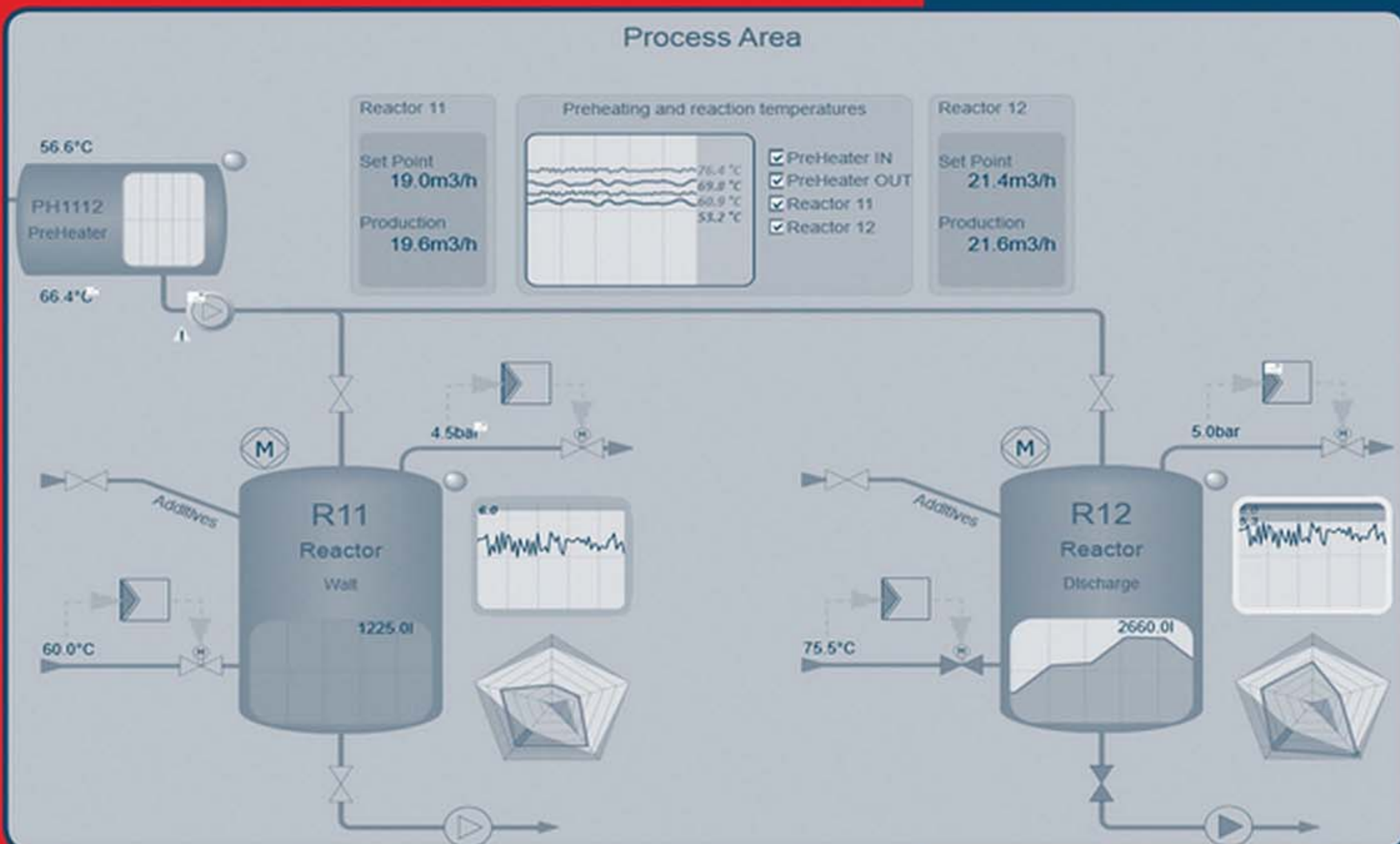
Process Dynamics and Control

4th Edition



Seborg | Edgar | Mellichamp | Doyle

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Fourth Edition

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To our families

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Thomas F. Edgar holds the Abell Chair in chemical engineering at the University of Texas at Austin and is Director of the UT Energy Institute. He earned a B.S. degree in chemical engineering from the University of Kansas and his Ph.D. from Princeton University. Before receiving his doctorate, he was employed by Continental Oil Company. His professional honors include the AIChE Colburn and Lewis Awards, ASEE Meriam-Wiley and Chemical Engineering Division Awards, ISA and AACC Education Awards, AACC Bellman Control Heritage Award, and AIChE Computing in Chemical Engineering Award. He has published over 500 papers in the field of process control, optimization, and mathematical modeling of processes such as separations, combustion, microelectronics processing, and energy systems. He is a co-author of *Optimization of Chemical Processes*, published by McGraw-Hill in 2001. Dr. Edgar was the president of AIChE in 1997, President of the American Automatic Control Council in 1989–1991 and is a member of the National Academy of Engineering.

Duncan A. Mellichamp is a founding faculty member of the Department of Chemical Engineering of the University of California, Santa Barbara. He is editor of an early book on data acquisition and control computing and has published more than 100 papers on process modeling, large scale/plantwide systems analysis, and computer control. He earned a B.S. degree from Georgia Tech and a Ph.D. from Purdue University with intermediate studies at the Technische Universität Stuttgart (Germany). He worked for four years with the Textile Fibers Department of the DuPont Company before joining UCSB. Dr. Mellichamp has headed several organizations, including the CACHE Corporation (1977), the UCSB Academic Senate (1990–1992), and the University of California Systemwide Academic Senate (1995–1997), where he served on the UC Board of Regents. He presently serves on the governing boards of several nonprofit organizations and as president of Opera Santa Barbara. Emeritus Professor since 2003, he still guest lectures and publishes in the areas of process profitability and plantwide control.

