



Mathematical Modelling Principles

CHAPTER

3

3.1 ■ INTRODUCTION

The models addressed in this chapter are based on fundamental theories or laws, such as the conservations of mass, energy, and momentum. Of many approaches to understanding physical systems, engineers tend to favor fundamental models for several reasons. One reason is the amazingly small number of principles that can be used to explain a wide range of physical systems; thus, fundamental principles *simplify* our view of nature. A second reason is the broad range of applicability of fundamental models, which allow extrapolation (with caution) beyond regions of immediate empirical experience; this enables engineers to evaluate potential changes in operating conditions and equipment and to design new plants. Perhaps the most important reason for using fundamental models in process control is the analytical expressions they provide relating key features of the physical system (flows, volumes, temperatures, and so forth) to its dynamic behavior. Since chemical engineers design the process, these relationships can be used to design processes that are as easy to control as possible, so that a problem created through poor process design need not be partially solved through sophisticated control calculations.

The presentation in this chapter assumes that the reader has previously studied the principles of modelling material and energy balances, with emphasis on steady-state systems. Those unsure of the principles should refer to one of the many introductory textbooks in the area (e.g., Felder and Rousseau, 1986; Himmelblau, 1982). In this chapter, a step-by-step procedure for developing fundamental models is presented that emphasizes dynamic models used to analyze the transient behavior

of processes and control systems. The procedure begins with a definition of goals and proceeds through formulation, solution, results analysis, and validation. Analytical solutions will be restricted to the simple integrating factor for this chapter and will be extended to Laplace transforms in the next chapter.

Experience has shown that the beginning engineer is advised to follow this procedure closely, because it provides a road map for the sequence of steps and a checklist of issues to be addressed at each step. Based on this strong recommendation, the engineer who closely follows the procedure might expect a guarantee of reaching a satisfactory result. Unfortunately, no such guarantee can be given, because a good model depends on the insight of the engineer as well as the procedure followed. In particular, several types of models of the same process might be used for different purposes; thus, the model formulation and solution should be matched with the problem goals. In this chapter, the modelling procedure is applied to several process examples, with each example having a goal that would be important in its own right and leads to insights for the later discussions of control engineering. This approach will enable us to complete the modelling procedure, including the important step of results analysis, and learn a great deal of useful information about the relationships between design, operating conditions, and dynamic behavior.

3.2 ■ A MODELLING PROCEDURE

Modelling is a task that requires creativity and problem-solving skills. A general method is presented in Table 3.1 as an aid to learning and applying modelling skills, but the engineer should feel free to adapt the procedure to the needs of

TABLE 3.1

Outline of fundamental modelling procedure

<ol style="list-style-type: none"> 1. Define goals <ol style="list-style-type: none"> a. Specific design decisions b. Numerical values c. Functional relationships d. Required accuracy 2. Prepare information <ol style="list-style-type: none"> a. Sketch process and identify system b. Identify variables of interest c. State assumptions and data 3. Formulate model <ol style="list-style-type: none"> a. Conservation balances b. Constitutive equations c. Rationalize (combine equations and collect terms) d. Check degrees of freedom e. Dimensionless form 4. Determine solution <ol style="list-style-type: none"> a. Analytical b. Numerical 	<ol style="list-style-type: none"> 5. Analyze results <ol style="list-style-type: none"> a. Check results for correctness <ol style="list-style-type: none"> 1. Limiting and approximate answers 2. Accuracy of numerical method b. Interpret results <ol style="list-style-type: none"> 1. Plot solution 2. Characteristic behavior like oscillations or extrema 3. Relate results to data and assumptions 4. Evaluate sensitivity 5. Answer "what if" questions 6. Validate model <ol style="list-style-type: none"> a. Select key values for validation b. Compare with experimental results c. Compare with results from more complex model
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particular problems. It is worth noting that the steps could be divided into two categories: steps 1 to 3 (model development) and steps 4 to 6 (model solution or simulation), because several solution methods could be applied to a particular model. All steps are grouped together here as an integrated modelling procedure, because this represents the vernacular use of the term *modelling* and stresses the need for the model and solution technique to be selected in conjunction to satisfy the stated goal successfully. Also, while the procedure is presented in a linear manner from step 1 to step 6, the reality is that the engineer often has to iterate to solve the problem at hand. Only experience can teach us how to “look ahead” so that decisions at earlier steps are made in a manner that facilitate the execution of later steps. Each step in the procedure is discussed in this section and is demonstrated for a simple stirred-tank mixing process.

Define Goals

Perhaps the most demanding aspect of modelling is judging the type of model needed to solve the engineering problem at hand. This judgment, summarized in the goal statement, is a critical element of the modelling task. The goals should be specific concerning the type of information needed. A specific numerical value may be needed; for example, “At what time will the liquid in the tank overflow?” In addition to specific numerical values, the engineer would like to determine semi-quantitative information about the characteristics of the system’s behavior; for example, “Will the level increase monotonically or will it oscillate?” Finally, the engineer would like to have further insight requiring functional relationships; for example, “How would the flow rate and tank volume influence the time that the overflow will occur?”

Another important factor in setting modelling goals is the accuracy of a model and the effects of estimated inaccuracy on the results. This factor is perhaps not emphasized sufficiently in engineering education—a situation that may lead to the false impression that all models have great accuracy over large ranges. The modelling and analysis methods in this book consider accuracy by recognizing likely errors in assumptions and data at the outset and tracing their effects through the modelling and later analysis steps. It is only through this careful analysis that we can be assured that designs will function properly in realistic situations.

EXAMPLE 3.1.

Goal. The dynamic response of the mixing tank in Figure 3.1 to a step change in the inlet concentration is to be determined, along with the way the speed and shape of response depend on the volume and flow rate. In this example, the outlet stream cannot be used for further production until 90% of the change in outlet concentration has occurred; therefore, a specific goal of the example is to determine how long after the step change the outlet stream reaches this composition.

Prepare Information

The first step is to identify the system. This is usually facilitated by sketching the process, identifying the key variables, and defining the boundaries of the system for which the balances will be formulated.

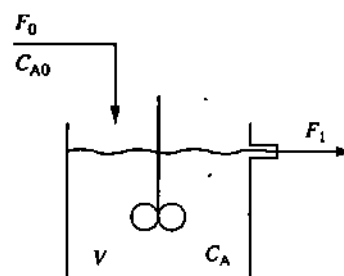


FIGURE 3.1

Continuous-flow stirred tank.



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The system, or control volume, must be a volume within which the important properties do not vary with position.

The assumption of a well-stirred vessel is often employed in this book because even though no such system exists in fact, many systems closely approximate this behavior. The reader should not infer from the use of stirred-tank models in this book that more complex models are never required. Modelling of systems via partial differential equations is required for many processes in which product quality varies with position; distributed models are required for many processes, such as paper and metals. Systems with no spatial variation in important variables are termed *lumped-parameter* systems, whereas systems with significant variation in one or more directions are termed *distributed-parameter* systems.

In addition to system selection, all models require information to predict a system's behavior. An important component of the information is the set of assumptions on which the model will be based; these are selected after consideration of the physical system and the accuracy required to satisfy the modelling goals. For example, the engineer usually is not concerned with the system behavior at the atomic level, and frequently not at the microscopic level. Often, but not always, the macroscopic behavior is sufficient to understand process dynamics and control. The assumptions used often involve a compromise between the goals of modelling, which may favor detailed and complex models, and the solution step, which favors simpler models.

A second component of the information is data regarding the physicochemical system (e.g., heat capacities, reaction rates, and densities). In addition, the external variables that are inputs to the system must be defined. These external variables, sometimes termed *forcing functions*, could be changes to operating variables introduced by a person (or control system) in an associated process (such as inlet temperature) or changes to the behavior of the system (such as fouling of a heat exchanger).

EXAMPLE 3.1.

Information. The system is the liquid in the tank. The tank has been designed well, with baffling and impeller size, shape, and speed such that the concentration should be uniform in the liquid (Foust et al., 1980).

Assumptions.

1. Well-mixed vessel
2. Density the same for A and solvent
3. Constant flow in

Data.

1. $F_0 = 0.085 \text{ m}^3/\text{min}$; $V = 2.1 \text{ m}^3$; $C_{A\text{init}} = 0.925 \text{ mole/m}^3$; $\Delta C_{A0} = 0.925 \text{ mole/m}^3$; thus, $C_{A0} = 1.85 \text{ mole/m}^3$ after the step
2. The system is initially at steady state ($C_{A0} = C_A = C_{A\text{init}}$ at $t = 0$)

Note that the inlet concentration, C_{A0} , remains constant after the step change has been introduced to this two-component system.

Formulate the Model

First, the important variables, whose behavior is to be predicted, are selected. Then the equations are derived based on fundamental principles, which usually can be divided into two categories: conservation and constitutive. The *conservation balances* are relationships that are obeyed by all physical systems under common assumptions valid for chemical processes. The conservation equations most often used in process control are the conservations of material (overall and component), energy, and momentum.

These conservation balances are often written in the following general form for a system shown in Figure 3.2:

$$\text{Accumulation} = \text{in} - \text{out} + \text{generation} \quad (3.1)$$

For a well-mixed system, this balance will result in an ordinary differential equation when the accumulation term is nonzero and in an algebraic equation when the accumulation term is zero. General statements of this balance for the conservation of material and energy follow.

OVERALL MATERIAL BALANCE.

$$\{\text{Accumulation of mass}\} = \{\text{mass in}\} - \{\text{mass out}\} \quad (3.2)$$

COMPONENT MATERIAL BALANCE.

$$\begin{aligned} \{\text{Accumulation of component mass}\} \\ = \{\text{component mass in}\} - \{\text{component mass out}\} \\ + \{\text{generation of component mass}\} \end{aligned} \quad (3.3)$$

ENERGY BALANCE.

$$\begin{aligned} \{\text{Accumulation of } U + \text{PE} + \text{KE}\} &= \{\text{ } U + \text{PE} + \text{KE in due to convection}\} \\ &- \{\text{ } U + \text{PE} + \text{KE out due to convection}\} \\ &+ Q - W \end{aligned} \quad (3.4)$$

which can be written for a system with constant volume as

$$\begin{aligned} \{\text{Accumulation of } U + \text{PE} + \text{KE}\} &= \{\text{ } H + \text{PE} + \text{KE in due to convection}\} \\ &- \{\text{ } H + \text{PE} + \text{KE out due to convection}\} \\ &+ Q - W_s \end{aligned} \quad (3.5)$$

where $H = U + pv = \text{enthalpy}$

KE = kinetic energy

PE = potential energy

pv = pressure times specific volume (referred to as flow work)

Q = heat transferred to the system from the surroundings

U = internal energy

W = work done by the system on the surroundings

W_s = shaft work done by the system on the surroundings

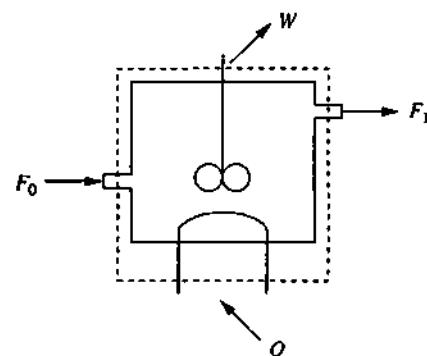


FIGURE 3.2

General lumped-parameter system.

The equations are selected to yield information on the key dependent variables whose behavior will be predicted within the defined system. The following guidelines provide assistance in selecting the proper balances.

- If the variable is *total liquid mass* in a tank or *pressure* in an enclosed gas-filled vessel, a material balance is appropriate.
- If the variable is *concentration* (mole/m³ or weight fraction, etc.) of a specific component, a component material balance is appropriate.
- If the variable is temperature, an energy balance is appropriate.

Naturally, the model may be developed to predict the behavior of several dependent variables; thus, models involving several balances are common.

In fact, the engineer should seek to predict the behavior of all important dependent variables using only fundamental balances. However, we often find that an insufficient number of balances exist to determine all variables. When this is the case, additional *constitutive equations* are included to provide sufficient equations for a completely specified model. Some examples of constitutive equations follow:

Heat transfer:	$Q = hA(\Delta T)$
Chemical reaction rate:	$r_A = k_0 e^{-E/RT} C_A$
Fluid flow:	$F = C_v(\Delta P/\rho)^{1/2}$
Equation of state:	$PV = nRT$
Phase equilibrium:	$y_i = K_i x_i$

The constitutive equations provide relationships that are not universally applicable but are selected to be sufficiently accurate for the specific system being studied. The applicability of a constitutive equation is problem-specific and is the topic of a major segment of the chemical engineering curriculum.

An important issue in deriving the defining model equations is "How many equations are appropriate?" By that we mean the proper number of equations to predict the dependent variables. The proper number of equations can be determined from the recognition that the model is correctly formulated when the system's behavior can be predicted from the model; thus, a well-posed problem should have no degrees of freedom. The number of *degrees of freedom* for a system is defined as

$$\text{DOF} = \text{NV} - \text{NE} \quad (3.6)$$

with DOF equal to the number of degrees of freedom, NV equal to the number of dependent variables, and NE equal to the number of independent equations. Not every symbol appearing in the equations represents a dependent variable; some are parameters that have known constant values. Other symbols represent external variables (also called *exogenous* variables); these are variables whose values are not dependent on the behavior of the system being studied. External variables may be constant or vary with time in response to conditions external to the system, such as a valve that is opened according to a specified function (e.g., a step). The value of each external variable must be known. NV in equation (3.6) represents the number of variables that depend on the behavior of the system and are to be evaluated through the model equations.



It is important to recognize that the equations used to evaluate NE must be *independent*; additional dependent equations, although valid in that they also describe the system, are not to be considered in the degrees-of-freedom analysis, because they are redundant and provide no independent information. This point is reinforced in several examples throughout the book. The three possible results in the degrees-of-freedom analysis are summarized in Table 3.2.

After the initial, valid model has been derived, a rationalization should be considered. First, equations can sometimes be combined to simplify the overall model. Also, some terms can be combined to form more meaningful groupings in the resulting equations. Combining terms can establish the key parameters that affect the behavior of the system; for example, control engineering often uses parameters like the time constant of a process, which can be affected by flows, volumes, temperatures, and compositions in a process. By grouping terms, many physical systems can be shown to have one of a small number of mathematical model structures, enabling engineers to understand the key aspects of these physical systems quickly. This is an important step in modelling and will be demonstrated through many examples.

A potential final modification in this step would be to transform the equation into dimensionless form. A dimensionless formulation has the advantages of (1) developing a general solution in the dimensionless variables, (2) providing a rationale for identifying terms that might be negligible, and (3) simplifying the repeated solution of problems of the same form. A potential disadvantage is some decrease in the ease of understanding. Most of the modelling in this book retains problem symbols and dimensions for ease of interpretation; however, a few general results are developed in dimensionless form.

EXAMPLE 3.1.

Formulation. Since this problem involves concentrations, overall and component material balances will be prepared. The overall material balance for a time

TABLE 3.2

Summary of degrees-of-freedom analysis

$$\text{DOF} = \text{NV} - \text{NE}$$

DOF = 0	The system is exactly specified , and the solution of the model can proceed.
DOF < 0	The system is overspecified , and in general, no solution to the model exists (unless all external variables and parameters take values that fortuitously satisfy the model equations). This is a symptom of an error in the formulation. The likely cause is either (1) improperly designating a variable(s) as a parameter or external variable or (2) including an extra, dependent equation(s) in the model. The model must be corrected to achieve zero degrees of freedom.
DOF > 0	The system is underspecified , and an infinite number of solutions to the model exists. The likely cause is either (1) improperly designating a parameter or external variable as a variable or (2) not including in the model all equations that determine the system's behavior. The model must be corrected to achieve zero degrees of freedom.

increment Δt is

$$\begin{aligned} \{\text{Accumulation of mass}\} &= \{\text{mass in}\} - \{\text{mass out}\} \\ (\rho V)_{(t+\Delta t)} - (\rho V)_t &= F_0 \rho \Delta t - F_1 \rho \Delta t \end{aligned} \quad (3.8)$$

with ρ = density. Dividing by Δt and taking the limit as $\Delta t \rightarrow 0$ gives

$$\frac{d(\rho V)}{dt} = V \frac{d\rho}{dt} + \rho \frac{dV}{dt} = \rho F_0 - \rho F_1 \quad (3.9)$$

The flow in, F_0 , is an external variable, because it does not depend on the behavior of the system. Because there is one equation and two variables (V and F_1) at this point, a constitutive expression is required for the flow out. Since the liquid exits by overflow, the flow out is related to the liquid level according to a weir equation, an example of which is given below (Foust et al., 1980).

$$F_1 = k_F \sqrt{L - L_w} \quad \text{for} \quad L > L_w \quad (3.10)$$

with k_F = constant, $L = V/A$, and L_w = level of the overflow weir. In this problem, the level is never below the overflow, and the height above the overflow, $L - L_w$, is very small compared with the height of liquid in the tank, L . Therefore, we will assume that the liquid level in the tank is approximately constant, and the flows in and out are equal, $F_0 = F_1 = F$

$$\frac{dV}{dt} = F_0 - F_1 = 0 \quad \therefore V = \text{constant} \quad (3.11)$$

This result, stated as an assumption hereafter, will be used for all tanks with overflow, as shown in Figure 3.1.

