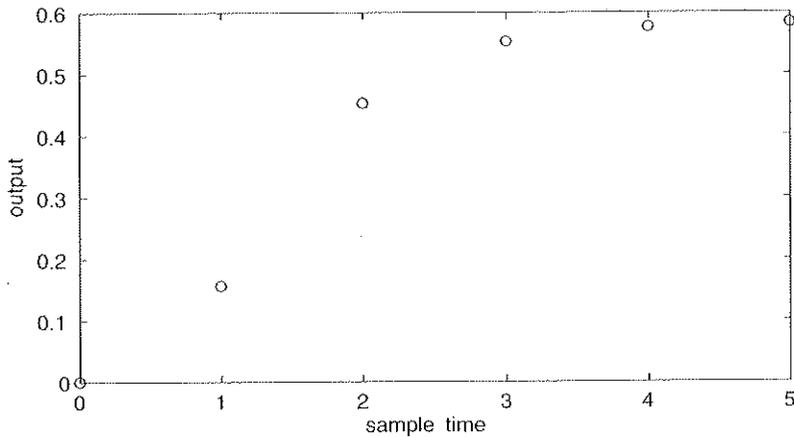


FIGURE 12.5 Step response data (same as Figure 12.4).

$$\mathbf{Y} = \begin{bmatrix} y(1) \\ y(2) \\ y(3) \\ y(4) \\ y(5) \end{bmatrix} = \begin{bmatrix} 0.1564 \\ 0.4522 \\ 0.5513 \\ 0.5770 \\ 0.5830 \end{bmatrix}$$

$$\Phi = \begin{bmatrix} \varphi(1)^T \\ \vdots \\ \varphi(5)^T \end{bmatrix} = \begin{bmatrix} y(0) & y(-1) & u(0) & u(-1) \\ \vdots & \vdots & \vdots & \vdots \\ y(4) & y(3) & u(4) & u(3) \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0.1564 & 0 & 1 & 1 \\ 0.4522 & 0.1564 & 1 & 1 \\ 0.5513 & 0.4522 & 1 & 1 \\ 0.5770 & 0.5513 & 1 & 1 \end{bmatrix}$$

The solution is:

$$\theta = (\Phi^T \Phi)^{-1} \Phi^T \mathbf{Y}$$

$$\begin{bmatrix} -a_1 \\ -a_0 \\ b_1 \\ b_0 \end{bmatrix} = \begin{bmatrix} 0.3513 \\ -0.0308 \\ 0.1564 \\ 0.2409 \end{bmatrix}$$

which are the same parameters that we found for the discrete transfer function model that was converted from the continuous model with a sample time of 0.75.

This simple example illustrated the step response of a perfectly modeled system (no measurement noise). The approach can also be applied to a system with arbitrary inputs and with noisy measurements. The data was analyzed in a batch fashion, that is, all of the data were collected before the parameter estimation was performed.

There are other approaches that are useful for estimating model parameters in real time, often using the model parameters to modify feedback control laws. These approaches are beyond the scope of this textbook. The MATLAB System Identification Toolbox is useful for these types of problems. A good reference is the text by Ljung.

## SUMMARY

There were multiple objectives to this chapter. The first was to introduce analytical solution techniques for boundary value ordinary differential equations. The second was to provide a concise review of techniques to solve linear initial value ordinary differential equations. The final objective was to introduce discrete-time models and discuss parameter estimation for these models.

For continuous-time models, the eigenvalues of the state-space model must have negative real portions for the system to be stable. Equivalently, the poles of the continuous transfer function models must be negative (the eigenvalues of the state-space model are equal to the poles of the transfer function model). Analogously, the eigenvalues of the discrete state-space model must have a magnitude less than one to be stable. Also, the poles of a discrete transfer function model must have magnitudes less than one to be stable.

Continuous-time input/output (transfer function) models with zeros that are positive exhibit inverse response. Similarly, discrete transfer function models with zeros that have a magnitude greater than one (yet have a negative real portion) exhibit inverse response.

## REFERENCES

The following text provides methods to solve boundary value ordinary differential equation models.

Rameriz, W.F. (1989). *Computational Methods for Process Simulation*. Boston: Butterworths.

Many process control textbooks provide coverage of linear discrete-time models. See, for example:

Ogunnaike, B.A., & W.H. Ray. (1994). *Process Dynamics, Modeling and Control*. New York: Oxford.

System identification (model parameter estimation) is covered in the text by Ljung

Ljung, L. (1987). *System Identification—Theory for the User*. Englewood Cliffs, NJ: Prentice-Hall.