Francis J. Doyle III is the Dean of the Harvard Paulson School of Engineering and Applied Sciences. He is also the John A. & Elizabeth S. Armstrong Professor of Engineering & Applied Sciences at Harvard University. He received his B.S.E. from Princeton, C.P.G.S. from Cambridge, and Ph.D. from Caltech, all in Chemical Engineering. Prior to his appointment at Harvard, Dr. Doyle held faculty appointments at Purdue University, the University of Delaware, and UCSB. He also held visiting positions at DuPont, Weyerhaeuser, and Stuttgart University. He is a Fellow of IEEE, IFAC, AAAS, and AIMBE; he is also the recipient of multiple research awards (including the AIChE Computing in Chemical Engineering Award) as well as teaching awards (including the ASEE Ray Fahien Award). He is the Vice President of the Technical Board of IFAC and is the President of the IEEE Control Systems Society in 2016.

Preface

Global competition, rapidly changing economic conditions, faster product development, and more stringent environmental and safety regulations have made process control increasingly important in the process industries. Process control and its allied fields of process modeling and optimization are critical in the development of more flexible and complex processes for manufacturing high-value-added products. Furthermore, the continuing development of improved and less-expensive digital technology has enabled high-performance measurement and control systems to become an essential part of industrial plants.

Overall, it is clear that the scope and importance of process control technology will continue to expand during the 21st century. Consequently, chemical engineers need to master this subject in order to be able to develop, design, and operate modern processing plants. The concepts of dynamic behavior, feedback, and stability are important for understanding many complex systems of interest to chemical engineers, such as bioengineering and advanced materials. An introductory process control course should provide an appropriate balance of theory and practice. In particular, the course should emphasize dynamic behavior, physical and empirical modeling, computer simulation, measurement and control technology, fundamental control concepts, and advanced control strategies. We have organized this book so that the instructor can cover the basic material while having the flexibility to include advanced topics on an individual basis. The textbook provides the basis for 10–30 weeks of instruction for a single course or a sequence of courses at either the undergraduate or first-year graduate levels. It is also suitable for self-study by engineers in industry. The book is divided into reasonably short chapters to make it more readable and modular. This organization allows some chapters to be omitted without a loss of continuity.

The mathematical level of the book is oriented toward a junior or senior student in chemical engineering who has taken at least one course in differential equations. Additional mathematical tools required for the analysis of control systems are introduced as needed. We emphasize process control techniques that are used in practice and provide detailed mathematical analysis only when it is essential for understanding the material. Key theoretical concepts are illustrated with numerous examples, exercises, and simulations.

Initially, the textbook material was developed for an industrial short course. But over the past 40 years, it has significantly evolved at the University of California, Santa Barbara, and the University of Texas at Austin. The first edition was published in 1989 and adopted by over 80 universities worldwide. In the second edition (2004), we added new chapters on the important topics of process monitoring, batch process control, and plantwide control. For the third edition (2011), we were very pleased to add a fourth co-author, Professor Frank Doyle (then at UCSB) and made major changes that reflect the evolving field of chemical and biological engineering. These previous editions have been very successful and translated into Japanese, Chinese, Korean, and Turkish.

General revisions for the fourth edition include reducing the emphasis on lengthy theoretical derivations and increasing the emphasis on analysis using widely available software: MATLAB®, Simulink®, and Mathematica. We have also significantly revised material on major topics including control system design, instrumentation, and troubleshooting to include new developments. In addition, the references at the end of each chapter have been updated and new exercises have been added.

Exercises in several chapters are based on MATLAB® simulations of two physical models, a distillation column and a furnace. Both the book and the MATLAB simulations are available on the book's website (*www.wiley.com/college/seborg*). National Instruments has provided multimedia modules for a number of examples in the book based on their LabVIEW™ software.

Revisions to the five parts of the book can be summarized as follows. Part I provides an introduction to process control and an in-depth discussion of process modeling. It is an important topic because control system design and analysis are greatly enhanced by the availability of a process model.

Steady-state and unsteady-state behavior of processes are considered in Part II (Chapters 3 through 7). Transfer functions and state-space models are used to characterize the dynamic behavior of linear and nonlinear systems. However, we have kept derivations using classical analytical methods (e.g., Laplace transforms) to a minimum and prefer the use of computer simulation to determine dynamic responses. In addition, the important topics of empirical models and their development from experimental data are considered.

Part III (Chapters 8 through 15) addresses the fundamental concepts of feedback and feedforward control. Topics include an overview of process instrumentation (Chapter 9) and control hardware and software that are necessary to implement process control (Chapter 8 and Appendix A). Chapters 8–10 have been extensively revised to include new developments and recent references, especially in the area of process safety. The design and analysis of feedback control systems is a major topic with emphasis on industry-proven methods for controller design, tuning, and troubleshooting. Frequency response analysis (Chapter 14) provides important insights into closed-loop stability and why control loops can oscillate. Part III concludes with a chapter on feedforward and ratio control.

Part IV (Chapters 16 through 22) is concerned with advanced process control techniques. The topics include digital control, multivariable control, process monitoring, batch process control, and enhancements of PID control, such as cascade control, selective control, and gain scheduling. Up-to-date chapters on real-time optimization and model predictive control (MPC) emphasize the significant impact these powerful techniques have had on industrial practice. Material on Plantwide Control (Appendices G–I) and other important appendices are located on the book's website: *www.wiley.com/college/seborg*.

The website contains errata for current and previous editions that are available to both students and instructors. In addition, there are resources that are available for instructors (only): the Solutions Manual, lecture slides, figures from the book, and a link to the authors' websites. In order to access these password-protected resources, instructors need to register on the website.