The next step is to formulate a material balance on component A. Since the tank is well-mixed, the tank and outlet concentrations are the same:

$$\left\{ \begin{array}{c} \text{Accumulation of} \\ \text{component A} \end{array} \right\} = \left\{ \begin{array}{c} \text{component} \\ \text{A in} \end{array} \right\} - \left\{ \begin{array}{c} \text{component} \\ \text{A out} \end{array} \right\} + \left\{ \begin{array}{c} \text{generation} \\ \text{of A} \end{array} \right\} \quad (3.12)$$

$$(MW_A V C_A)_{t+\Delta t} - (MW_A V C_A)_t = (MW_A F C_{A0} - MW_A F C_A) \Delta t \quad (3.13)$$

with C_A being moles/volume of component A and MW_A being its molecular weight, and the generation term being zero, because there is no chemical reaction. Dividing by Δt and taking the limit as $\Delta t \rightarrow 0$ gives

$$MW_A V \frac{dC_A}{dt} = MW_A F (C_{A0} - C_A) \quad (3.14)$$

One might initially believe that another balance on the only other component, solvent S, could be included in the model:

$$MW_S V \frac{dC_S}{dt} = MW_S F (C_{S0} - C_S) \quad (3.15)$$

with C_S the moles/volume and MW_S the molecular weight. However, equation (3.9) is the sum of equations (3.14) and (3.15); thus, only two of the three equations are independent. Therefore, only equations (3.11) and (3.14) are required for the model and should be considered in determining the degrees of freedom. The following analysis shows that the model using only independent equations is exactly specified:

Variables:	C_A and F_1	
External variables:	F_0 and C_{A0}	DOF = NV - NE = 2 - 2 = 0
Equations:	(3.11) and (3.14)	



Note that the variable t representing time must be specified to use the model for predicting the concentration at a particular time.



The model is formulated assuming that parameters do not change with time, which is not exactly correct but can be essentially true when the parameters change slowly and with small magnitude during the time considered in the dynamic modelling problem. What constitutes a “small” change depends on the problem, and a brief sensitivity analysis is included in the results analysis of this example to determine how changes in the volume and flow would affect the answer to this example.

Mathematical Solution

Determining the solution is certainly of importance. However, the engineer should realize that the solution is implicitly contained in the results of the Information and Formulation steps; the solution simply “figures it out.” The engineer would like to use the solution method that gives the most insight into the system. Therefore, analytical solutions are preferred in most cases, because they can be used to (1) calculate specific numerical values, (2) determine important functional relationships among design and operating variables and system behavior, and (3) give insight into the sensitivity of the result to changes in data. These results are so highly prized that we often make assumptions to enable us to obtain analytical solutions; the most frequently used approximation is linearizing nonlinear terms, as covered in Section 3.4.

In some cases, the approximations necessary to make analytical solutions possible introduce unacceptable errors into the results. In these cases, a numerical solution to the equations is employed, as described in Section 3.5. Although the numerical solutions are never exact, the error introduced can usually be made quite small, often much less than the errors associated with the assumptions and data in the model; thus, properly calculated numerical solutions can often be considered essentially exact. The major drawback to numerical solutions is loss of insight.

EXAMPLE 3.1.

Solution. The model in equation (3.14) is a linear, first-order ordinary differential equation that is not separable. However, it can be transformed into a separable form by an integrating factor, which becomes more easily recognized when the differential equation is rearranged in the standard form as follows (see Appendix B):

$$\frac{dC_A}{dt} + \frac{1}{\tau} C_A = \frac{1}{\tau} C_{A0} \quad \text{with} \quad \frac{V}{F} = \frac{2.1 \text{ m}^3}{0.085 \text{ m}^3/\text{min}} = 24.7 \text{ min} = \tau \equiv \text{time constant} \quad (3.16)$$

The parameter τ is termed the *time constant* of the system and will appear in many models. The equation can be converted into separable form by multiplying both sides by the integrating factor, and the resulting equation can be solved directly:

$$\text{Integrating factor} = IF = \exp\left(\int \frac{1}{\tau} dt\right) = e^{t/\tau}$$

$$e^{t/\tau} \left(\frac{dC_A}{dt} + \frac{1}{\tau} C_A \right) = e^{t/\tau} \frac{dC_A}{dt} + C_A \frac{de^{t/\tau}}{dt} = \frac{d(e^{t/\tau} C_A)}{dt} = \frac{C_{A0}}{\tau} e^{t/\tau} \quad (3.17)$$

$$\int d(C_A e^{t/\tau}) = \int \frac{C_{A0} e^{t/\tau}}{\tau} dt = \frac{C_{A0}}{\tau} \int e^{t/\tau} dt$$

$$C_A e^{t/\tau} = \frac{C_{A0} \tau}{\tau} e^{t/\tau} + I$$

$$C_A = C_{A0} + I e^{-t/\tau}$$

Note that the integration was simplified by the fact that C_{A0} is constant after the step change (i.e., for $t > 0$). The initial condition is $C_A(t) = C_{Ainit}$ at $t = 0$, which can be used to evaluate the constant of integration, I . This formulation implies that the time t is measured from the introduction of the step change.

$$I = C_{Ainit} - C_{A0} \quad \therefore C_A = C_{A0} + (C_{Ainit} - C_{A0}) e^{-t/\tau} \quad (3.18)$$

$$(C_A - C_{Ainit}) = [C_{A0} - (C_{A0})_{init}](1 - e^{-t/\tau})$$

The final equation has used the extra relationship that $(C_{A0})_{init} = C_{Ainit}$. Substituting the numerical values gives

$$C_A - 0.925 = (C_{A0} - 0.925)(1 - e^{-t/24.7})$$

Two important aspects of the dynamic behavior can be determined from equation (3.18). The first is the "speed" of the dynamic response, which is characterized by the time constant, τ . The second is the steady-state gain, which is defined as

$$\text{Steady-state gain} = K_p = \frac{\Delta \text{output}}{\Delta \text{input}} = \frac{\Delta C_A}{\Delta C_{A0}} = 1.0$$

Note that in this example the time constant depends on the equipment (V) and operation of the process (F), and the steady-state gain is independent of these design and operating variables. These values are *not* generally applicable to other processes.

Results Analysis

The first phase of the results analysis is to evaluate whether the solution is correct, at least to the extent that it satisfies the formulation. This can be partially verified by ensuring that the solution obeys some limiting criteria that are more easily derived than the solution itself. For example, the result

- Satisfies initial and final conditions
- Obeys bounds such as adiabatic reaction temperature
- Contains negligible errors associated with numerical calculations
- Obeys semi-quantitative expectations, such as the sign of the output change

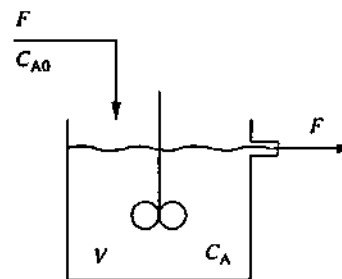
Next, the engineer should "interrogate" the mathematical solution to elicit the information needed to achieve the original modelling goals. Determining specific numerical values is a major part of the results analysis, because engineers need to make quantitative decisions on equipment size, operating conditions, and so



h. However, results analysis should involve more extensive interpretation of the solution. When meaningful, results should be plotted, so that key features like oscillations or extrema (maximum or minimum) will become apparent. Important features should be related to specific parameters or groups of parameters to assist in understanding the behavior. Also, the sensitivity of the result to changes in assumptions or data should be evaluated. Sometimes this is referred to as *what-if* analysis, where the engineer determines what happens if a parameter changes by a specified amount. A thorough results analysis enables the engineer to understand the result of the formulation and solution steps.

EXAMPLE 3.1.

Results analysis. The solution in equation (3.18) is an exponential curve as shown in Figure 3.3. The shape of the curve is monotonic, with the maximum rate of change occurring when the inlet step change is entered. The manner in which the variable changes from its initial to final values is influenced by the time constant (τ), which in this problem is the volume divided by the flow. Thus, the same dynamic response could be obtained for any stirred tank with values of flow and volume that give the same value of the time constant. It is helpful to learn a few values of this curve, which we will see so often in process control. The values for the change in concentration for several values of time after the step are noted in the following table.



A Modelling
Procedure

Time from step	Percent of final steady-state change in output
0	0
τ	63.2
2τ	86.5
3τ	95.0
4τ	98.2

The specific quantitative question posed in the goal statement involves determining the time until 90 percent of the change in outlet concentration has occurred. This time can be calculated by setting $C_A = C_{A\text{init}} + 0.9(C_{A0} - C_{A\text{init}})$ in equation (3.18), which on rearrangement gives

$$t = -\tau \ln \left(\frac{0.1[(C_A)_{\text{init}} - C_{A0}]}{(C_A)_{\text{init}} - C_{A0}} \right) = -(24.7)(-2.30) = 56.8 \text{ min}$$

Note that this is time from the introduction of the step change, which, since the step is introduced at $t = 10$, becomes 66.8 in Figure 3.3. One should ask how important the specification is; if it is critical, a sensitivity analysis should be performed. For example, if the volume and flow are not known exactly but can change within ± 5 percent of their base values, the time calculated above is not exact. The range for this time can be estimated from the bounds on the parameters that influence the time constant:

$$\text{Maximum } t = -\frac{(2.1)(1.05)}{(0.085)(0.95)}(-2.30) = 62.8 \text{ min}$$

$$\text{Minimum } t = -\frac{(2.1)(0.95)}{(0.085)(1.05)}(-2.30) = 51.4 \text{ min}$$

Given the estimated inaccuracy in the data, one should wait at least 62.8 (not 56.8)

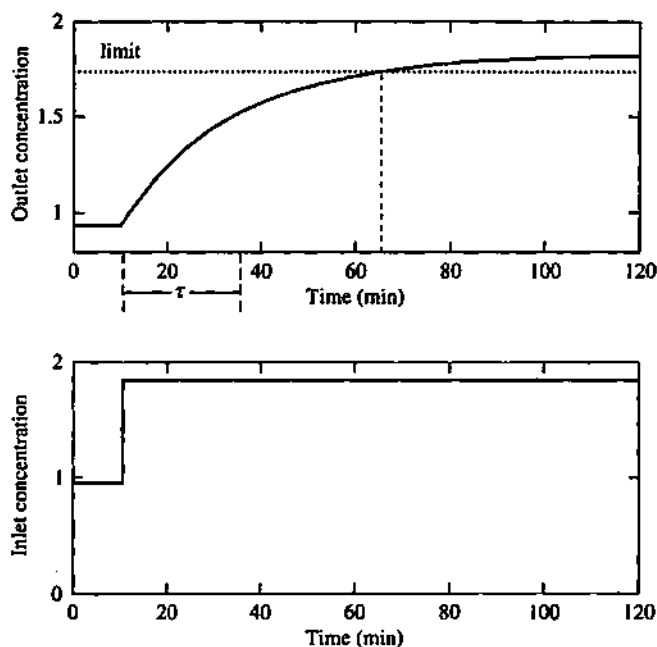


FIGURE 3.3
Dynamic result for Example 3.1.

minutes after the step to be sure that 90 percent of the concentration change has occurred.

VALIDATION. Validation involves determining whether the results of steps 1 through 5 truly represent the physical process with the required fidelity for the specified range of conditions. The question to be evaluated is, “Does the model represent the data well enough that the engineering task can be performed using the model?” Since we know that all models are simplified representations of the true, complex physical world, this question must be evaluated with careful attention to the application of the model. We do not have enough background in control engineering at this point, so the sensitivity of process and control design to modelling errors must be deferred to a later point in the book; however, all methods will be based on models, so this question will be addressed frequently because of its central importance.

While the sensitivity analysis in step 5 could build confidence that the results are likely to be correct, a comparison with empirical data is needed to evaluate the validity of the model. One simple step is to compare the results of the model with the empirical data in a graph. If parameters are adjusted to improve the fit of the model to the data, consideration should be taken of the amount the parameters must be adjusted to fit the data; adjustments that are too large raise a warning that the model may be inadequate to describe the physical system.

It is important to recognize that no set of experiences can validate the model. Good comparisons only demonstrate that the model has not been invalidated by the data; another experiment could still find data that is not properly explained by the model. Thus, no model can be completely validated, because this would require an infinite number of experiments to cover the full range of conditions. However, data from a few experiments can characterize the system in a limited range of operating variables. Experimental design and modelling procedures for empirical models are the topic of Chapter 6.

EXAMPLE 3.1.

Validation. The mixing tank was built, the experiment was performed, and samples of the outlet material were analyzed. The data points are plotted in Figure 3.4 along with the model prediction. By visual evaluation and considering the accuracy of each data point, one would accept the model as “valid” (or, more accurately, not invalid) for most engineering applications.

The modelling procedure presented in this section is designed to ensure that the most common issues are addressed in a logical order. While the procedure is important, the decisions made by the engineer have more impact on the quality of the result than the procedure has. Since no one is prescient, the effects of early assumptions and formulations may not be appropriate for the goals. Thus, a thorough analysis of the results should be performed so that the sensitivity of the conclusions to model assumptions and data is clearly understood. If the conclusion is unduly sensitive to assumptions or data, an iteration would be indicated, employing a more

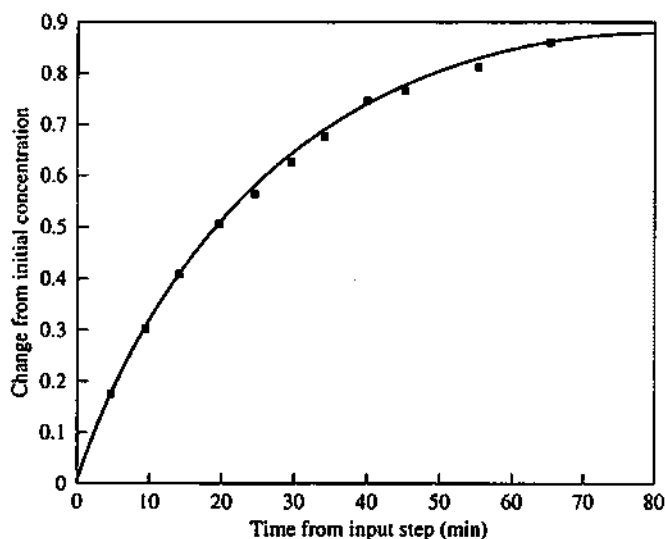


FIGURE 3.4

Comparison of empirical data (squares) and model (line) for Example 3.1.

rigorous model or more accurate data. Thus, the procedure contains the essence of the modelling process and provides an opportunity for evaluation and improvement.

3.3 ■ MODELLING EXAMPLES

Most people learn modelling by *doing modelling*, not observing results of others! The problems at the end of the chapter, along with many solved and unsolved problems in the references and resources, provide the reader with ample opportunity to develop modelling skills. To assist the reader in applying the procedure to a variety of problems, this section includes a few more solved example problems with solutions. In all examples, steps 1 to 5 are performed, but validation is not.

EXAMPLE 3.2. Isothermal CSTR

The dynamic response of a continuous-flow, stirred-tank chemical reactor (CSTR) will be determined in this example and compared with the stirred-tank mixer in Example 3.1.

Goal. Determine the dynamic response of a CSTR to a step in the inlet concentration. Also, the reactant concentration should never go above 0.85 mole/m³. If an alarm sounds when the concentration reaches 0.83 mole/m³, would a person have enough time to respond? What would a correct response be?

Information. The process is the same as shown in Figure 3.1, and therefore, the system is the liquid in the tank. The important variable is the reactant concentration in the reactor.

Assumptions. The same as for the stirred-tank mixer.

Data. The flow, volume, and inlet concentrations (before and after the step) are the same as for the stirred-tank mixer in Example 3.1.