## STUDENT EXERCISES

1. Consider the following second-order boundary value problem:

$$\frac{d^2x}{dz^2} + 4 \frac{dx}{dz} + \frac{7}{4}x = 0$$

where:

$$x(z = 0) = 2$$

$$x(z = 1) = 1$$

Show that, by defining  $x_1 = x$  and  $x_2 = dx/dz$ , the following equations are obtained:

$$dx_1/dz = x_2$$

$$dx_2/dz = -\frac{7}{4}x_1 - 4x_2$$

and that one of the initial conditions is:

$$x_1(z = 0) = 2$$

We see that  $x_2(z = 0)$  must be “guessed,” then the two equations can be integrated (using `ode45`) from  $z = 0$  to  $z = 1$ . The value of  $x_1$  at  $z = 1$  is then checked; if  $x_1(z = 1)$  is not equal to 1 (within an acceptable tolerance) then values of  $x_2(z = 0)$  are iteratively guessed until the final value is satisfied. This method is known as the “shooting method”. Use `fzero` to solve for the initial condition that satisfies the end boundary value.

2. Consider the reaction/dispersion equation

$$\frac{\partial C_A}{\partial t} = -v_z \frac{\partial C_A}{\partial z} + \tilde{D}_{AZ} \frac{\partial^2 C_A}{\partial z^2} - k C_A$$

let:  $C = \frac{C_A}{C_{A0}} = \text{dimensionless concentration}$

and:  $y = \frac{z}{L} = \text{dimensionless axial distance}$

define:  $\tau = \frac{\tilde{D}_{AZ} t}{L^2} = \text{dimensionless time}$

$P_e = \frac{v_z L}{D_{AZ}} = \text{Peclet number}$

and:  $D_a = \frac{k L^2}{D_{AZ}} = \text{Damkohler number}$

to show that: 
$$\frac{\partial C}{\partial \tau} = -P_e \frac{\partial C}{\partial y} + \frac{\partial^2 C}{\partial y^2} - D_a C \quad (12.2)$$

Find the dimensionless form of the Danckwerts boundary conditions at steady-state:

$$v_z C_{A0} = v_z C_A(0^+) - \tilde{D}_{AZ} \frac{dC_A(0^+)}{dz}$$

and: 
$$\frac{dC_A(L)}{dz} = 0$$

- a. Perform steady-state calculations (analytically) using the Danckwerts boundary conditions for:
- $P_e = 1, D_a = 1, 10, 25$  (compare on same plot)
  - $P_e = 10, D_a = 1, 10, 25, 100$  (compare on same plot)
  - $P_e = 25, D_a = 1, 10, 25, 100$  (compare on same plot)
  - $P_e = 100, D_a = 1, 10, 25, 100$  (compare on same plot)
3. Consider the following continuous state-space model:

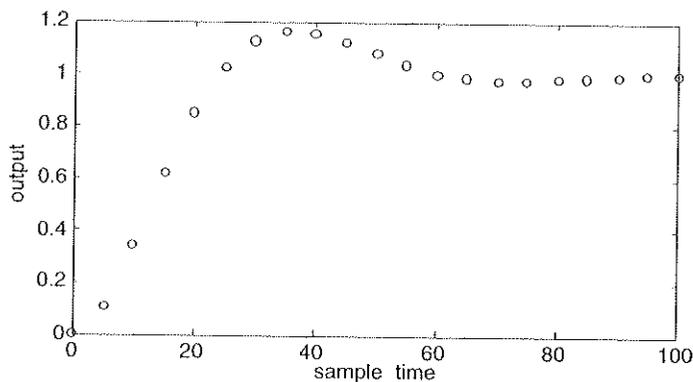
$$A = \begin{bmatrix} -3.6237 & 0 \\ 0.8333 & -2.9588 \end{bmatrix}$$

$$B = \begin{bmatrix} 5.5051 \\ -1.2660 \end{bmatrix}$$

$$C = [0 \quad 1]$$

$$D = 0$$

- Find the continuous transfer function model.
  - For a sample time of 0.25, find the discrete state-space and transfer function models.
  - Compare the step responses of the continuous and discrete models. What do you observe?
4. Consider a unit step change made at  $k = 0$ , resulting in the output response shown in the plot and table below.



$k$	0	1	2	3	4	5	6	7	8	9	10	11
$y$	0	0.1044	0.3403	0.6105	0.8494	1.0234	1.1244	1.1616	1.1531	1.1184	1.0746	1.0336
$k$	12	13	14	15	16	17	18	19	20			
$y$	1.0023	0.9828	0.9744	0.9742	0.9790	0.9860	0.9929	0.9985	1.0022			

Estimate the parameters for a discrete linear model with the form:

$$\mathbf{g}(z) = \frac{b_1 z^{-1} + b_0 z^{-2}}{1 - a_1 z^{-1} - a_0 z^{-2}}$$