We gratefully acknowledge the very helpful suggestions and reviews provided by many colleagues in academia and industry: Joe Alford, Anand Asthagiri, Karl Åström, Tom Badgwell, Michael Baldea, Max Barolo, Noel Bell, Larry Biegler, Don Bartusiak, Terry Blevins, Dominique Bonvin, Richard Braatz, Dave Camp, Jarrett Campbell, I-Lung Chien, Will Cluett, Oscar Crisalle, Patrick Daugherty, Bob Deshotels, Rainer Dittmar, Jim Downs, Ricardo Dunia, David Ender, Stacy Firth, Rudiyanto Gunawan, Juergen Hahn, Sandra Harris, John Hedengren, Karlene Hoo, Biao Huang, Babu Joseph, Derrick Kozub, Jietae Lee, Bernt Lie, Cheng Ling, Sam Mannan, Tom McAvoy, Greg McMillan, Randy Miller, Samir Mitragotri, Manfred Morari, Duane Morningred, Kenneth Muske, Mark Nixon, Srinivas Palanki, Bob Parker, Michel Perrier, Mike Piovoso, Joe Qin, Larry Ricker, Dan Rivera, Derrick Rollins, Alan Schneider, Sirish Shah, Mikhail Skliar, Sigurd Skogestad, Tyler Soderstrom, Ron Sorensen, Dirk Thiele, John Tsing, Ernie Vogel, Doug White, Willy Wojsznis, and Robert Young.

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In the spirit of this continuous improvement, we are interested in receiving feedback from students, faculty, and practitioners who use this book. We hope you find it to be useful.

Dale E. Seborg
Thomas F. Edgar
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Chapter 1

Introduction to Process Control

CHAPTER CONTENTS

In recent years the performance requirements for process plants have become increasingly difficult to satisfy. Stronger competition, tougher environmental and safety regulations, and rapidly changing economic conditions have been key factors. Consequently, product quality specifications have been tightened and increased emphasis has been placed on more profitable plant operation. A further complication is that modern plants have become more difficult to operate because of the trend toward complex and highly integrated processes. Thus, it is difficult to prevent disturbances from propagating from one unit to other interconnected units.

In view of the increased emphasis placed on safe, efficient plant operation, it is only natural that the subject of *process control* has become increasingly important in recent years. Without computer-based process control systems, it would be impossible to operate modern plants safely and profitably while satisfying product quality and environmental requirements. Thus, it is important for chemical engineers to have an understanding of both the theory and practice of process control.

The two main subjects of this book are *process dynamics* and *process control*. The term *process dynamics* refers to unsteady-state (or transient) process behavior. By contrast, most of the chemical engineering curricula emphasize steady-state and equilibrium conditions in such courses as material and energy balances, thermodynamics, and transport phenomena. But the topic of process dynamics is also very important. Transient operation occurs during important situations such as start-ups and shutdowns, unusual process disturbances, and planned transitions from one product grade to another. Consequently, the first part of this book is concerned with process dynamics.

The primary objective of process control is to maintain a process at the desired operating conditions, safely and economically, while satisfying environmental and product quality requirements. The subject of process control is concerned with how to achieve these goals. In large-scale, integrated processing plants such as oil refineries or ethylene plants, thousands of process variables such as compositions, temperatures, and pressures are measured and must be controlled. Fortunately, thousands of process variables (mainly flow rates) can usually be manipulated for this purpose. Feedback control systems compare measurements with their desired values and then adjust the manipulated variables accordingly.

Feedback control is a fundamental concept that is absolutely critical for both biological and manmade systems. Without feedback control, it would be very difficult, if not impossible, to keep complicated systems at the desired conditions. Feedback control is embedded in many modern devices that we take for granted: computers, cell phones, consumer electronics, air conditioning, automobiles, airplanes, as well as automatic control systems for industrial processes. The scope and history of feedback control and automatic control systems have been well described elsewhere (Mayr, 1970; Åström and Murray, 2008; Blevins and Nixon, 2011).

For living organisms, feedback control is essential to achieve a stable balance of physiological variables, a condition that is referred to as *homeostasis*. In fact, homeostasis is considered to be a defining feature of physiology (Widmaier *et al.*, 2011). In biology, feedback control occurs at many different levels including gene, cellular, metabolic pathways, organs, and even entire ecosystems. For the human body, feedback is essential to regulate critical physiological variables (e.g., temperature, blood pressure, and glucose concentration) and processes (e.g., blood circulation, respiration, and digestion). Feedback is also an important concept in education and the social sciences, especially economics (Rao, 2013) and psychology (Carver and Scheier, 1998).

As an introduction to the subject, we next consider representative process control problems in several industries.

1.1 REPRESENTATIVE PROCESS CONTROL PROBLEMS

The foundation of process control is *process understanding*. Thus, we begin this section with a basic question: what is a process? For our purposes, a brief definition is appropriate:

> ***Process:*** *The conversion of feed materials to products using chemical and physical operations. In practice, the term* process *tends to be used for both the processing operation and the processing equipment.*

There are three broad categories of processes: continuous, batch, and semibatch. Next, we consider representative processes and briefly summarize key control issues.

1.1.1 Continuous Processes

Four continuous processes are shown schematically in Fig. 1.1:

(a) ***Tubular heat exchanger.*** A process fluid on the tube side is cooled by cooling water on the shell side. Typically, the exit temperature of the process fluid is controlled by manipulating the cooling water flow rate. Variations in the inlet temperatures and the process fluid flow rate affect the heat exchanger operation. Consequently, these variables are considered to be disturbance variables.

(b) ***Continuous stirred-tank reactor (CSTR).*** If the reaction is highly exothermic, it is necessary to control the reactor temperature by manipulating the flow rate of coolant in a jacket or cooling coil. The feed conditions (composition, flow rate, and temperature) can be manipulated variables or disturbance variables.

(c) ***Thermal cracking furnace.*** Crude oil is broken down ("cracked") into a number of lighter petroleum fractions by the heat transferred from a burning fuel/air mixture. The furnace temperature and amount of excess air in the flue gas can be controlled by manipulating the fuel flow rate and the fuel/air ratio. The crude oil composition and the heating quality of the fuel are common disturbance variables.