1. $F = 0.085 \text{ m}^3/\text{min}$; $V = 2.1 \text{ m}^3$; $(C_{A0})_{\text{init}} = 0.925 \text{ mole/m}^3$; $\Delta C_{A0} = 0.925 \text{ mole/m}^3$.
2. The chemical reaction is first-order, $r_A = -kC_A$ with $k = 0.040 \text{ min}^{-1}$.
3. The heat of reaction is negligible, and no heat is transferred to the surroundings.

Formulation. Based on the model of the stirred-tank mixer, the overall material balance again yields $F_0 = F_1 = F$. To determine the concentration of reactant, a component material balance is required, which is different from that of the mixing tank because there is a (negative) generation of component A as a result of the chemical reaction.

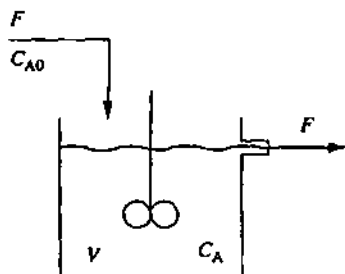
$$\left\{ \begin{array}{c} \text{Accumulation of} \\ \text{component A} \end{array} \right\} = \left\{ \begin{array}{c} \text{component} \\ \text{A in} \end{array} \right\} - \left\{ \begin{array}{c} \text{component} \\ \text{A out} \end{array} \right\} + \left\{ \begin{array}{c} \text{generation} \\ \text{of A} \end{array} \right\} \quad (3.19)$$

$$(MW_A V C_A)_{t+\Delta t} - (MW_A V C_A)_t = (MW_A F C_{A0} - MW_A F C_A - MW_A V k C_A) \Delta t \quad (3.20)$$

Again, dividing by $MW_A(\Delta t)$ and taking the limit as $\Delta t \rightarrow 0$ gives

$$\frac{dC_A}{dt} + \frac{1}{\tau} C_A = \frac{F}{V} C_{A0} \quad \text{with the time constant } \tau = \frac{V}{F + V k} \quad (3.21)$$

The degrees-of-freedom analysis yields one equation, one variable (C_A), two external variables (F and C_{A0}), and two parameters (V and k). Since the number of variables is equal to the number of equations, the degrees of freedom are zero, and the model is exactly specified.





Equation (3.21) is a nonseparable linear ordinary differential equation, which can be solved by application of the integrating factor:

$$\begin{aligned} \text{IF} &= \exp\left(\int \frac{1}{\tau} dt\right) = e^{t/\tau} \\ \frac{d(C_A e^{t/\tau})}{dt} &= \frac{F}{V} C_{A0} e^{t/\tau} \\ \int d(C_A e^{t/\tau}) &= \frac{F C_{A0}}{V} \int e^{t/\tau} dt \\ C_A e^{t/\tau} &= \frac{F C_{A0} \tau}{V} e^{t/\tau} + I \\ C_A &= \frac{F \tau}{V} C_{A0} + I e^{-t/\tau} \end{aligned} \quad (3.22)$$

The data give the initial condition of the *inlet* concentration of 0.925 mole/m³ at the time of the step, $t = 0$. The initial steady-state *reactor* concentration can be determined from the data and equation (3.21) with $dC_A/dt = 0$.

$$\begin{aligned} (C_A)_{\text{init}} &= \frac{F}{F + V k} (C_{A0})_{\text{init}} \\ &= \frac{0.085}{0.085 + (2.1)(0.040)} 0.925 = 0.465 \frac{\text{mole}}{\text{m}^3} \end{aligned}$$

The constant of integration can be evaluated to be

$$I = \frac{F[(C_{A0})_{\text{init}} - (C_{A0})]}{F + V k} = \frac{-F(\Delta C_{A0})}{F + V k}$$

This can be substituted in equation (3.22) to give

$$\begin{aligned} C_A &= \frac{F C_{A0}}{F + V k} - \frac{F(\Delta C_{A0})}{F + V k} e^{-t/\tau} \\ &= (C_A)_{\text{init}} + \frac{F}{F + V k} [C_{A0} - (C_{A0})_{\text{init}}] (1 - e^{-t/\tau}) \end{aligned} \quad (3.23)$$

This can be rearranged with $K_p = F/(F + V k)$ to give the change in reactor concentration.

$$\begin{aligned} C_A - (C_A)_{\text{init}} &= K_p \Delta C_{A0} (1 - e^{-t/\tau}) \\ \Delta C_A &= (0.503)(0.925)(1 - e^{-t/\tau}) \end{aligned}$$

Again, the time constant determines the “speed” of the response. Note that in this example, the time constant depends on the equipment (V), the operation (F), and the chemical reaction (k), and that by comparing equations (3.16) and (3.21) the time constant for the chemical reactor is always shorter than the time constant for the mixer, using the same values for F and V . Their numerical values are

$$\begin{aligned} \tau &= \frac{V}{F + V k} = \frac{2.1}{0.085 + 2.1(0.040)} = 12.4 \text{ min} \\ K_p &= \frac{F}{F + V k} = \frac{0.085}{0.085 + 2.1(0.04)} = 0.503 \frac{\text{mole/m}^3}{\text{mole/m}^3} \end{aligned}$$

Thus, the steady-state gain and time constant in this example depend on equipment design and operating conditions.

Results analysis. First, the result from equation (3.23) is calculated and plotted. As shown in Figure 3.5a, the reactant concentration increases as an exponential function to its final value without overshoot or oscillation. In this case, the

concentration exceeds its maximum limit; therefore, a corrective action was evaluated. The concentration reaches the alarm limit in 19.6 minutes after the start (29.6 minutes in the figure) and exceeds the maximum limit after 22.5 minutes. The sensitivity of this result can be evaluated from the analytical solution; in particular, the dependence of the time constant on variables and parameters is given in equation (3.21). The time difference between the alarm and the dangerous condition is too short for a person to respond reliably, because other important events may be occurring simultaneously.

Since a response is required, the safety response should be automated; safety systems are discussed in Chapter 24. A proper response can be determined by considering equation (3.21). The goal is to ensure that the reactor concentration decreases immediately when the corrective manipulation has been introduced. One manner (for this, but not all processes) would be to decrease the inlet concentration to its initial value, so that the rate of change of C_A would be negative without delay. The transient response obtained by implementing this strategy when the alarm value is reached is shown in Figure 3.5b. The model for the response after the alarm value has been reached, 29.6 minutes, is of the same form as equation (3.23), with the same time constant and gain.

EXAMPLE 3.3. Two isothermal CSTR reactors

A problem similar to the single CSTR in Example 3.2 is presented, with the only difference that two series reactors are included as shown in Figure 3.6. Each tank is one-half the volume of the tank in Example 3.2.

Goal. The same as that of Example 3.2, with the important concentration being in the second reactor. Determine the time when this concentration exceeds 0.85 mole/m^3 .

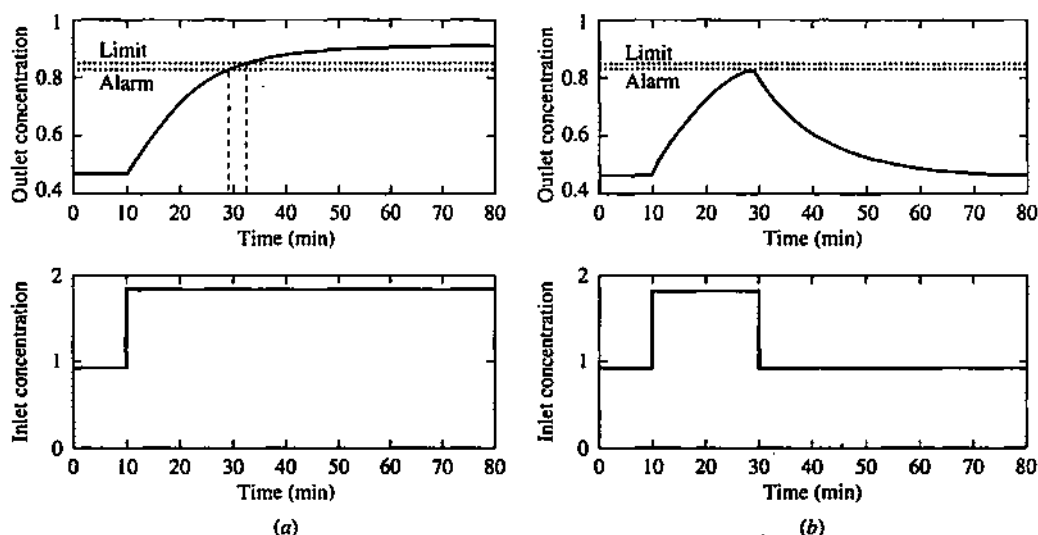


FIGURE 3.5

Results for Example 3.2: (a) without action at the alarm value; (b) with action at the alarm value.

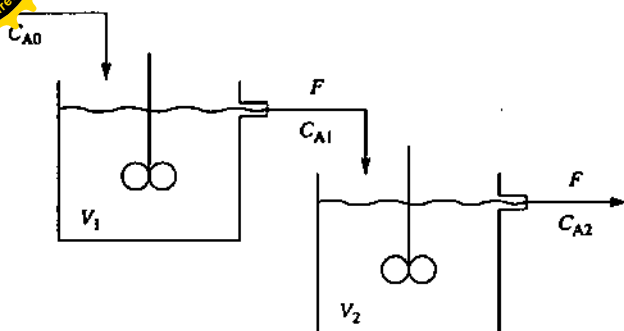


FIGURE 3.6
Two CSTRs in series.

Information. The two systems are the liquid in each tank. The data is the same as in Example 3.2, except that $V_1 = V_2 = 1.05 \text{ m}^3$.

1. $F = 0.085 \text{ m}^3/\text{min}$; $(C_{A0})_{\text{ini}} = 0.925 \text{ mole/m}^3$; $\Delta C_{A0} = 0.925 \text{ mole/m}^3$.
2. The chemical reaction is first-order, $\tau_A = -kC_A$ with $k = 0.040 \text{ min}^{-1}$.
3. The reactor is well mixed and isothermal.

Formulation. Again, due to the assumptions for the overflow tanks, the volumes in the two tanks can be taken to be constant, and all flows are constant and equal. The value of the concentration in the second tank is desired, but it depends on the concentration in the first tank. Therefore, the component balances on both tanks are formulated.

$$\text{First tank: } V_1 \frac{dC_{A1}}{dt} = F(C_{A0} - C_{A1}) - V_1 k C_{A1} \quad (3.24)$$

$$\text{Second tank: } V_2 \frac{dC_{A2}}{dt} = F(C_{A1} - C_{A2}) - V_2 k C_{A2} \quad (3.25)$$

The result is two linear ordinary differential equations, which in general must be solved simultaneously. Note that the two equations could be combined into a single second-order differential equation; thus, the system is second-order.

Before proceeding to the solution, we should discuss a common error in formulating a model for this example. The engineer might formulate one component material balance, as given in the following.

Incorrect model

System: liquid in both tanks

$$\text{Component balance: } \frac{dC_{A2}}{dt} = F(C_{A0} - C_{A2}) - V k C_{A2}$$

The choice of the system is *not correct*, because a balance on component A (C_{A2}) must have a constant concentration of component A that is independent of location *within the system*. This condition is satisfied by the second tank, but not by both tanks. Also, the reaction rate depends on the concentration, which is different for the two tanks. Therefore, the correct model includes two component balances, one for each tank. Note that the correct model includes a balance for an *intermediate variable*, C_{A1} , that is not a goal of the modelling but is required to determine C_{A2} .

$$V_1 + V_2 k = F \quad \rightarrow \quad C_{A1} + C_{A2} = 1$$

$$F C_{A0} = F C_{A1} + V_1 k C_{A1}$$

$$= C_{A1} (F + V_1 k)$$

Solution. In equations (3.24) and (3.25), the balance on the first tank does not involve the concentration in the second tank and thus can be solved independently from the equation representing the second reactor. (More general methods for solving simultaneous linear differential equations, using Laplace transforms, are presented in the next chapter.) The solution for the first balance can be seen to be exactly the same form as the result for Example 3.2, equation (3.23). The analytical expression for the concentration at the outlet of the first tank can be substituted into equation (3.25) to give the model which must be solved. In this solution, the subscript "s" designates the *initial* steady-state value of the variable before the step, and no subscript indicates the variable after the step; also, $\Delta C_{A0} = C_{A0} - C_{A0s}$. Therefore, the model for C_{A2} after the substitution of equation (3.23) is

$$\tau \frac{dC_{A2}}{dt} + C_{A2} = KC_{A1} = K[KC_{A0s} + K\Delta C_{A0}(1 - e^{-t/\tau})] \quad (3.26)$$

Since the two reactors are identical (and linear), the steady-state gains and time constant for both are identical, i.e.,

$$K = F_1/(F_1 + V_1k) = F_2/(F_2 + V_2k) = 0.669 \quad (\text{outlet mole/m}^3)/(\text{inlet mole/m}^3) \\ \tau = V_1/(F_1 + V_1k) = V_2/(F_2 + V_2k) = 8.25 \quad \text{min} \quad (3.27)$$

Equation (3.26) can be solved by applying the integrating factor method.

$$\text{IF} = \exp\left(\int \frac{1}{\tau} dt\right) = e^{t/\tau}$$

$$\frac{d(C_{A2}e^{t/\tau})}{dt} = K[KC_{A0s} + K\Delta C_{A0}(1 - e^{-t/\tau})] \frac{e^{t/\tau}}{\tau} \quad (3.28)$$

$$C_{A2} = K^2 \left(\frac{C_{A0s}}{\tau} \int e^{t/\tau} dt + \frac{\Delta C_{A0}}{\tau} \int e^{t/\tau} dt - \frac{\Delta C_{A0}}{\tau} \int e^{-t/\tau} e^{t/\tau} dt \right) e^{-t/\tau}$$

$$C_{A2} = K^2 \left(C_{A0s} + \Delta C_{A0} - \frac{\Delta C_{A0}}{\tau} t e^{-t/\tau} \right) + I e^{-t/\tau}$$

The integration constant can be evaluated using the initial condition of the reactor concentration, which can be determined by setting $dC_{A2}/dt = 0$ in equation (3.26) to give $C_{A2} = K^2(C_{A0s})$ at $t = 0$.

$$K^2 C_{A0s} = K^2 \left(C_{A0s} + \Delta C_{A0} - \frac{\Delta C_{A0}}{\tau} t e^{-t/\tau} \right) + I e^{-t/\tau} \quad \text{when } t = 0$$

$$\therefore I = -K^2 \Delta C_{A0}$$

Substituting the expression for the integration constant into equation (3.28) gives the final expression for the concentration in the second reactor.

$$C_{A2} = K^2 \left[C_{A0s} + \Delta C_{A0}(1 - e^{-t/\tau}) - \Delta C_{A0} \left(\frac{t}{\tau} \right) e^{-t/\tau} \right] \quad (3.29)$$

The data can be substituted into equation (3.29) to give

$$C_{A2} = 0.414 + 0.414(1 - e^{-t/8.25}) - 0.050 t e^{-t/8.25} \quad (3.30)$$

Results analysis. The shape of the transient of the concentration in the second of two reactors in Figure 3.7 is very different from the transient for one reactor in Figure 3.3. The second-order response for this example has a sigmoidal or "S" shape, with a derivative that goes through a maximum at an inflection point and reduces to zero at the new steady state. Also, the total conversion of reactant is different from Example 3.2, although the total reactor volume is the same in

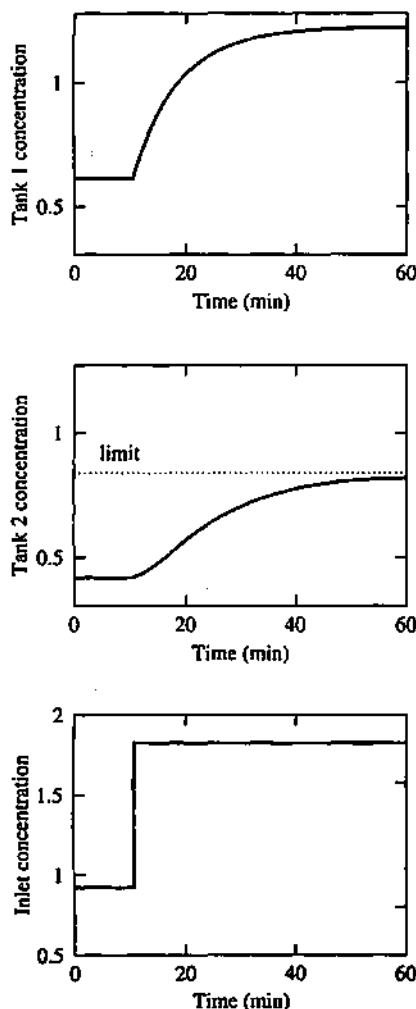


FIGURE 3.7

Dynamic responses for Example 3.3.

in cases. The increased conversion in the two-reactor system is due to the higher concentration of the reactant in the first reactor. In fact, the concentration of the second reactor does not reach the alarm or limiting values after the step change for the parameters specified, although the close approach to the alarm value indicates that a slight change could lead to an alarm.