(d) ***Kidney dialysis unit.*** This medical equipment is used to remove waste products from the blood of human patients whose own kidneys are failing or have failed. The blood flow rate is maintained by a pump, and "ambient conditions," such

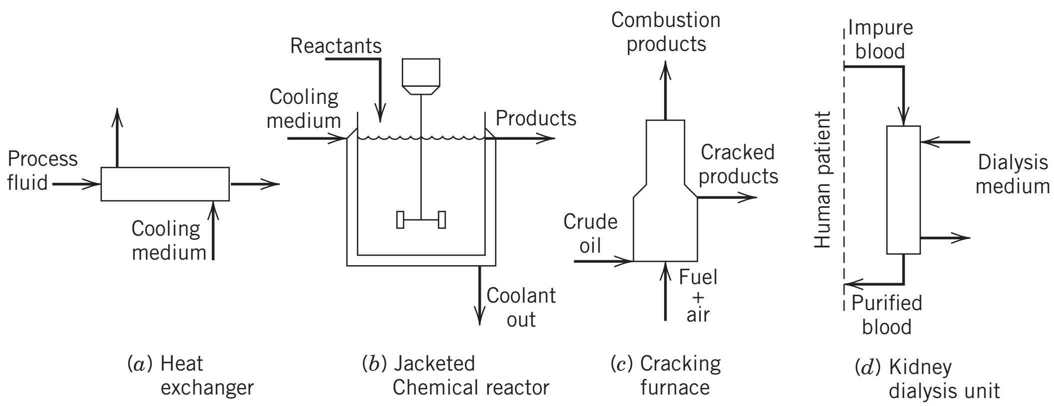

Figure 1.1 Some typical continuous processes.

as temperature in the unit, are controlled by adjusting a flow rate. The dialysis is continued long enough to reduce waste concentrations to acceptable levels.

For each of these four examples, the process control problem has been characterized by identifying three important types of process variables.

- *Controlled variables (CVs):* The process variables that are controlled. The desired value of a controlled variable is referred to as its *set point*.
- *Manipulated variables (MVs):* The process variables that can be adjusted in order to keep the controlled variables at or near their set points. Typically, the manipulated variables are flow rates.
- *Disturbance variables (DVs):* Process variables that affect the controlled variables but cannot be manipulated. Disturbances generally are related to changes in the operating environment of the process: for example, its feed conditions or ambient temperature. Some disturbance variables can be measured on-line, but many cannot such as the crude oil composition for Process (c), a thermal cracking furnace.

The specification of CVs, MVs, and DVs is a critical step in developing a control system. The selections should be based on process knowledge, experience, and control objectives.

1.1.2 Batch and Semibatch Processes

Batch and semibatch processes are used in many process industries, including microelectronics, pharmaceuticals, specialty chemicals, and fermentation. Batch and semibatch processes provide needed flexibility for multiproduct plants, especially when products change frequently and production quantities are small. Figure 1.2 shows four representative batch and semibatch processes:

(e) ***Jacketed batch reactor.*** In a batch reactor, an initial charge (e.g., reactants and catalyst) is placed in the reactor, agitated, and brought to the desired starting conditions. For exothermic reactions, cooling jackets are used to keep the reactor temperature at or near the desired set point. Typically, the reactor temperature is regulated by adjusting the coolant flow rate. The endpoint composition of the batch can be controlled by adjusting the temperature set point and/or the *cycle time*, the time period for reactor operation. At the end of the batch, the reactor contents are removed and either stored or transferred to another process unit such as a separation process.

(f) ***Semibatch bioreactor.*** For a semibatch reactor, one of the two alternative operations is used: (i) a reactant is gradually added as the batch proceeds or (ii) a product stream is withdrawn during the reaction. The first configuration can be used to reduce the side reactions while the second configuration allows the reaction equilibrium to be changed by withdrawing one of the products (Fogler, 2010).

For bioreactors, the first type of semibatch operation is referred to as a *fed-batch operation*; it is shown in Fig. 1.2(f). In order to better regulate the growth of the desired microorganisms, a nutrient is slowly added in a predetermined manner.

(g) ***Semibatch digester in a pulp mill.*** Both continuous and semibatch digesters are used in paper manufacturing to break down wood chips in order to extract the cellulosic fibers. The end point of the chemical reaction is indicated by the kappa number, a measure of lignin content. It is controlled to a desired value by adjusting the digester temperature, pressure, and/or cycle time.

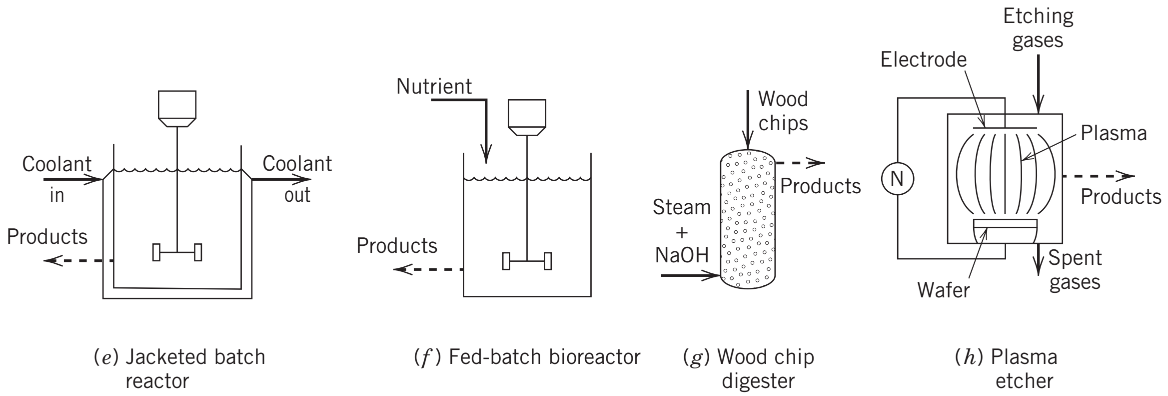

Figure 1.2 Some typical processes whose operation is noncontinuous. (Dashed lines indicate product removal after the operation is complete.)