The action upon exceeding the alarm limit in the second reactor would not be as easily determined for this process, since equation (3.25) shows that decreasing the inlet concentration to the first reactor does not ensure that the derivative of the second reactor's concentration will be negative. The system has "momentum," which makes it more difficult to influence the output of the second reactor immediately.

EXAMPLE 3.4. On/off room heating

The heating of a dwelling with an on/off heater was discussed in Section 1.2. The temperature was controlled by a feedback system, and semi-quantitative arguments led to the conclusion that the temperature would oscillate. In this section, a very simple model of the system is formulated and solved.

Goal. Determine the dynamic response of the room temperature. Also, ensure that the furnace does not have to switch on or off more frequently than once per 3 minutes, to allow the combustion zone to be purged of gases before reignition.

Information. The system is taken to be the air inside the dwelling. A sketch of the system is given in Figure 1.2. The important variables are the room temperature and the furnace on/off status.

Assumptions.

1. The air in the room is well mixed.
2. No transfer of material to or from the dwelling occurs.
3. The heat transferred depends only on the temperature difference between the room and the outside environment.
4. No heat is transferred from the floor or ceiling.
5. Effects of kinetic and potential energies are negligible.

Data.

1. The heat capacity of the air C_V is $0.17 \text{ cal/(g}^\circ\text{C)}$, density is 1190 g/m^3 .
2. The overall heat transfer coefficient, $UA = 45 \times 10^3 \text{ cal/(}^\circ\text{C h)}$.
3. The size of the dwelling is 5 m by 5 m by 3 m high.
4. The furnace heating capacity Q_h is either 0 (off) or 1.5×10^6 (on) cal/h.
5. The furnace heating switches instantaneously at the values of 17°C (on) and 23°C (off).
6. The initial room temperature is 20°C and the initial furnace status is "off."
7. The outside temperature T_a is 10°C .

Formulation. The system is defined as the air inside the house. To determine the temperature, an energy balance should be formulated, and since no material is transferred, no material balance is required. The application of the energy balance in equation (3.5) to this system gives

$$\frac{dU}{dt} = (0) - (0) + Q - W, \quad (3.31)$$

The shaft work is zero. From principles of thermodynamics and heat transfer, the following expressions can be used for a system with negligible accumulation of

potential and kinetic energy:

$$\frac{dU}{dt} = \rho V C_v \frac{dT}{dt} \quad Q = -UA(T - T_o) + Q_h \quad (3.32)$$

with

$$Q_h = \begin{cases} 0 & \text{when } T > 23^\circ\text{C} \\ 1.5 \times 10^6 & \text{when } T < 17^\circ\text{C} \\ \text{unchanged} & \text{when } 17 < T < 23^\circ\text{C} \end{cases}$$

to give

$$\rho V C_v \frac{dT}{dt} = -UA(T - T_o) + Q_h \quad (3.33)$$

The degrees of freedom for this formulation is zero since the model has two equations, two variables (T and Q_h), four parameters (UA , C_v , V , and ρ), and one external variable (T_o). Thus, the system is exactly specified with equation (3.33), when the status of the heating has been defined by equation (3.32).

Solution. Rearranging equation (3.33) gives the following linear ordinary differential equation:

$$\frac{dT}{dt} + \frac{1}{\tau} T = \frac{UA T_o + Q_h}{V \rho C_v} \quad \text{with } \tau = \frac{V \rho C_v}{UA} \quad (3.34)$$

Equation (3.34) is a linear differential equation when the value of heat transferred, Q_h , is *constant*. As described in the example data, Q_h has one of two constant values, depending on the status of the furnace heating. Thus, the equation can be solved using the integrating factor with one value of Q_h until the switching value of temperature is reached; then, the equation is solved with the appropriate value of Q_h until the next switch occurs. The solution for equation (3.34) is given in the following:

$$T - T_{\text{init}} = (T_{\text{final}} - T_{\text{init}})(1 - e^{-t/\tau}) \quad (3.35)$$

where

- t = time from step in Q_h
- τ = time constant = 0.34 h
- T_{final} = final value of T as $t \rightarrow \infty = T_o + Q_h/UA$
 - = 10°C when $Q_h = 0$
 - = 43.3°C when $Q_h = 1.5 \times 10^6$
- T_{init} = the value of T when a step in Q_h occurs

Results analysis. First, the numerical result is determined and plotted in Figure 3.8. From the initial condition with the furnace off, the temperature decreases according to equation (3.35) until the switch value of 17°C is reached. Then, the furnace heating begins instantaneously (Q_h changes from 0 to 1.5×10^6), and since the system is first-order with no “momentum,” the temperature immediately begins to increase. This procedure is repeated as the room temperature follows a periodic trajectory between 17 and 23°C .

The analytical solution provides insight into how to alter the behavior of the system. The time constant is proportional to the mass in the room, which seems reasonable. Also, it is inversely proportional to the heat transfer coefficient, since the faster the heat transfer, the more quickly the system reaches an equilibrium with its surroundings; therefore, insulating the house will decrease UA and increase the time constant. Finally, the time constant does not depend on the heating by the furnace, which is the forcing function of the system; therefore, increasing the capacity of the furnace will not affect the time constant, although it will affect the time between switches.

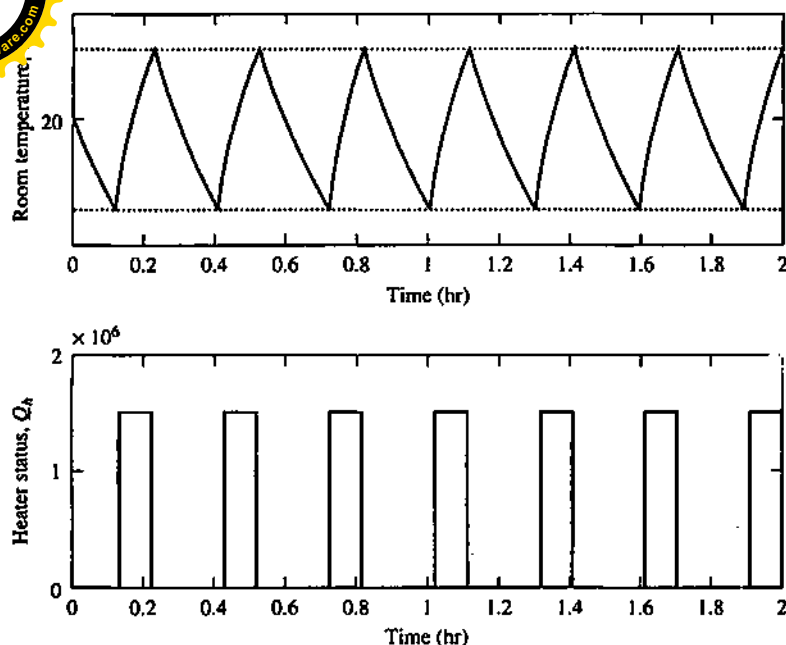


FIGURE 3.8
Dynamic response for Example 3.4.

The goals of the modelling exercise have been satisfied. The temperature has been determined as a function of time, and the switching frequency of the furnace has been determined to be over 3 minutes; that is, longer than the minimum limit. However, a switch could occur much faster due to a sudden change in outside temperature or to a disturbance such as a door being opened, which would allow a rapid exchange of warm and cold air. Therefore, a special safety system would be included to ensure that the furnace would not be restarted until a safe time period after shutting off.

Building heating and air conditioning have been studied intensively, and more accurate data and models are available (McQuiston and Parker, 1988). Also, some extensions to this simple example are suggested in question 3.9 at the end of the chapter (adding capacitance, changing UA , and including ventilation).

This example is the first quantitative analysis of a continuous feedback control system. The simplicity of the model and the on/off control approach facilitated the solution while retaining the essential characteristics of the behavior. For most industrial processes, the oscillations associated with on/off control are unacceptable, and more complex feedback control approaches, introduced in Part III, are required to achieve acceptable dynamic performance.

3.4 ■ LINEARIZATION

The models in the previous sections were easily solved because they involved linear equations, which were a natural result of the conservation balances and constitutive relationships for the specific physical systems. However, the conservation and constitutive equations are nonlinear for most systems, and general methods for

developing analytical solutions for nonlinear models are not available. An alternative is numerical simulation, covered later in this chapter, which can produce accurate solutions for specific numerical values but usually offers much less understanding. Fortunately, methods exist for obtaining approximate linearized solutions to nonlinear systems, and experience over decades has demonstrated that linearized methods of control systems analysis provide very useful results for many (but not all) realistic processes. Therefore, this section introduces the important method for developing approximate linear models.

First, the concept of *linearity* needs to be formally defined. This will be done using the concept of an *operator*, which transforms an input variable into an output variable.

An operator \mathcal{F} is linear if it satisfies the properties of additivity and proportionality, which are included in the following superposition, where x_1 are variables and a and b are constants:

$$\mathcal{F}(ax_1 + bx_2) = a\mathcal{F}(x_1) + b\mathcal{F}(x_2) \quad (3.36)$$

We can test any term in a model using equation (3.36) to determine whether it is linear. A few examples are given in the following table.

Function	Check for linearity	Is check satisfied?
$\mathcal{F}(x) = kx$	$k(ax_1 + bx_2) \stackrel{?}{=} kax_1 + kbx_2$	Yes
$\mathcal{F}(x) = kx^{1/2}$	$k(ax_1 + bx_2)^{1/2} \stackrel{?}{=} k(ax_1)^{1/2} + k(bx_2)^{1/2}$	No

Next, it is worthwhile considering the dynamic behavior of a process, such as the stirred-tank heat exchanger shown in Figure 3.9, subject to changes in the feed temperature and cooling fluid flow rate. For a linear system, the result of the two changes is the sum of the results from each change individually. The responses to step changes in the feed temperature (at $t = 5$) and cooling medium flow rate (at $t = 20$) are shown in Figure 3.10. The responses in parts *a* and *b* are the effects of each disturbance individually, and the response in part *c* is the total effect, which for this linear process is the sum of the two individual effects. Note that the true physical system experiences only the response in Figure 3.10c; the individual responses are the linear predictions for each input change. (The model for this system will be derived in Example 3.7.) This concept, as an approximation to real nonlinear processes, is used often in analyzing process control systems.

A linearized model can be developed by approximating each nonlinear term with its linear approximation. A nonlinear term can be approximated by a Taylor series expansion to the n th order about a point if derivatives up to n th order exist at the point; the general expressions for functions of one and two variables are given in Table 3.3.

The term R is the remainder and depends on the order of the series. A few examples of nonlinear terms that commonly occur in process models, along with

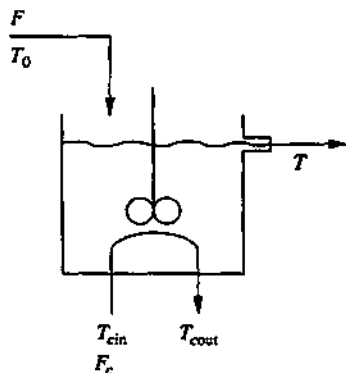


FIGURE 3.9
Stirred tank with heat exchanger.

Taylor series for functions of one and two variables

Function of one variable about x_s

$$F(x) = F(x_s) + \left. \frac{dF}{dx} \right|_{x_s} (x - x_s) + \frac{1}{2!} \left. \frac{d^2F}{dx^2} \right|_{x_s} (x - x_s)^2 + R \quad (3.38)$$

Function of two variables about x_{1s}, x_{2s}

$$\begin{aligned} F(x_1, x_2) = & F(x_{1s}, x_{2s}) + \left. \frac{\partial F}{\partial x_1} \right|_{x_{1s}, x_{2s}} (x_1 - x_{1s}) + \left. \frac{\partial F}{\partial x_2} \right|_{x_{1s}, x_{2s}} (x_2 - x_{2s}) \\ & + \frac{1}{2!} \left. \frac{\partial^2 F}{\partial x_1^2} \right|_{x_{1s}, x_{2s}} (x_1 - x_{1s})^2 + \frac{1}{2!} \left. \frac{\partial^2 F}{\partial x_2^2} \right|_{x_{1s}, x_{2s}} (x_2 - x_{2s})^2 \\ & + \left. \frac{\partial^2 F}{\partial x_1 \partial x_2} \right|_{x_{1s}, x_{2s}} (x_1 - x_{1s})(x_2 - x_{2s}) + R \end{aligned} \quad (3.39)$$

their linear approximations about x_s , are the following:

$$\begin{aligned} F(x) = x^{1/2} \quad & F(x) \approx x_s^{1/2} + \frac{1}{2} x_s^{-1/2} (x - x_s) \\ F(x) = \frac{x}{1+ax} \quad & F(x) \approx \frac{x_s}{1+ax_s} + \frac{1}{(1+ax_s)^2} (x - x_s) \end{aligned}$$

The accuracy of the linearization can be estimated by comparing the magnitude of the remainder, R' , to the linear term. For a linear Taylor series approximation in one variable,

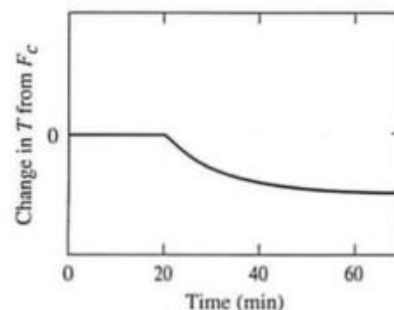
$$R' = \left. \frac{1}{2} \frac{d^2F}{dx^2} \right|_{x=\xi} (x - x_s)^2 \quad \text{with } \xi \text{ between } x \text{ and } x_s \quad (3.37)$$

The accuracy of a sample linearization is depicted in Figure 3.11. From this figure and equation (3.37), it can be seen that the accuracy of the linear approximation is relatively better when (1) the second-order derivative has a small magnitude (there is little curvature) and (2) the region about the base point is small. The successful application of linearization to process control systems is typically justified by the small region of operation of a process when under control. Although the uncontrolled system might operate over a large region because of disturbances in input variables, the controlled process variables should operate over a much smaller range, where the linear approximation often is adequate. Note that the accuracy of the linearization would in general depend on the normal operating point x_s .

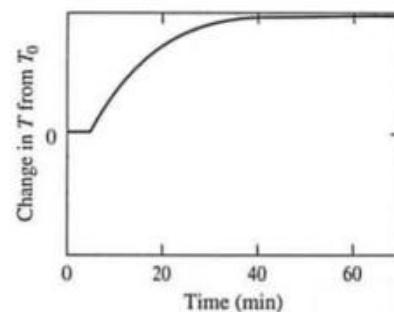
Several modelling examples of linearized models are now given, with the linearized results compared with the nonlinear results. In all cases, the models will be expressed in deviation variables, such as $x - x_s$, where the subscript s represents the steady-state value of the variable. The deviation variable will always be designated with a prime (').

Deviation variable: $(x - x_s) = x'$ with x_s = steady-state value

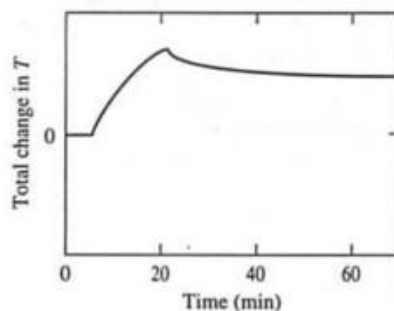
Linearization



(a)



(b)



(c)

FIGURE 3.10

Response of the linear system in Figure 3.9 to positive step changes in two input variables, T_0 and F_c .