(h) ***Plasma etcher in semiconductor processing.*** A single wafer containing hundreds of printed circuits is subjected to a mixture of etching gases under conditions suitable to establish and maintain a plasma (a high voltage applied at high temperature and extremely low pressure). The unwanted material on a layer of a microelectronics circuit is selectively removed by chemical reactions. The temperature, pressure, and flow rates of etching gases to the reactor are controlled by adjusting electrical heaters and control valves.

Next, we consider an illustrative example in more detail.

1.2 ILLUSTRATIVE EXAMPLE—A BLENDING PROCESS

A simple blending process is used to introduce some important issues in control system design. Blending operations are commonly used in many industries to ensure that final products meet customer specifications.

A continuous, stirred-tank blending system is shown in Fig. 1.3. The control objective is to blend the two inlet streams to produce an outlet stream that has the desired composition. Stream 1 is a mixture of two chemical species, A and B. We assume that its mass flow rate w_1 is constant, but the mass fraction of A, x_1, varies with time. Stream 2 consists of pure A and thus $x_2 = 1$. The mass flow rate of Stream 2, w_2, can be manipulated using a control valve. The mass fraction of A in the outlet stream is denoted by x and the desired value (set point) by x_{sp}. Thus for this control problem, the controlled variable is x, the manipulated variable is w_2, and the disturbance variable is x_1.

Next we consider two questions.

Design Question. *If the nominal value of x_1 is $\overline{x}_1$, what nominal flow rate $\overline{w}_2$ is required to produce the desired outlet concentration, x_{sp}?*

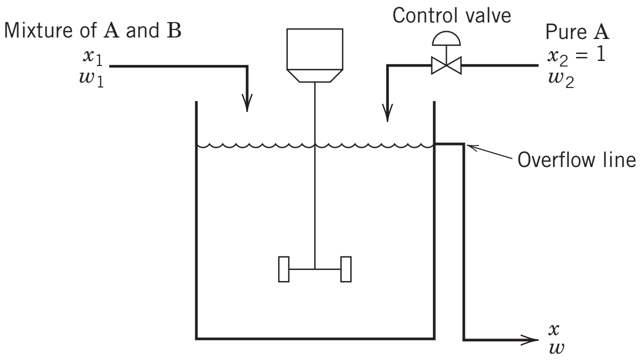

Figure 1.3 Stirred-tank blending system.

To answer this question, we consider the steady-state material balances:

Overall balance:

$$0 = \overline{w}_1 + \overline{w}_2 - \overline{w} \tag{1-1}$$

Component A balance:

$$0 = \overline{w}_1\overline{x}_1 + \overline{w}_2\overline{x}_2 - \overline{w}\,\overline{x} \tag{1-2}$$

The overbar over a symbol denotes its nominal steady-state value, for example, the value used in the process design. According to the process description, $\overline{x}_2 = 1$ and $\overline{x} = x_{sp}$. Solving Eq. 1-1 for $\overline{w}$, substituting these values into Eq. 1-2, and rearranging gives

$$\overline{w}_2 = \overline{w}_1 \frac{x_{sp} - \overline{x}_1}{1 - x_{sp}} \tag{1-3}$$

Equation 1-3 is the design equation for the blending system. If our assumptions are correct and if $x_1 = \overline{x}_1$, then this value of w_2 will produce the desired result, $x = x_{sp}$. But what happens if conditions change?

Control Question. *Suppose that inlet concentration x_1 varies with time. How can we ensure that the outlet composition x remains at or near its desired value, x_{sp}?*

As a specific example, assume that x_1 increases to a constant value that is larger than its nominal value, $\overline{x}_1$. It is clear that the outlet composition will also increase due to the increase in inlet composition. Consequently, at this new steady state, $x > x_{sp}$.

Next we consider several strategies for reducing the effects of x_1 disturbances on x.

Method 1. *Measure x and adjust w_2.* It is reasonable to measure controlled variable x and then adjust w_2 accordingly. For example, if x is too high, w_2 should be reduced; if x is too low, w_2 should be increased. This control strategy could be implemented by a person (*manual control*). However, it would normally be more convenient and economical to automate this simple task (*automatic control*).

Method 1 can be implemented as a simple control algorithm (or control law),

$$w_2(t) = \overline{w}_2 + K_c[x_{sp} - x(t)] \tag{1-4}$$

where K_c is a constant called the *controller gain*. The symbols, $w_2(t)$ and $x(t)$, indicate that w_2 and x change with time. Equation 1-4 is an example of *proportional control*, because the change in the flow rate, $w_2(t) - \overline{w}_2$, is proportional to the deviation from the set point, $x_{sp} - x(t)$. Consequently, a large deviation from set point produces a large corrective action, while a small deviation results in a small corrective action. Note that we require K_c to be positive because w_2 must increase when x decreases, and vice versa. However, in other control applications, negative values of K_c are appropriate, as discussed in Chapter 8.

A schematic diagram of Method 1 is shown in Fig. 1.4. The outlet concentration is measured and transmitted to the controller as an electrical signal. (Electrical signals are shown as dashed lines in Fig. 1.4.) The controller executes the control law and sends an appropriate electrical signal to the control valve. The control valve opens or closes accordingly. In Chapters 8 and 9, we consider process instrumentation and control hardware in more detail.

Method 2. *Measure x_1, adjust w_2.* As an alternative to Method 1, we could measure disturbance variable x_1 and adjust w_2 accordingly. Thus, if $x_1 > \overline{x}_1$, we would decrease w_2 so that $w_2 < \overline{w}_2$. If $x_1 < \overline{x}_1$, we would increase w_2. A control law based on Method 2 can be obtained from Eq. 1-3 by replacing $\overline{x}_1$ with $x_1(t)$ and $\overline{w}_2$ with $w_2(t)$:

$$w_2(t) = \overline{w}_1 \frac{x_{sp} - x_1(t)}{1 - x_{sp}} \tag{1-5}$$

The schematic diagram for Method 2 is shown in Fig. 1.5. Because Eq. 1-3 is valid only for steady-state conditions, it is not clear just how effective Method 2 will be during the transient conditions that occur after an x_1 disturbance.

Method 3. *Measure x_1 and x, adjust w_2.* This approach is a combination of Methods 1 and 2.

Method 4. *Use a larger tank.* If a larger tank is used, fluctuations in x_1 will tend to be damped out as a result of the larger volume of liquid. However, increasing tank size is an expensive solution due to the increased capital cost.

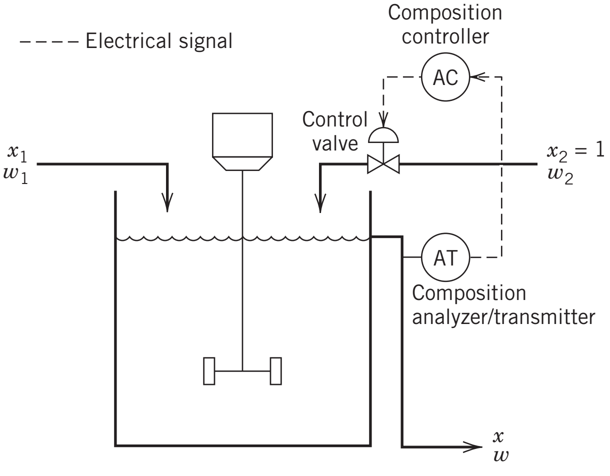

Figure 1.4 Blending system and Control Method 1.

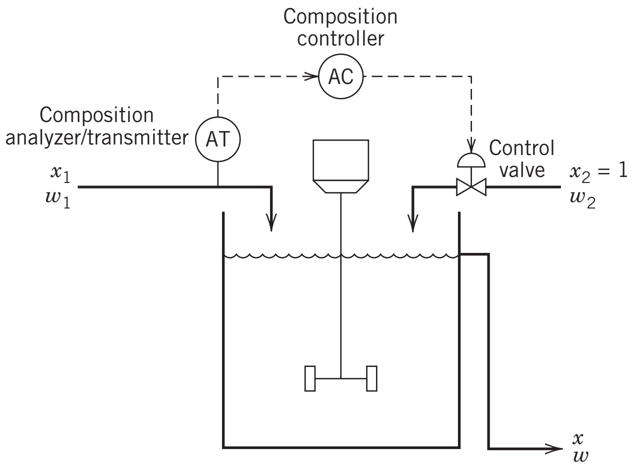

Figure 1.5 Blending system and Control Method 2.

1.3 CLASSIFICATION OF PROCESS CONTROL STRATEGIES

Next, we will classify the four blending control strategies of the previous section and discuss their relative advantages and disadvantages. Method 1 is an example of a *feedback control* strategy. The distinguishing feature of feedback control is that the controlled variable is measured, and that the measurement is used to adjust the manipulated variable. For feedback control, the disturbance variable is *not* measured.

It is important to make a distinction between *negative feedback* and *positive feedback*. In the engineering literature, negative feedback refers to the desirable situation in which the corrective action taken by the controller forces the controlled variable toward the set point. On the other hand, when positive feedback occurs, the controller makes things worse by forcing the controlled variable farther away from the set point. For example, in the blending control problem, positive feedback takes place if $K_c < 0$, because w_2 will increase when x increases.[1] Clearly, it is of paramount importance to ensure that a feedback control system incorporates negative feedback rather than positive feedback.

An important advantage of feedback control is that corrective action occurs regardless of the source of the disturbance. For example, in the blending process, the feedback control law in Eq. 1-4 can accommodate disturbances in w_1, as well as x_1. Its ability to handle disturbances of unknown origin is a major reason why feedback control is the dominant process control strategy. Another important advantage is that feedback

[1]Note that social scientists use the terms negative feedback and positive feedback in a very different way. For example, they would say that teachers provide "positive feedback" when they compliment students who correctly do assignments. Criticism of a poor performance would be an example of "negative feedback."

control reduces the sensitivity of the controlled variable to unmeasured disturbances and process changes. However, feedback control does have a fundamental limitation: no corrective action is taken until after the disturbance has upset the process, that is, until after the controlled variable deviates from the set point. This shortcoming is evident from the control law of Eq. 1-4.

Method 2 is an example of a *feedforward control strategy*. The distinguishing feature of feedforward control is that the disturbance variable is measured, but the controlled variable is not. The important advantage of feedforward control is that corrective action is taken *before* the controlled variable deviates from the set point. Ideally, the corrective action will cancel the effects of the disturbance so that the controlled variable is not affected by the disturbance. Although ideal cancelation is generally not possible, feedforward control can significantly reduce the effects of measured disturbances, as discussed in Chapter 15.

Feedforward control has three significant disadvantages: (i) the disturbance variable must be measured (or accurately estimated), (ii) no corrective action is taken for unmeasured disturbances, and (iii) a process model is required. For example, the feedforward control strategy for the blending system (Method 2) does not take any corrective action for unmeasured w_1 disturbances. In principle, we could deal with this situation by measuring both x_1 and w_1 and then adjusting w_2 accordingly. However, in industrial applications, it is generally uneconomical to attempt to measure all potential disturbance variables. A more practical approach is to use a combined feedforward–feedback control system, in which feedback control provides corrective action for unmeasured disturbances, while feedforward control reacts to measured disturbances before the controlled variable is upset. Consequently, in industrial applications, feedforward control is normally used in combination with feedback control. This approach is illustrated by Method 3, a combined feedforward–feedback control strategy because both x and x_1 are measured.

Table 1.1 Concentration Control Strategies for the Blending System

Method	Measured Variable	Manipulated Variable	Category
1	x	w_2	FB
2	x_1	w_2	FF
3	x_1 and x	w_2	FF/FB
4	—	—	Design change

FB = feedback control; FF = feedforward control; FF/FB = feedforward control and feedback control.