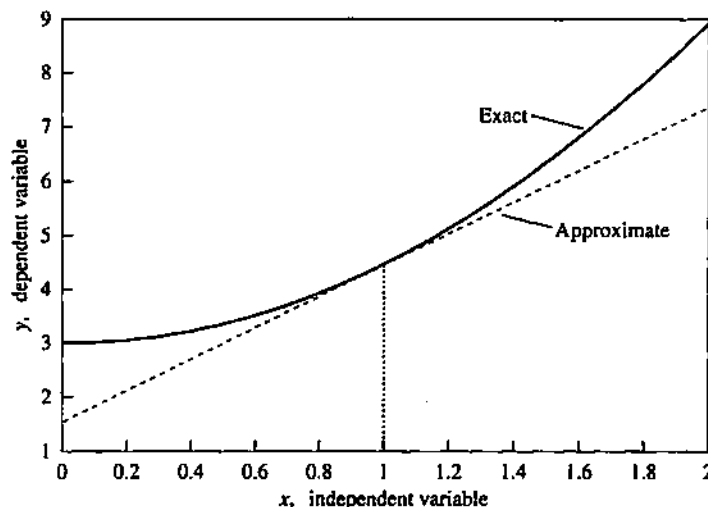


FIGURE 3.11

Comparison of a nonlinear function $y = (1.5x^2 + 3)$ with its linear approximation about $x_s = 1$.

A deviation variable simply translates the variable value (x) by a constant, and the value of the variable (x) is easily recovered by adding the initial steady-state value x_s to its deviation value, x' . The use of deviation variables is not necessary and provides no advantage at this point in our analysis. However, expressing a model in deviation variables will be shown in Chapter 4 to provide a significant simplification in the analysis of dynamic systems; therefore, we will begin to use them here for all linear or linearized systems.

EXAMPLE 3.5. Isothermal CSTR

The solution to the single-tank CSTR problem in Example 3.2 is now presented for a second-order chemical reaction.

Goal. Determine the transient response of the tank concentration in response to a step in the inlet concentration for the nonlinear and linearized models.

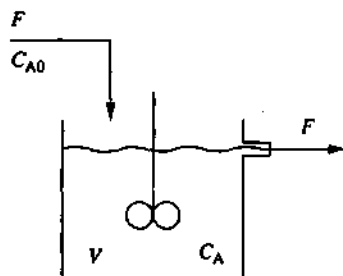
Information. The process equipment and flow are the same as shown in Figure 3.1. The important variable is the reactant concentration in the reactor.

Assumptions. The same as in Example 3.1.

Data. The same as in Example 3.2 except the chemical reaction rate is second-order, with $r_A = -kC_A^2$ and $k = 0.5[(\text{mole}/\text{m}^3) \text{ min}]^{-1}$.

1. $F = 0.085 \text{ m}^3/\text{min}$; $V = 2.1 \text{ m}^3$; $(C_{A0})_{\text{init}} = 0.925 \text{ mole}/\text{m}^3$; $\Delta C_{A0} = 0.925 \text{ mole}/\text{m}^3$; $(C_A)_{\text{init}} = 0.236 \text{ mole}/\text{m}^3$.
2. The reactor is isothermal.

Formulation. The formulation of the equations and analysis of degrees of freedom are the same as in Example 3.2 except that the rate term involves the reactant





concentration to the second power.

$$V \frac{dC_A}{dt} = F(C_{A0} - C_A) - V k C_A^2 \quad (3.40)$$

To more clearly evaluate the model for linearity, the values for all constants (in this example) can be substituted into equation (3.40), giving the following:

$$(2.1) \frac{dC_A}{dt} = (0.085)(1.85 - C_A) - (2.1)(0.50)C_A^2$$

The only nonlinear term in the equation is the second-order concentration term in the rate expression. This term can be linearized by expressing it as a Taylor series and retaining only the linear terms:

$$C_A^2 \approx C_{As}^2 + 2C_{As}(C_A - C_{As}) \quad (3.41)$$

Recall that C_{As} is evaluated by setting the derivative to zero in equation (3.40) and solving for C_A , with C_{A0} having its initial value before the input perturbation, because the linearization is about the initial steady state. The approximation is now substituted in the process model:

$$V \frac{dC_A}{dt} = F(C_{A0} - C_A) - [V k C_{As}^2 + 2V k C_{As}(C_A - C_{As})] \quad (3.42)$$

The model can be expressed in deviation variables by first repeating the linearized model, equation (3.42), which is valid for any time, at the steady-state point, when the variable is equal to its steady-state value:

$$0 = V \frac{dC_{As}}{dt} = F(C_{A0s} - C_{As}) - [V k C_{As}^2 + 2V k C_{As}(C_{As} - C_{As})] \quad (3.43)$$

Then equation (3.43) can be subtracted from equation (3.42) to give the equation in deviation variables:

$$V \frac{dC'_A}{dt} = F(C'_{A0} - C'_A) - 2V k C_{As} C'_A \quad (3.44)$$

The resulting model is a first-order, linear ordinary differential equation, which can be rearranged into the standard form:

$$\frac{dC'_A}{dt} + \frac{1}{\tau} C'_A = \frac{F}{V} C'_{A0} \quad \text{with } \tau = \frac{V}{F + 2V k C_{As}} = 3.62 \text{ min} \quad (3.45)$$

Solution. Since the input forcing function is again a simple step, the analytical solution can be derived by a straightforward application of the integrating factor:

$$C'_A = C'_{A0} \left(\frac{F}{F + 2V k C_{As}} \right) (1 - e^{-t/\tau}) = \Delta C_{A0} K_p (1 - e^{-t/\tau})$$

with

$$K_p = \frac{F}{F + 2V k C_{As}} = 0.146 \quad \text{and} \quad \Delta C_{A0} = 0.925 \text{ mole/m}^3 \quad (3.46)$$

The data can be substituted into this expression to give

$$C'_A = (0.925)(0.146)(1 - e^{-t/3.62})$$

Results Analysis. The linearized solution from equation (3.46) is plotted in Figure 3.12 in comparison with the solution to the original nonlinear differential equation, equation (3.40). The linear solution can be seen to give a good semi-quantitative description of the true process response.



CHAPTER 3 Mathematical Modelling Principles

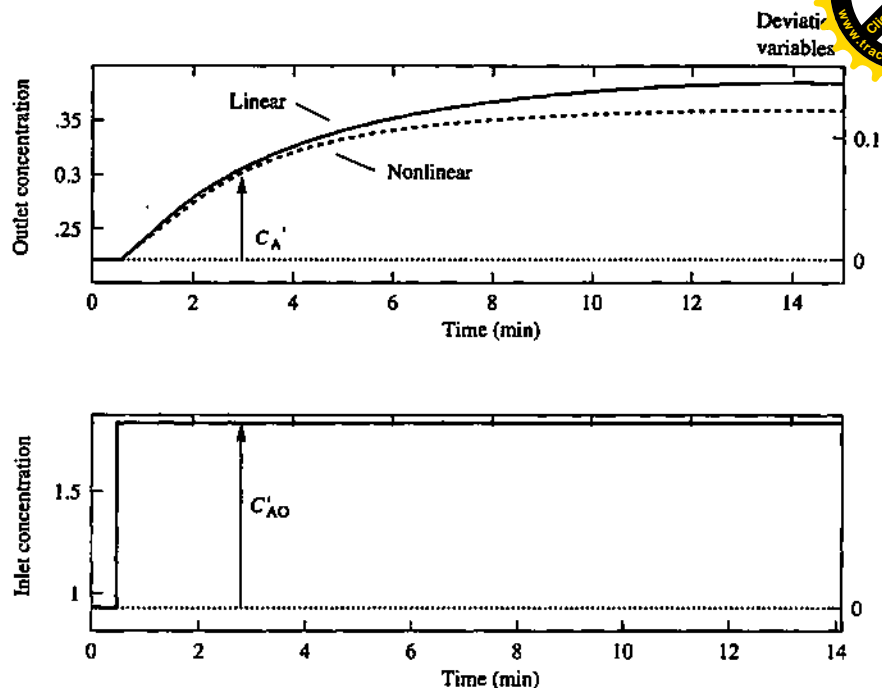


FIGURE 3.12

Dynamic responses for Example 3.5.

An important advantage of the linearized solution is in the analytical relationships. For example, the time constants and gains of the three similar continuous-flow stirred-tank processes—mixer, linear reactor, and linearized model of nonlinear reactor—are summarized in Table 3.4. These results can be used to learn how process equipment design and process operating conditions affect the dynamic responses. Clearly, the analytical solutions provide a great deal of useful information on the relationship between design and operating conditions and dynamic behavior.

TABLE 3.4

Summary of linear or linearized models for single stirred-tank systems

Physical system	Is the system linear?	Time constant (τ)	Steady-state gain, K_p
Example 3.1 (CST mixing)	Yes	V/F	1.0
Example 3.2 (CSTR with first-order reaction)	Yes	$V/(F + Vk)$	$F/(F + Vk)$
Example 3.5 (CSTR with second-order reaction)	No	$V/(F + 2VkC_{A0})$ (linearized model)	$F/(F + 2VkC_{A0})$ (linearized model)

EXAMPLE 3.6. Tank draining

The level and flow through a partially opened restriction out of the tank system in Figure 3.13 is considered in this example.

Goal. Determine a model for this system. Evaluate the accuracies of the linearized solutions for small (10 m³/h) and large (60 m³/h) step changes in the inlet flow rate.

Information. The system is the liquid in the tank, and the important variables are the level and flow out.

Assumptions.

1. The density is constant.
2. The cross-sectional area of the tank, A , does not change with height.

Data.

1. The initial steady-state conditions are (i) flows = $F_0 = F_1 = 100$ m³/h and (ii) level = $L = 7.0$ m.
2. The cross-sectional area is 7 m².

Formulation. The level depends on the total amount of liquid in the tank; thus, the conservation equation selected is an overall material balance on the system.

$$\rho A \frac{dL}{dt} = \rho F_0 - \rho F_1 \quad (3.47)$$

This single balance does not provide enough information, because there are two unknowns, F_1 and L . Thus, the number of degrees of freedom (1) indicates that another equation is required. An additional equation can be provided to determine F_1 without adding new variables, through a momentum balance on the liquid in the exit pipe. In essence, another subproblem is defined to formulate this balance. The major assumptions for this subproblem are that

1. The system is at quasi-steady state, since the dynamics of the pipe flow will be fast with respect to the dynamics of the level.
2. The total pressure drop is due to the restriction.
3. Conventional macroscopic flow equations, using relationships for friction factors and restrictions, can relate the flow to the pressure driving force (Foust et al., 1980; Bird, Stewart, and Lightfoot, 1960).

With these assumptions, which relate the flow out to the liquid level in the tank, the balance becomes

$$F_1 = f(F_1)(P_a + \rho L - P_a)^{0.5} = k_{F1} L^{0.5} \quad (3.48)$$

with P_a constant. The system with equations (3.47) and (3.48) and with two variables, F_1 and L , is exactly specified. After the equations are combined, the system can be described by a single first-order differential equation:

$$A \frac{dL}{dt} = F_0 - k_{F1} L^{0.5} \quad (3.49)$$

To more clearly evaluate the model for linearity, the values for all constants (flow, area, and $k_{F1} = 37.8$) can be substituted into equation (3.49), giving the following:

$$(7) \frac{dL}{dt} = (100 + 10) - (37.8) L^{0.5}$$

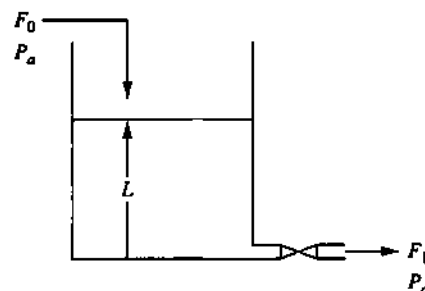


FIGURE 3.13

Level in draining tank for Example 3.6.

Linearization

The only nonlinear term in the equation is the square root of level, which can be linearized as shown in the following:

$$L^{0.5} \approx L_s^{0.5} + 0.5L_s^{-0.5}(L - L_s) \quad (3.50)$$

This expression can be used to replace the nonlinear term. The resulting equation, after subtracting the linearized balance at steady-state conditions and noting that the input is a constant step (i.e., $F'_0 = \Delta F_0$), is

$$A \frac{dL'}{dt} = \Delta F_0 - (0.5k_{F1}L_s^{-0.5})L' \quad (3.51)$$

Solution. The linearized differential equation can be rearranged and solved as before.

$$\frac{dL'}{dt} + \frac{1}{\tau}L' = \frac{1}{A}\Delta F_0 \quad \text{with } \tau = \frac{A}{0.5k_{F1}L_s^{-0.5}} \quad (3.52)$$

giving the solution

$$L' = \frac{\tau \Delta F_0}{A} + Ie^{-t/\tau} \quad (3.53)$$

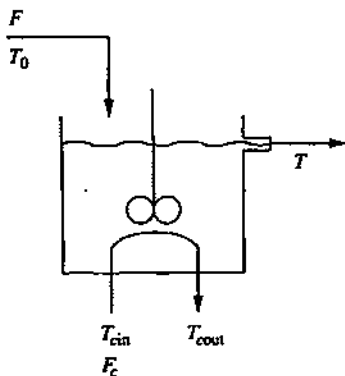
The initial condition is that $L' = 0$ at $t = 0$, with time measured from the input step; thus, $I = -\tau \Delta F_0/A$. Substitution gives

$$\begin{aligned} L' &= \frac{\tau \Delta F_0}{A}(1 - e^{-t/\tau}) \\ &= \Delta F_0 K_p(1 - e^{-t/\tau}) \quad \text{with } K_p = \frac{\tau}{A} = \frac{1}{0.5k_{F1}L_s^{-0.5}} \end{aligned} \quad (3.54)$$

For this example,

$$\begin{aligned} k_{F1} &= \frac{F_{1s}}{L_s^{0.5}} = \frac{100 \text{ m}^3/\text{h}}{\sqrt{7} \text{ m}^{0.5}} = 37.8 \frac{\text{m}^3/\text{h}}{\text{m}^{0.5}} \quad \tau = 0.98 \text{ h} \quad K_p = 0.14 \frac{\text{m}}{\text{m}^3/\text{h}} \\ L' &= 0.14 \Delta F_0(1 - e^{-t/0.98}) \end{aligned}$$

Results analysis. The solution of the linearized model indicates an exponential response to a step change. The results for the small and large step changes in flow in are plotted in Figure 3.14a and b, respectively. The solution to the approximate linearized model is quite accurate for the small step; however, it is inaccurate for a large step, even predicting an impossible *negative* level at the final steady state. The general trend that the linearized model should be more accurate for a small than for a large step conforms to the previous discussion of the Taylor series. Also, the large variation of the level, which for the larger input step is not maintained close to its initial condition as shown in Figure 3.14b, suggests that the linear solution might not be very accurate.



EXAMPLE 3.7. Stirred-tank heat exchanger

To provide another simple example of an energy balance, the stirred-tank heat exchanger in Figure 3.9 is considered.

Goal. The dynamic response of the tank temperature to a step change in the coolant flow is to be determined.

Information. The system is the liquid in the tank.

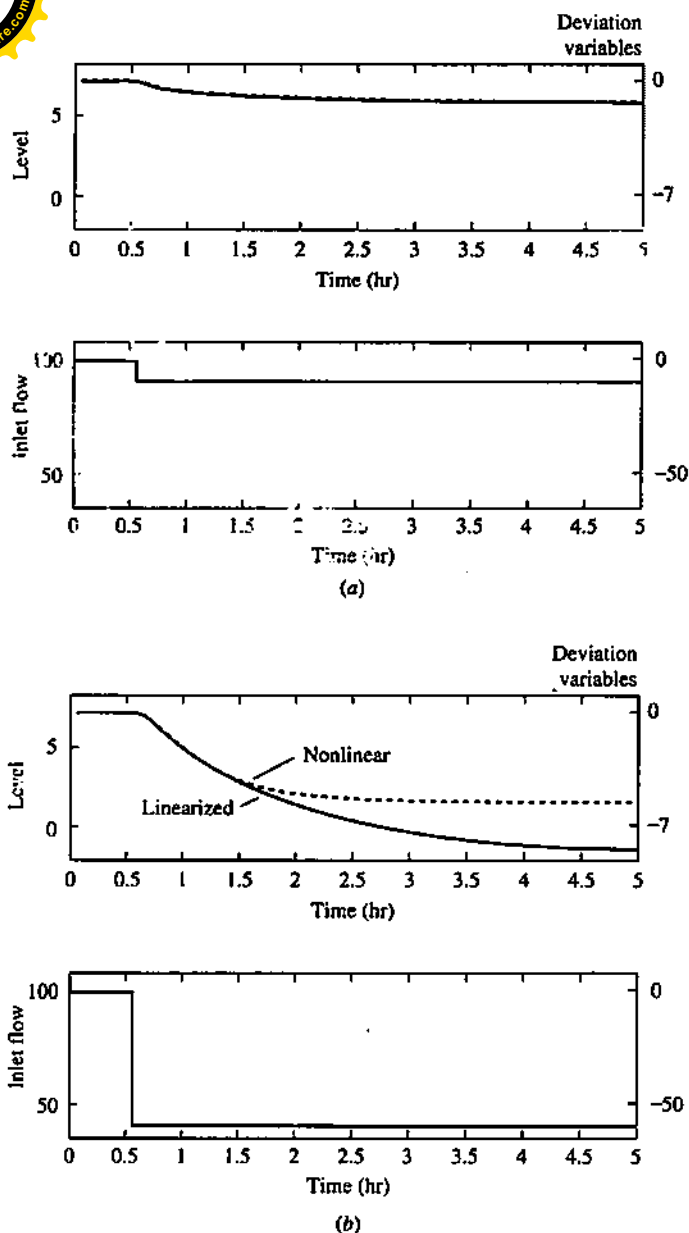


FIGURE 3.14

Dynamic responses for Example 3.6: (a) for a small input change (linearized and nonlinear essentially the same curve); (b) for a large input change.