Finally, Method 4 consists of a process design change and thus is not really a control strategy. The four strategies for the stirred-tank blending system are summarized in Table 1.1.

1.3.1 Process Control Diagrams

Next we consider the equipment that is used to implement control strategies. For the stirred-tank mixing system under feedback control (Method 1) in Fig. 1.4, the exit concentration x is controlled and the flow rate w_2 of pure species A is adjusted using proportional control. To consider how this feedback control strategy could be implemented, a block diagram for the stirred-tank control system is shown in Fig. 1.6. The operation of the feedback control system can be summarized as follows:

1. *Analyzer and transmitter:* The tank exit concentration is measured by an analyzer and then the measurement is converted to a corresponding electrical current signal by a transmitter.

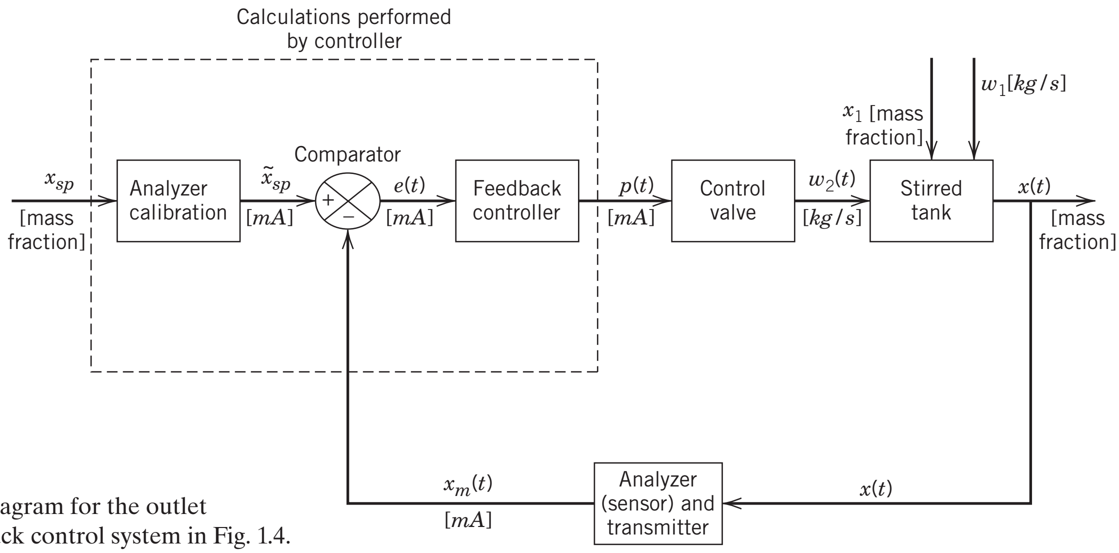

Figure 1.6 Block diagram for the outlet composition feedback control system in Fig. 1.4.

2. *Feedback controller:* The controller performs three distinct calculations. First, it converts the actual set point x_{sp} into an equivalent internal signal $\tilde{x}_{sp}$. Second, it calculates an error signal $e(t)$ by subtracting the measured value $x_m(t)$ from the set point $\tilde{x}_{sp}$, that is, $e(t) = \tilde{x}_{sp} - \tilde{x}_m(t)$. Third, controller output $p(t)$ is calculated from the proportional control law similar to Eq. 1-4.
3. *Control valve:* The controller output $p(t)$ in this case is a DC current signal that is sent to the control valve to adjust the valve stem position, which in turn affects flow rate $w_2(t)$. (The controller output signal is traditionally denoted by p because early controllers were pneumatic devices with pneumatic (pressure) signals as inputs and outputs.)

The block diagram in Fig. 1.6 provides a convenient starting point for analyzing process control problems. The physical units for each input and output signal are also shown. Note that the schematic diagram in Fig. 1.4 shows the *physical connections* between the components of the control system, while the block diagram shows the *flow of information* within the control system. The block labeled "control valve" has $p(t)$ as its input signal and $w_2(t)$ as its output signal, which illustrates that the signals on a block diagram can represent either a physical variable such as $w_2(t)$ or an instrument signal such as $p(t)$.

Each component in Fig. 1.6 exhibits behavior that can be described by a differential or algebraic equation. One of the tasks facing a control engineer is to develop suitable mathematical descriptions for each block; the development and analysis of such dynamic models are considered in Chapters 2–7.

The elements of the block diagram (Fig. 1.6) are discussed in detail in future chapters. Sensors, transmitters, and control valves are presented in Chapter 9, and the feedback controllers are considered in Chapter 8.

The feedback control system in Fig. 1.6 is shown as a single, standalone controller. However, for industrial applications, it is more economical to have a digital computer implement multiple feedback control loops. In particular, networks of digital computers can be used to implement thousands of feedback and feedforward control loops. Computer control systems are the subject of Appendix A and Chapter 17.

1.4 A MORE COMPLICATED EXAMPLE—A DISTILLATION COLUMN

The blending control system in the previous section is quite simple, because there is only one controlled variable and one manipulated variable. For most practical applications, there are multiple controlled variables and multiple manipulated variables. As a representative example, we consider the distillation column in Fig. 1.7, with five controlled variables and five manipulated variables. The controlled variables are product compositions, x_D and x_B, column pressure, P, and the liquid levels in the reflux drum and column base, h_D and h_B. The five manipulated variables are product flow rates, D and B, reflux flow, R, and the heat duties for the condenser and reboiler, Q_D and Q_B. The heat duties are adjusted via the control valves on the coolant and heating medium lines. The feed stream is assumed to come from an upstream unit. Thus, the feed flow rate cannot be manipulated, but it can be measured and used for feedforward control.