Assumptions.

1. The tank is well insulated, so that negligible heat is transferred to the surroundings.
2. The accumulation of energy in the tank walls and cooling coil is negligible compared with the accumulation in the liquid.

3. The tank is well mixed.
4. Physical properties are constant.
5. The system is initially at steady state.

Data. $F = 0.085 \text{ m}^3/\text{min}$; $V = 2.1 \text{ m}^3$; $T_i = 85.4^\circ\text{C}$; $\rho = 10^6 \text{ g/m}^3$; $C_p = 1 \text{ cal/(g}^\circ\text{C)}$; $T_0 = 150^\circ\text{C}$; $T_{\text{cin}} = 25^\circ\text{C}$; $F_c = 0.50 \text{ m}^3/\text{min}$; $C_{pc} = 1 \text{ cal/(g}^\circ\text{C)}$; $\rho_c = 10^6 \text{ g/m}^3$; $a = 1.41 \times 10^5 \text{ cal/min}^\circ\text{C}$; $b = 0.50$.

Formulation. Overall material and energy balances on the system are required to determine the flow and temperature from the tank. The overall material balance is the same as for the mixing tank, with the result that the level is approximately constant and $F_0 = F_1 = F$. For this system, the kinetic and potential energy accumulation terms are zero, and their input and output terms cancel if they are not zero. The energy balance is as follows:

$$\frac{dU}{dt} = \{H_0\} - \{H_1\} + Q - W, \quad (3.55)$$

Also, it is assumed (and could be verified by calculations) that the shaft work is negligible. Now, the goal is to express the internal energy and enthalpy in measurable variables. This can be done using the following thermodynamic relationships (Smith and Van Ness, 1987):

$$dU/dt = \rho V C_v dT/dt \approx \rho V C_p dT/dt \quad (3.56)$$

$$H_i = \rho C_p F_i (T_i - T_{\text{ref}}) \quad (3.57)$$

Note that the heat capacity at constant volume is approximated as the heat capacity at constant pressure, which is acceptable for this liquid system. Substituting the relationships in equations (3.56) and (3.57) into (3.55) gives

$$\rho V C_p \frac{dT}{dt} = \rho C_p F [(T_0 - T_{\text{ref}}) - (T_1 - T_{\text{ref}})] + Q \quad (3.58)$$

This is the basic energy balance on the tank, which is one equation with two variables, T and Q . To complete the model, the heat transferred must be related to the tank temperature and the external variables (coolant flow and temperature). Thus, a subproblem involving the energy balance on the liquid in the cooling coils is now defined and solved (Douglas, 1972). The assumptions are

1. The coil liquid is at a quasi-steady state.
2. The coolant physical properties are constant.
3. The driving force for heat transfer can be approximated as the *average* between the inlet and outlet.

With these assumptions, the energy balance on the cooling coil is

$$T_{\text{cout}} = T_{\text{cin}} - \frac{Q}{\rho_c C_{pc} F_c} \quad (3.59)$$

The subscript c refers to the coolant fluid. Now, two constitutive relationships are employed to complete the model. The heat transferred can be expressed as

$$Q = -UA(\Delta T)_{\text{lm}} \approx -UA \left[\frac{(T - T_{\text{cin}}) + (T - T_{\text{cout}})}{2} \right] \quad (3.60)$$

The heat transfer coefficient would depend on both film coefficients and the wall resistance. For many designs the outer film resistance in the stirred tank and the wall resistance would be small compared with the inner film resistance; thus,

$h_{10} A$. The inner film coefficient can be related to the flow by an empirical relationship of the form (Foust et al., 1980)

$$UA = aF_c^b \quad (3.61)$$

Equations (3.59) to (3.61) can be combined to eliminate T_{coul} and UA to give the following expression for the heat transferred:

$$Q = -\frac{aF_c^{b+1}}{F_c + \frac{aF_c^b}{2\rho_c C_{pc}}}(T - T_{\text{cin}}) \quad (3.62)$$

This solution to the subproblem expresses the heat transferred in terms of the specified, external variables (F_c and T_{cin}) and the tank temperature, which is the dependent variable to be determined. Equation (3.62) can be substituted into equation (3.58) to give the final model for the stirred-tank exchanger.

$$V\rho C_p \frac{dT}{dt} = C_p \rho F(T_0 - T) - \frac{aF_c^{b+1}}{F_c + \frac{aF_c^b}{2\rho_c C_{pc}}}(T - T_{\text{cin}}) \quad (3.63)$$

The degrees-of-freedom analysis results in one variable (T), one equation (3.63), four external variables (T_{cin} , T_0 , and F are assumed constant, and F_c can change with time), and seven parameters. Thus, the model is exactly specified.

To evaluate the linearity of the model, all constants (for this example) are substituted into equation (3.63) to give the following:

$$(2.1 \times 10^6) \frac{dT}{dt} = (0.85 \times 10^6)(150 - T) - \frac{1.41 \times 10^5 F_c^{0.5}}{F_c + (0.141) F_c^{0.5}}(T - 25)$$

The model is nonlinear because of the F_c terms and the product of F_c times T . Therefore, the second term in equation (3.63) must be linearized using the Taylor series in two variables, which yields the following result:

$$Q = Q_s - UA_s^*(T - T_s) + K_{F_c}(F_c - F_{cs}) \quad (3.64)$$

$$Q_s = \left(\frac{-aF_c^{b+1}(T - T_{\text{cin}})}{F_c + \frac{aF_c^b}{2\rho_c C_{pc}}} \right), \quad (3.65)$$

$$UA_s^* = \left(\frac{aF_c^{b+1}}{F_c + \frac{aF_c^b}{2\rho_c C_{pc}}} \right), \quad K_{F_c} = \left[\frac{-abF_c^b \left(F_c + \frac{a}{b} \frac{F_c^b}{2\rho_c C_{pc}} \right) (T - T_{\text{cin}})}{\left(F_c + \frac{aF_c^b}{2\rho_c C_{pc}} \right)^2} \right],$$

The linear approximation can be used to replace the nonlinear term, and again the equation can be expressed in deviation variables:

$$VC_p \rho \frac{dT'}{dt} = F\rho C_p(-T') - UA_s^* T' + K_{F_c} F_c' \quad (3.66)$$

Solution. The resulting approximate model is a linear first-order ordinary differential equation that can be solved by applying the integrating factor.

$$\frac{dT'}{dt} + \frac{1}{\tau} T' = \frac{K_{F_c}}{V\rho C_p} F_c' \quad \text{with } \tau = \left(\frac{F}{V} + \frac{UA_s^*}{V\rho C_p} \right)^{-1} \quad (3.67)$$

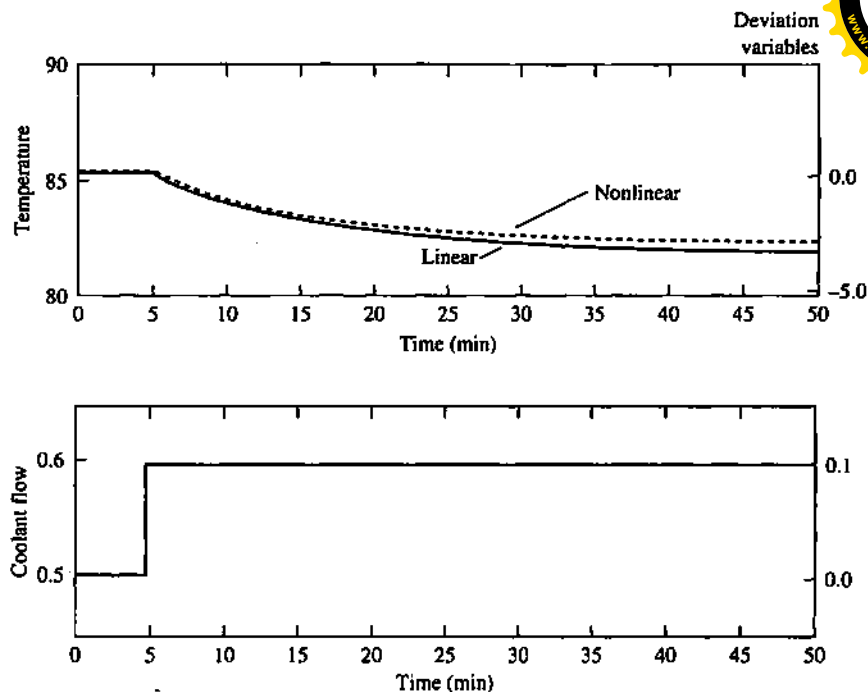


FIGURE 3.15

Dynamic response for Example 3.7.

For a step change in the coolant flow rate at $t = 0$ and $T'(0) = 0$, the solution is given by

$$T' = \frac{K_{Fc} \Delta F_c \tau}{V \rho C_p} (1 - e^{-t/\tau}) = \Delta F_c K_p (1 - e^{-t/\tau}) \quad (3.68)$$

The linearized coefficients can be calculated to be $K_{Fc} = -5.97 \times 10^6$ ([cal/min]/[m³/min]), $K_T = -9.09 \times 10^4$ ([cal/min]/°C). The steady-state gain and time constant can be determined to be

$$K_p = \frac{K_{Fc} \tau}{V \rho C_p} = -33.9 \frac{^\circ\text{C}}{\text{m}^3/\text{min}} \quad \tau = \left(\frac{F}{V} + \frac{UA_s^*}{V \rho C_p} \right)^{-1} = 11.9 \text{ min}$$

Results analysis. The solution gives an exponential relationship between time and the variable of interest. The approximate linearized response is plotted in Figure 3.15 along with the solution to the nonlinear model. For the magnitude of the step change considered, the linearized approximation provides a good estimate of the true response.

The analytical linearized approximation provides relationships between the transient response and process design and operation. For example, since $UA_s^* > 0$, equation (3.67) demonstrates that the time constant for the heat exchanger is always smaller than the time constant for the same stirred tank without a heat exchanger, for which $\tau = V/F$.

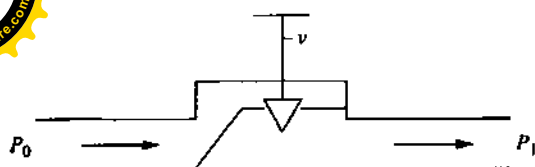


FIGURE 3.16

Simplified schematic of flow through valve.

EXAMPLE 3.8. Flow manipulation

As explained briefly in Chapter 1, process control requires a manipulated variable that can be adjusted independently by a person or automation system. Possible manipulated variables include motor speed and electrical power, but the manipulated variable in the majority of process control systems is valve opening, which influences the flow of gas, liquid, or slurry. Therefore, it is worthwhile briefly considering a model for the effect of valve opening on flow. A simplified system is shown in Figure 3.16, which is described by the following macroscopic energy balance (Foust et al., 1980; Hutchinson, 1976).

$$F = C_v v \sqrt{\frac{P_0 - P_1}{\rho}} \quad (3.69)$$

where C_v = inherent valve characteristic
 v = valve stem position, related to percent open
 F = volumetric flow rate

The valve stem position is changed by a person, as with a faucet, or by an automated system. The inherent valve characteristic depends in general on the stem position; also, the pressures in the pipe would depend on the flow and, thus, the stem position. For the present, the characteristic and pressures will be considered to be approximately constant. In that case, the flow is a linear function of the valve stem position:

$$F' = C_v \sqrt{\frac{P_0 - P_1}{\rho}} v' = K_v v' \quad \text{with } K_v = C_v \sqrt{\frac{P_0 - P_1}{\rho}} \quad (3.70)$$

Thus, linear or linearized models involving flow can be expressed as a function of valve position using equation (3.70). This is the expression used for many of the models in the next few chapters. More detail on the industrial flow systems will be presented in Chapters 7 (automated valve design) and 16 (variable characteristics and pressures).

The procedure for linearization in this section has applied classical methods to be performed by the engineer. Software systems can perform algebra and calculus; therefore, linearization can be performed via special software. One well-known software system for analytical calculations is Maple™. We will continue to use the “hand” method because of the simplicity of the models. Whether the models are linearized by hand or using software, the engineer should always thoroughly understand the effects of design and operating variables on the gains, time constant, and dead time.

The examples in this section have demonstrated the ease with which linearization can be applied to dynamic process models. As shown in equation (3.37), a second-order term in the Taylor series gives insight into the accuracy of the linear approximation. However, there is no simple manner for evaluating whether a linear approximation is appropriate, since the sensitivity of the modelling results depends on the formulation, input variables, parameters, and, perhaps most importantly, the goals of the modelling task. An analytical method for estimating the effects of the second-order terms in the Taylor series on the results of the dynamic model is available (Douglas, 1972); however, it requires more effort than the numerical solution of the original nonlinear equations. Therefore, the analytical method using higher-order terms in the Taylor series is not often used, although it might find application for a model solved frequently.

One quick check on the accuracy of the linearized model is to compare the final values, as time goes to infinity, of the nonlinear and linearized models. If they differ by too much, with this value specific to the problem, then the linearized model would be deemed to be of insufficient accuracy. If the final values are close enough, the dynamic responses could still differ and would have to be evaluated. Also, values of the time constants and gain at the initial and final conditions can be determined; if they are significantly different, the linearized model is not likely to provide adequate accuracy. The reader will be assisted in making these decisions by numerous examples in this book that evaluate linearized control methods applied to nonlinear processes.

The predictions from a linearized dynamic model are sufficiently accurate for most control system design calculations if the values of steady-state gain and time constant(s) are similar throughout the transient, i.e., from the initial to final conditions.

The more complete approach for checking accuracy is to compare results from the linearized and full nonlinear models, with the nonlinear model solved using numerical methods, as discussed in the next section. Fundamental models can require considerable engineering effort to develop and solve for complex processes, so this approach is usually reserved for processes that are poorly understood or known to be highly nonlinear. In practice, engineers often learn by experience which processes in their plants can be analyzed using linearized models.

Again, this experience indicates that in the majority of cases, linear models are adequate for process control. An additional advantage of approximate linear models is the insight they provide into how process parameters and operating conditions affect the transient response.

3.5 ■ NUMERICAL SOLUTIONS OF ORDINARY DIFFERENTIAL EQUATIONS

There are situations in which accurate solutions of the nonlinear equations are required. Since most systems of nonlinear algebraic and differential equations cannot be solved analytically, approximate solutions are determined using numerical methods. Many numerical solution methods are available, and a thorough coverage of the topic would require a complete book (for example, Carnahan et al., 1969,



(Maron and Lopez, 1991). However, a few of the simplest numerical methods for solving ordinary differential equations will be introduced here, and they will be adequate, if not the most efficient, for most of the problems in this book.

Numerical methods do not find analytical solutions like the expressions in the previous sections; they provide a set of points that are “close” to the true solution of the differential equation. The general concept for numerical solutions is to use an initial value (or values) of a variable and an approximation of the derivative over a single step to determine the variable after the step. For example, the solution to the differential equation

$$\frac{dy}{dt} = f(y, t) \quad \text{with } y|_{t=t_i} = y_i \quad (3.71)$$

can be approximated from $t = t_i$ to $t = t_{i+1}$, with $\Delta t = t_{i+1} - t_i$, by a linear Taylor series approximation to give

$$\begin{aligned} y_{i+1} &\approx y_i + \left[\frac{dy}{dt} \right]_{t_i} (t_{i+1} - t_i) \\ y_{i+1} &\approx y_i + f(y_i, t) \Delta t \end{aligned} \quad (3.72)$$

The procedure in equation (3.72) is the *Euler* numerical integration method (Carnahan et al., 1969). This procedure can be repeated for any number of time steps to yield the approximate solution over a time interval.

Numerical methods can include higher-order terms in the Taylor series to improve the accuracy. The obvious method would be to determine higher-order terms in the Taylor series in equation (3.72); however, this would require algebraic manipulations that are generally avoided, although they could be practical with computer algebra. A manner has been developed to achieve the equivalent accuracy by evaluating the first derivative term at several points within the step. The result is presented here without derivation; the derivation is available in most textbooks on numerical analysis (Maron and Lopez, 1991). There are many forms of the solution, all of which are referred to as Runge-Kutta methods. The following equations are one common form of the Runge-Kutta fourth-order method:

$$y_{i+1} = y_i + \frac{\Delta t}{6} (m_1 + 2m_2 + 2m_3 + m_4) \quad (3.73)$$

with $m_1 = f(y_i, t_i)$

$$m_2 = f\left(y_i + \frac{\Delta t}{2} m_1, t_i + \frac{\Delta t}{2}\right)$$

$$m_3 = f\left(y_i + \frac{\Delta t}{2} m_2, t_i + \frac{\Delta t}{2}\right)$$

$$m_4 = f(y_i + \Delta t m_3, t_i + \Delta t)$$

All numerical methods introduce an error at each step, due to the loss of the higher-order terms in the Taylor series, and these errors accumulate as the integration proceeds. Since the accumulated error depends on how well the function is approximated, the Euler and Runge-Kutta methods have different accumulated errors. The Euler accumulated error is proportional to the step size; the Runge-Kutta error in equation (3.73) depends on the step size to the fourth power. Thus, the Euler method requires a smaller step size for the same accuracy as Runge-Kutta; this is partially offset by fewer calculations per step required for the Euler

method. Since the errors from both methods increase with increasing step size, a very small step size might be selected for good accuracy, but a very small step size has two disadvantages. First, it requires a large number of steps and, therefore, long computing times to complete the entire simulation. Second, the use of too small a step size results in a very small change in y , perhaps so small as to be lost due to round-off. Therefore, an intermediate range of step sizes exists, in which the approximate numerical solution typically provides the best accuracy.

The engineer must choose the step size Δt to be the proper size to provide adequate accuracy. The proper step size is relative to the dynamics of the solution; thus, a key parameter is $\Delta t/\tau$, with τ being the smallest time constant appearing in a linear(ized) model. As a very rough initial estimate, this parameter could be taken to be approximately 0.01. Then, solutions can be determined at different step sizes; the region in which the solution does not change significantly, as compared with the accuracy needed to achieve the modelling goal, indicates the proper range of step size. There are numerical methods that monitor the error during the problem solution and adjust the step size during the solution to achieve a specified accuracy (Maron and Lopez, 1991).

Some higher-order systems have time constants that differ greatly (e.g., $\tau_1 = 1$ and $\tau_2 = 5000$); these systems are referred to as *stiff*. When explicit numerical methods such as Euler and Runge-Kutta are used for these systems, the step size must be small relative to the *smallest* time constant for good accuracy (and stability), but the total interval must be sufficient for the longest time constant to respond. Thus, the total number of time steps can be extremely large, and computer resources can be exorbitant. One solution method is to approximate part of the system as a quasi-steady state; this was done in several of the previous examples in this chapter, such as Example 3.7, where the coolant energy balance was modelled as a steady-state process. When this is not possible, the explicit numerical methods described above are not appropriate, and *implicit* numerical methods, which involve iterative calculations at each step, are recommended (Maron and Lopez, 1991).

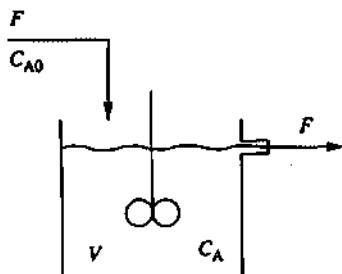
Either the Euler or the Runge-Kutta method should be sufficient for the problems encountered in this book, but not for all realistic process control simulations. Recommendations on algorithm selection are available in the references already noted, and various techniques have been evaluated (Enwright and Hull, 1976). The numerical methods are demonstrated by application to examples.

EXAMPLE 3.9. Isothermal CSTR

In Example 3.5 a model of an isothermal CSTR with a second-order chemical reaction was derived and an approximate linear model was solved. The nonlinear model cannot be solved analytically; therefore, a numerical solution is presented. The Euler method can be used, which involves the solution of the following equation at each step, i :

$$C_{A,i+1} = C_{A,i} + \Delta t \left(\frac{F}{V} (C_{A0} - C_{A,i}) + k C_{A,i}^2 \right) \quad (3.74)$$

An appropriate step size was found by trial and error to be 0.05. (Note that $\Delta t/\tau = 0.014$.) The numerical solution is shown in Figure 3.12 as the result from the nonlinear model.





In summary, numerical methods provide the capability of solving complex, nonlinear ordinary differential equations. Thus, the engineer can formulate a model to satisfy the modelling goals without undue concern for determining an analytical solution. This power in developing specific solutions is achieved at a loss in engineering insight, so that the linearized solutions are often derived to establish relationships.

3.6 ■ THE NONISOTHERMAL CHEMICAL REACTOR

One of the most important processes for the engineer is the chemical reactor because of its strong influence on product quality and profit. The dynamic behaviors of chemical reactors vary from quite straightforward to highly complex, and to evaluate the dynamic behavior, the engineer often must develop fundamental models. A simple model of a nonisothermal chemical reactor is introduced here with a sample dynamic response, and further details on modelling a continuous-flow stirred-tank reactor (CSTR) are presented in Appendix C along with additional aspects of its dynamic behavior. In this introduction, the reactor shown in Figure 3.17 is modelled; it is a well-mixed, constant-volume CSTR with a single first-order reaction, exothermic heat of reaction, and a cooling coil. The system is the liquid in the reactor. Since the concentration changes, a component material balance is required, and since heat is transferred and the heat of reaction is significant, an energy balance is required. Thus, the following two equations must be solved simultaneously to determine the dynamic behavior of the system:

Material balance on component A:

$$\frac{dC_A}{dt} = F(C_{A0} - C_A) - V k_0 e^{-E/RT} C_A \quad (3.75)$$

Energy balance:

$$\begin{aligned} \frac{dT}{dt} = & F\rho C_p(T_0 - T) + \frac{aF_c^b}{F_c + aF_c^b/2\rho_c C_{pc}}(T - T_c) \\ & + (-\Delta H_{rxn})V k_0 e^{-E/RT} C_A \end{aligned} \quad (3.76)$$

The second term on the right-hand side of the energy balance represents the heat transferred via the cooling coil, with the heat transfer coefficient a function of the coolant flow rate as described in Example 3.7.

The dynamic behavior of the concentration of the reactant and temperature to a step change in the cooling flow can be determined by solving equations (3.75) and (3.76). Since these equations are highly nonlinear, they are solved numerically here, using data documented in Section C.2 of Appendix C. The dynamic behaviors of the concentration and temperature to a step in coolant flow are shown in Figure 3.18. Note that for *this case*, the dynamic behavior is underdamped, yielding oscillations that damp out with time. (You may have experienced this type of behavior in an automobile with poor springs and shock absorbers when the suspension oscillates for a long time after striking a bump in the road.) Certainly, the large oscillations over a long time can lead to undesired product quality.

Not all chemical reactors behave with this underdamped behavior; many are more straightforward with overdamped dynamics, while a few are much more challenging. However, the engineer cannot determine the dynamic behavior of

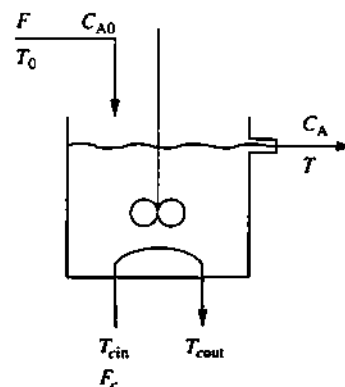


FIGURE 3.17

Continuous-flow stirred-tank
chemical reactor with
cooling coil.

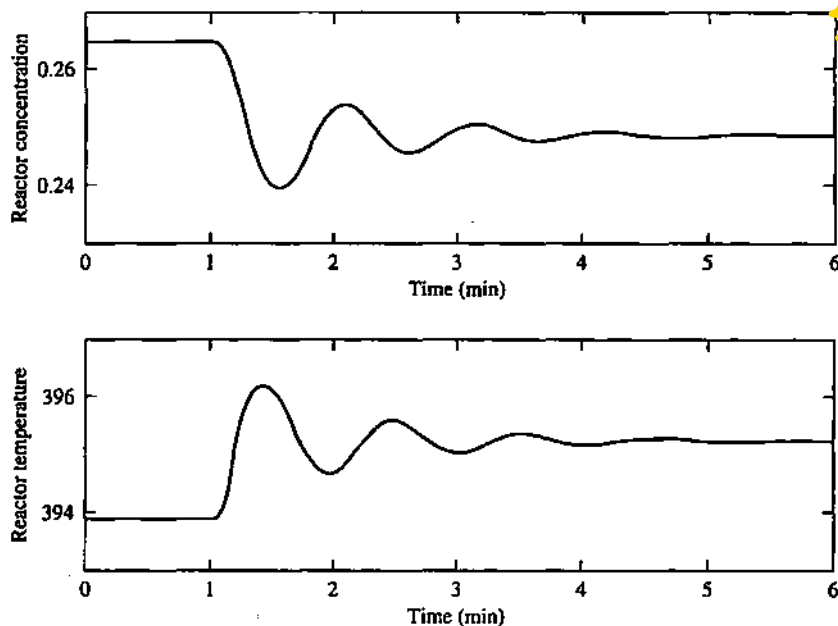


FIGURE 3.18

Dynamic response of a CSTR to a step change in coolant flow of $-1 \text{ m}^3/\text{min}$ at $t = 1$.

a reactor based on the physical structure, such as a CSTR or packed bed, or on specific design parameters. Therefore, the engineer must apply modelling and analysis to predict the dynamic behavior. Hopefully, your interest will be piqued by this example, and you will refer to the detailed reactor modelling and analysis found in Appendix C.

3.7 ■ CONCLUSIONS

The procedure in Table 3.1 provides a road map for developing, solving, and interpreting mathematical models based on fundamental principles. In addition to predicting specific behavior, these models provide considerable insight into the relationship between the process equipment and operating conditions and dynamic behavior. A thorough analysis of results is recommended in all cases so that the sensitivity of the solution to assumptions and data can be evaluated.

Perhaps the most important concept is

Modelling is a goal-oriented task, so the proper model depends on its application.

The models used in process control are developed to relate each input variable (cause) to the output variable (effect). The modelling approach enables us to reach this goal by (1) developing the fundamental model and (2) deriving the linearized



Models for each input output dynamic response. The approach can be demonstrated by repeating the model for the isothermal CSTR with first-order kinetics derived in Example 3.2.

$$V \frac{dC_A}{dt} = F(C_{A0} - C_A) - V k C_A \quad (3.77)$$

In this discussion, we will consider the situation in which the feed flow rate can be regulated by a valve, while the feed concentration is determined by upstream equipment that causes unregulated variations in the concentration. Thus,

C_A = key output variable

F = manipulated input variable

C_{A0} = disturbance input variable

Equation (3.77) can be linearized and expressed in deviation variables to give the following approximate model:

$$\tau \frac{dC'_A}{dt} + C'_A = K_F F' + K_{CA0} C'_{A0} \quad (3.78)$$

with

$$\tau = V/(F + V k)$$
$$K_F = (C_{A0} - C_A)/(F_s + V k)$$
$$K_{CA0} = F/(F + V k)$$

A model for each input can be derived by assuming that the other input is constant (zero deviation) to give the following *two models*, one for each input, in the standard form.

Effect of the disturbance:

$$\tau \frac{dC'_A}{dt} + C'_A = K_{CA0} C'_{A0} \quad (3.79)$$

Effect of the manipulated variable:

$$\tau \frac{dC'_A}{dt} + C'_A = K_F F' \quad (3.80)$$

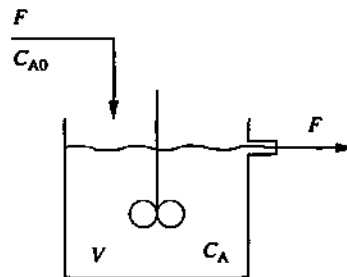
Note that separate models are needed to represent the dynamics between the two inputs and the output; thus, the single-component material balance yields two input/output models. If more input variables were considered, for example, temperature, additional input/output models would result.

This modelling approach provides very important information about the dynamic behavior of the process that can be determined from the values of the steady-state gains and the time constants. The definitions of the key parameters are summarized in the following:

Parameter	Symbol	Definition	Units
Steady-state gain	K	Output/input	$(\Delta \text{output}/\Delta \text{input})_{ss}$
Time constant	τ	Multiplies derivative in standard model form	Time



Conclusions



The values of these parameters can be used to estimate the magnitude and speed of the effects of the input changes on the output variable. This modelling procedure enables the engineer to relate the dynamic behavior of a process to the equipment sizes, physical properties, rate processes, and operating conditions. For example, the steady-state effect of the flow disturbance (F) depends on its gain (K_F), which is affected by the equipment (V), chemistry (k), and operating conditions (F , C_{A0} , and C_{As}). Recall that we are compromising accuracy through linearization to achieve these insights.

The engineer should interpret linearized models to determine the factors influencing dynamic behavior, i.e., influencing the gains and time constants.

As we build understanding of process control in later chapters, this interpretation will prove invaluable in designing process with favorable dynamics and designing feedback process control calculations.

The observant reader may have noticed the similarities among the behaviors of many of the examples in this chapter. These similarities will lead to important generalizations, presented in Chapter 5, about the dynamics of processes that can be represented by simple sets of differential equations: one ordinary differential equation (first-order system), two equations (second-order system), and so forth. However, before exploring these generalities, some useful mathematical methods are introduced in Chapter 4. These mathematical methods are selected to facilitate the analysis of process control systems using models like the ones developed in this chapter and will be used extensively in the remainder of the book.

REFERENCES

- Bird, R., W. Stewart, and E. Lightfoot, *Transport Phenomena*, Wiley, New York, 1960.
- Carnahan, B., H. Luther, and J. Wilkes, *Applied Numerical Methods*, Wiley, New York, 1969.
- Douglas, J., *Process Dynamics and Control, Volume I, Analysis of Dynamic Systems*, Prentice-Hall, Englewood Cliffs, NJ, 1972.
- Enwright, W., and T. Hull, *SIAM J. Numer. Anal.*, 13, 6, 944–961 (1976).
- Felder, R., and R. Rousseau, *Elementary Principles of Chemical Processes* (2nd ed.), Wiley, New York, 1986.
- Foust, A., L. Wenzel, C. Clump, L. Maus, and L. Andersen, *Principles of Unit Operations*, Wiley, New York, 1980.
- Himmelblau, D., *Basic Principles and Calculations in Chemical Engineering*, Prentice-Hall, Englewood Cliffs, NJ, 1982.
- Hutchinson, J. (ed.), *ISA Handbook of Control Valves* (2nd ed.), Instrument Society of America, Research Triangle Park, NC, 1976.
- Levenspiel, O., *Chemical Reaction Engineering*, Wiley, New York, 1972.
- Maron, M., and R. Lopez, *Numerical Analysis, A Practical Approach* (3rd ed.), Wadsworth, Belmont, CA, 1991.



McQuiston, F., and J. Parker, *Heating, Ventilation, and Air Conditioning* (3rd ed.), Wiley, New York, 1988.

Smith, J., and H. Van Ness, *Introduction to Chemical Engineering Thermodynamics* (4th ed.), McGraw-Hill, New York, 1987.



Additional Resources

ADDITIONAL RESOURCES

The following references, in addition to Douglas (1972), discuss goals and methods of fundamental modelling for steady-state and dynamic systems in chemical engineering.

Aris, R., *Mathematical Modelling Techniques*, Pitman, London, 1978.

Denn, M., *Process Modeling*, Pitman Publishing, Marshfield, MA, 1986.

Franks, R., *Modelling and Simulation in Chemical Engineering*, Wiley-Interscience, New York, 1972.

Friedly, J., *Dynamic Behavior of Processes*, Prentice-Hall, Englewood Cliffs, NJ, 1972.

Himmelblau, D., and K. Bishoff, *Process Analysis and Simulation, Deterministic Systems*, Wiley, New York, 1968.

Luyben, W., *Process Modelling, Simulation, and Control for Chemical Engineers* (2nd ed.), McGraw-Hill, New York, 1989.

Guidance on the formulation, analysis, and efficient numerical computation of the sensitivity of the solution of differential equations to parameters is given in the following.

Leis, J., and M. Kramer, "The Simultaneous Solution and Sensitivity Analysis of Systems Described by Ordinary Differential Equations," *ACM Trans. on Math. Software*, 14, 1, 45–60 (1988).

Tomovic, R., and M. Vokobratovic, *General Sensitivity Theory*, Elsevier, New York, 1972.

The following reference presents methods for evaluating feasible operating conditions and economic optima in processes.

Edgar, T., and D. Himmelblau, *Optimization of Chemical Processes*, McGraw-Hill, New York, 1988.

The following reference discusses modelling as applied to many endeavors and gives examples in other disciplines, such as economics, biology, social sciences, and environmental sciences.

Murthy, D., N. Page, and E. Rodin, *Mathematical Modelling*, Pergamon Press, Oxford, 1990.

Stirred tanks are applied often in chemical engineering. Details on their design and performance can be found in the following reference.

Oldshue, J., *Fluid Mixing Technology*, McGraw-Hill, New York, 1983.

In answering the questions in this chapter (and future chapters), careful attention should be paid to the modelling methods and results. The following summary of the modelling method is provided to assist in this analysis.

- Define the system and determine the balances and constitutive relations used.
- Analyze the degrees of freedom of the model.
- Determine how the design and operating values influence key results like gains and time constants.
- Determine the shape of the dynamic response. Is it monotonic, oscillatory, etc.?
- If nonlinear, estimate the accuracy of the linearized result.
- Analyze the sensitivity of the dynamic response to parameter values.
- Discuss how you would validate the model.

QUESTIONS

- 3.1. The chemical reactor in Example 3.2 is to be modelled, with the goal of determining the concentration of the product C_B as a function of time for the same input change. Extend the analytical solution to answer this question.
- 3.2. The series of two tanks in Example 3.3 are to be modelled with $V_1 + V_2 = 2.1$ and $V_1 = 2V_2$. Repeat the analysis and solution for this situation.
- 3.3. The step input is changed to an impulse for Example 3.3. An impulse is a “spike” with a (nearly) instantaneous duration and nonzero integral; physically, an impulse would be achieved by rapidly dumping extra component A into the first tank. Solve for the outlet concentration of the second tank after an impulse of M moles of A is put into the first tank.
- 3.4. A batch reactor with the parameters in Example 3.2 is initially empty and is filled at the inlet flow rate, with the outlet flow being zero. Determine the concentration of A in the tank during the filling process. After the tank is full, the outlet flow is set equal to the inlet flow; that is, the reactor is operated like a continuous-flow CSTR. Determine the concentration of A to the steady state.
- 3.5. The system in Example 3.1 has an input concentration that varies as a sine with amplitude A and frequency ω . Determine the outlet concentration for this input.
- 3.6. The level-flow system in Figure Q3.6 is to be analyzed. The flow F_0 is constant. The flow F_3 depends on the valve opening but not on the levels, whereas flows F_1 and F_2 depend on the varying pressures (i.e., levels). The system is initially at steady state, and a step increase in F_3 is made by adjusting the valve. Determine the dynamic response of the levels and flows using an approximate linear model. Without specific numerical values, sketch the approximate dynamic behavior of the variables.
- 3.7. The behavior of the single CSTR with the kinetics shown below is considered in this question. The goal is to control the concentration of product D in the effluent. Your supervisor proposes the feed concentration of reactant

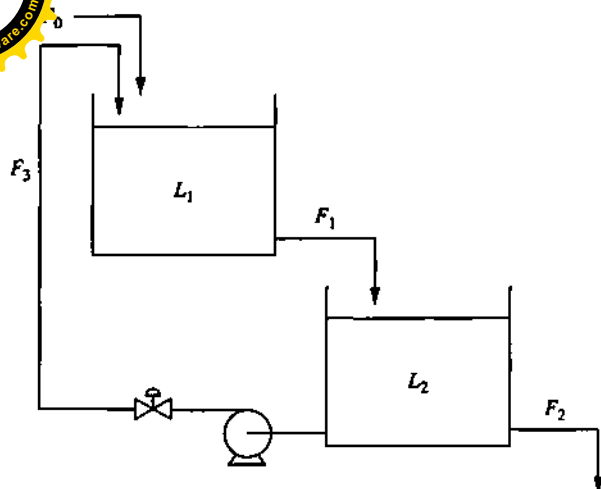


FIGURE Q3.6

A as the manipulated variable for a *feedback controller*. Is this a good idea?



In answering this question, you may use the following information: (1) the tank is well mixed and has a constant volume and temperature; (2) all components have the same molecular weights and densities; (3) all reactions are elementary; thus, in this case they are all first-order; (4) the volumetric feed flow is constant (F) and contains only component A (C_{A0}).

- Starting with fundamental balances, derive the model (differential equations) that must be solved to determine the behavior of the concentration of component D.
- Express the equations from part (a) in linear(ized) deviation variables and define the time constants and gains.
- Does a causal relationship exist between C_{A0} and C_D ?

- 3.8. The level-flow system in Figure Q3.8 is to be analyzed. The flow into the system, F_0 , is independent of the system pressures. The feed is entirely liquid, and the first vessel is closed and has a nonsoluble gas in the space above the nonvolatile liquid. The flows F_1 and F_2 depend only on the pressure drops, because the restrictions in the pipes are fixed. Derive the linearized model for this system in response to a step change in F_0 , solve the equations, and, without specific numerical values, sketch the dynamic responses.

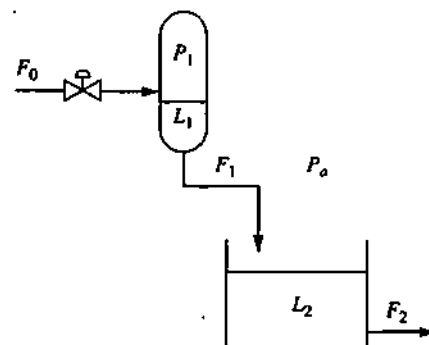


FIGURE Q3.8

- 3.9. The room heating Example 3.4 is reconsidered; for the following situations, each representing a single change from the base case, reformulate the model as needed and determine the dynamic behavior of the temperature and heating status.

- (a) Due to leaks, a constant flow into and out of the room exists. Assume that the volume of air in the room is changed every hour with entering air at the outside temperature.
- (b) A mass of material (e.g., furniture) is present in the room. Assume that this mass is always in equilibrium with the air; that is, the heat exchange is at quasi-steady state. The mass is equivalent to 200 kg of wood.
- (c) The ambient temperature decreases to -10°C .
- (d) The duty of the furnace is reduced to 0.50×10^6 when on.
- (e) The heat transferred to the room does not change instantaneously when the furnace status changes. The relationship between the heat generated in the furnace (Q_f), which changes immediately when the switch is activated, and the heat to the room (Q_h) is

$$\tau_Q \frac{dQ_h}{dt} = Q_f - Q_h \quad \text{with } \tau_Q = 0.10 \text{ h}$$

- 3.10. Determine the dynamic responses for a +10 percent change in inlet flow rate in place of the original input change for one or more of Examples 3.2, 3.5, and 3.7. Determine whether the model must be linearized in each case. For cases that require linearization, estimate the errors introduced and compare a numerical solution with the approximate, linear dynamic response.
- 3.11. A stirred-tank heater could have an external jacket with saturated steam condensing in the jacket to heat the tank. Assume that this modification has been made to the system in Example 3.7 and derive an analytical expression for the response of the tank temperature to a step change in the steam pressure. Begin by sketching the system and listing assumptions.
- 3.12. The tank draining problem in Example 3.6 has been modified to remove the restriction (partially opened valve) in the outlet line. Now, the line is simply a pipe. Reformulate and solve the problem for the two following cases, each with a pipe long enough that end conditions are negligible.
 - (a) The flow in the outlet pipe is laminar.
 - (b) The flow in the outlet pipe is turbulent.
- 3.13. Answer the following questions.
 - (a) Explain what is meant by a stiff system of differential equations. Under what conditions (changing values of parameters) would the equations in Example 3.3 be stiff? If they were stiff, suggest several ways to solve them numerically. Would this stiffness affect the accuracy of the analytical solutions of the linearized model?
 - (b) The analysis of degrees of freedom suggests that terms that are constant in the current examples be separated into two categories: parameters and external variables. Why would this be useful for future analysis of feedback control systems? Suggest two subcategories for the external variables and why they might be useful for feedback control analysis.
 - (c) The degrees-of-freedom analysis should define the proper number of equations for a model. Suppose that the following model were proposed for Example 3.6.

$$A \frac{dL}{dt} = F_0 - F_1 \quad (5)(2) = 10$$



When F_0 is constant, this model has two equations and two unknown variables, L and F_1 . Explain why this model does not satisfy the degrees-of-freedom analysis and provide a mathematical test that can be applied to potential equation sets.

- (d) Is it possible for a model to be linear for one external input perturbation and nonlinear for another? Explain and give examples.
- (e) Give the equations to be solved at every time step for an Euler integration of the nonisothermal chemical reactor model in equations (3.75) and (3.76).

3.14. The chemical reactor in Example 3.3 is considered in this question. The only change to the problem is the input function; here, the inlet concentration is returned to its initial value in a step 5 minutes after the initial step increase.

- (a) Determine the dynamic response of the concentration of both tanks.
- (b) Compare your answer to the shape of the plot in Figure 3.5b and explain similarities and differences.
- (c) Based on your results in (a) and (b), discuss how you would design an emergency system to prevent the concentration of A in the second tank from exceeding a specified maximum value. Discuss the variables F and C_{A0} as potential manipulated variables, and select the value to which the manipulated variable should be set when the action limit is reached. Also, discuss how you would determine the value of the action limit.

3.15. The dynamic response of the CSTR shown in Figure 3.1 is to be determined as follows.

Assumptions: (i) well mixed, (ii) isothermal, (iii) constant density, and (iv) constant volume.

Data: $V = 2 \text{ m}^3$; $F = 1 \text{ m}^3/\text{h}$; $C_{A0}(0) = 0.5 \text{ mole}/\text{m}^3$.

Reaction: $A \rightarrow \text{Products}$

with

$$\begin{aligned}r_A &= -k_1 C_A / (1 + k_2 C_A) \text{ mole}/(\text{m}^3\text{h}) \\k_1 &= 1.0 \text{ h}^{-1} \\k_2 &= 1.0 \text{ m}^3/\text{mole}\end{aligned}$$

- (a) Formulate the model for the dynamic response of the concentration of A.
- (b) Linearize the equation in (a).
- (c) Analytically solve the linearized equation for a step change in the inlet concentration of A, C_{A0} .
- (d) Give the equation(s) for the numerical solution of the “exact” nonlinear equation derived in (a). You may use any of the common numerical methods for solving ordinary differential equations.
- (e) Calculate the transients for the (analytical) linearized and (numerical) nonlinear models. Graph the results for both the nonlinear and linearized predictions for two cases, both of which start from the initial conditions given above and have the magnitudes (1) $\Delta C_{A0} = 0.5$ and (2) $\Delta C_{A0} = 4.0$. Provide an annotated listing of your program or spreadsheet.
- (f) Discuss the accuracy of the linearized solutions compared with solutions to the “exact” nonlinear equations for these two cases.

3.16. Discuss whether linearized dynamic models would provide accurate representations of the dynamic results for

- (a) Example 3.2 with $\Delta C_{A0} = -0.925$ moles/m³
- (b) Example 3.7 for $\Delta F_c = -9.25$ m³/min

3.17. A stirred-tank mixer has two input streams: F_A which is pure component A, and F_B , which has no A. The system is initially at steady state, and the flow F_A is constant. The flow of B changes according to the following description: From time $0 \rightarrow t_1$, $F'_B(t) = \alpha t$ (a ramp from the initial condition); and from time $t_1 \rightarrow \infty$, $F'_B(t) = \alpha t_1$ (constant at the value reached at t_1). The following assumptions may be used:

- (1) The densities of the two streams are constant and equal, and there is no density change on mixing.
- (2) The volume of the liquid in the tank is constant.
- (3) The tank is well mixed.
- (a) Sketch the process, define the system, and derive the basic balance for the weight fraction of A in the exit stream, X_A .
- (b) Derive the linearized balance in deviation variables.
- (c) Solve the equation for the forcing function, $F'_B(t)$, defined above. (Hint: You may want to develop two solutions, first from $0 \rightarrow t_1$ and then $t_1 \rightarrow \infty$.)
- (d) Sketch the dynamic behavior of $F'_B(t)$ and $X'_A(t)$.

3.18. In the tank system in Figure 3.13, the outflow drains through the outlet pipe with a restriction as in Example 3.6, and in this question, a first-order chemical reaction occurs in the tank. Given the following data, plot the operating window, i.e., the range of possible steady-state operating conditions, with coordinates of level and concentration of A. Discuss the effect of changing reactor temperature on the operating window, if any.

Design parameters: Cross-sectional area = 0.30 m², maximum level = 4.0 m. The chemical reaction is first-order with $k_0 = 2.28 \times 10^7$ (h⁻¹) and $E/R = 5000$ K. The base-case conditions can be used to back-calculate required parameters. The base case data are $T = 330$ K, $L = 3.33$ m, $F = 10$ m³/h, and $C_A = 0.313$ mole/m³. The external variables can be adjusted over the following ranges: $0.20 \leq C_{A0} \leq 0.70$ and $3.0 \leq F \leq 12.5$.

3.19. A system of well-mixed tanks and blending is shown in Figure Q3.19. The delays in the pipes are negligible, the flow rates are constant, and the streams have the same density. Step changes are introduced in C_{A1} at t_1 and C_{A2} at t_2 , with $t_2 > t_1$. Determine the transient responses of C_{A3} , C_{A4} , and C_{A5} .

3.20. Determining the sensitivity of modelling results to parameters is a key aspect of results analysis. For the result from Example 3.2,

$$C_A = C_{A\text{init}} + \Delta C_{A0} K_p (1 - e^{-t/\tau})$$

- (a) Determine analytical expressions for the sensitivity of the output variable C_A to small (differential) changes in the parameters, K_p , τ , forc-

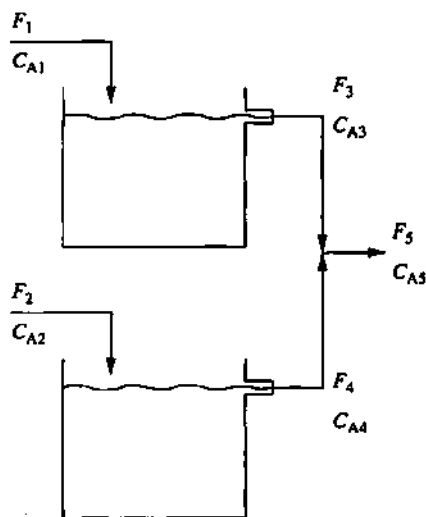


FIGURE Q3.19



ing function magnitude ΔC_{A0} , and initial steady state, $C_{A\text{init}}$. These sensitivity expressions should be functions of time.

- (b) For each result in (a), plot the sensitivities over their trajectories and discuss whether the answer makes sense physically.

- 3.21. Another experiment was performed to validate the fact that the vessel in Example 3.1 was well mixed. In this experiment, the vessel was well insulated and brought to steady state. Then a step change was introduced to the inlet temperature. The following data represents the operating conditions, and the dynamic data is given in Table Q3.21.

Data: $V = 2.7 \text{ m}^3$, $F = 0.71 \text{ m}^3/\text{min}$, $T_{0\text{init}} = 103.5^\circ\text{C}$, $T_0 = 68^\circ\text{C}$.

- (a) Formulate the energy balance for this system, and solve for the expected dynamic response of the tank temperature.
(b) Compare your prediction with the data.
(c) Given the two experimental results in Figure 3.4 and this question for the same equipment, discuss your conclusions on the assumption that the system is well mixed.
(d) Is there additional information that would help you in (c)?
- 3.22. The dynamic response of the reactant concentration in the reactor, C_A , to a change in the inlet concentration, C_{A0} , for an isothermal, constant-volume, constant-density CSTR with a single chemical reaction is to be evaluated. The reaction rate is modelled by

$$r_A = -\frac{k_1 C_A}{1 + k_2 C_A}$$

Determine how the approximate time constant of the linearized model of the process relating C_A to C_{A0} changes as k_1 and k_2 range from 0 to infinity. Explain how your answer makes sense.

TABLE Q3.22

Time	Temperature
0	103.5
.4	102
1.2	96
1.9	91
2.7	87
3.4	84
4.2	81
5.0	79
6.5	76
8.5	73