A conventional *multiloop control* strategy for this distillation column would consist of five feedback control loops. Each control loop uses a single manipulated variable to control a single controlled variable. But how

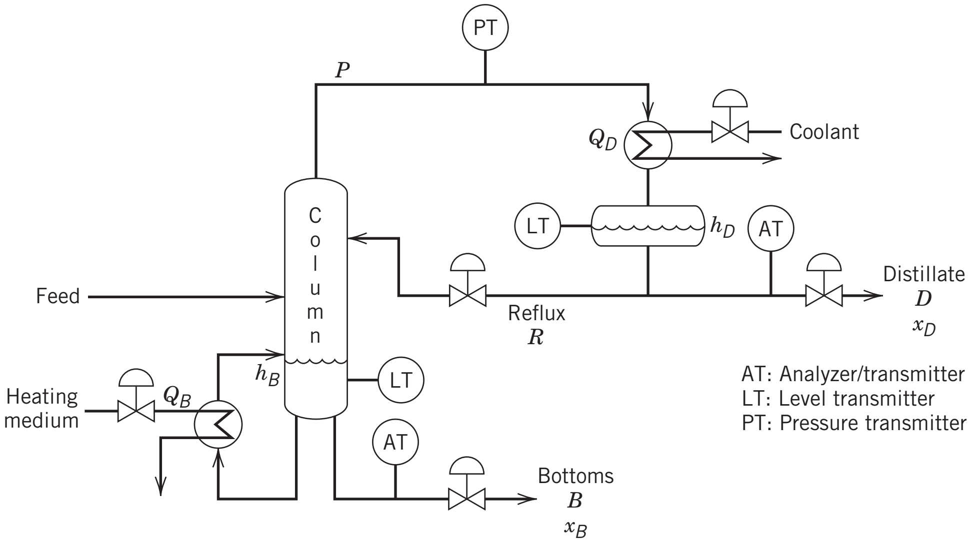

Figure 1.7 Controlled and manipulated variables for a typical distillation column.

should the controlled and manipulated variables be paired? The total number of different multiloop control configurations that could be considered is 5!, or 120. Many of these control configurations are impractical or unworkable, such as any configuration that attempts to control the base level h_B by manipulating distillate flow D or condenser heat duty Q_D. However, even after the infeasible control configurations are eliminated, there are still many reasonable configurations left. Thus, there is a need for systematic techniques that can identify the most promising multiloop configurations. Fortunately, such tools are available and are discussed in Chapter 18.

In control applications, for which conventional multiloop control systems are not satisfactory, an alternative approach, *multivariable control*, can be advantageous. In multivariable control, each manipulated variable is adjusted based on the measurements of at least two controlled variables rather than only a single controlled variable, as in multiloop control. The adjustments are based on a dynamic model of the process that indicates how the manipulated variables affect the controlled variables. Consequently, the performance of multivariable control, or any model-based control technique, will depend heavily on the accuracy of the process model. A specific type of multivariable control, *model predictive control*, has had a major impact on industrial practice, as discussed in Chapter 20.

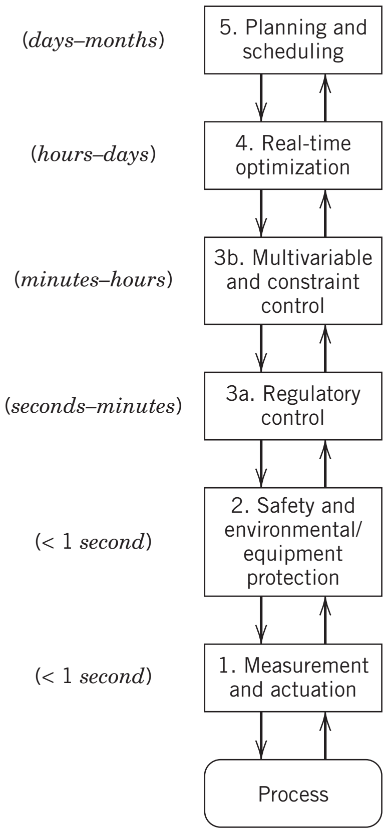

Figure 1.8 Hierarchy of process control activities.

1.5 THE HIERARCHY OF PROCESS CONTROL ACTIVITIES

As mentioned earlier, the chief objective of process control is to maintain a process at the desired operating conditions, safely and economically, while satisfying environmental and product quality requirements. So far, we have emphasized one process control activity, keeping controlled variables at specified set points. But there are other important activities that we will now briefly describe.

In Fig. 1.8, the process control activities are organized in the form of a hierarchy with required functions at lower levels and desirable, but optional, functions at higher levels. The time scale for each activity is shown on the left side. Note that the frequency of execution is much lower for the higher-level functions.

Measurement and Actuation (Level 1)

Instrumentation (e.g., sensors and transmitters) and actuation equipment (e.g., control valves) are used to measure process variables and implement the calculated control actions. These devices are interfaced to the control system, usually digital control equipment such as a digital computer. Clearly, the measurement and actuation functions are an indispensable part of any control system.

Safety and Environmental/Equipment Protection (Level 2)

The Level 2 functions play a critical role by ensuring that the process is operating safely and satisfies environmental regulations. As discussed in Chapter 10, process safety relies on the principle of *multiple protection layers* that involve groupings of equipment and human actions. One layer includes process control functions, such as alarm management during abnormal situations, and *safety instrumented systems* for emergency shutdowns. The safety equipment (including sensors and control valves) operates independently of the regular instrumentation used for regulatory control in Level 3a. Sensor validation techniques can be employed to confirm that the sensors are functioning properly.

Regulatory Control (Level 3a)

As mentioned earlier, successful operation of a process requires that key process variables such as flow rates, temperatures, pressures, and compositions be operated at or close to their set points. This Level 3a activity, *regulatory control*, is achieved by applying standard feedback and feedforward control techniques (Chapters 11–15). If the standard control techniques are not satisfactory, a variety of advanced control techniques are available (Chapters 16–18). In recent years, there has been increased interest in monitoring control system performance (Chapter 21).

Multivariable and Constraint Control (Level 3b)

Many difficult process control problems have two distinguishing characteristics: (i) significant interactions occur among key process variables and (ii) inequality constraints for manipulated and controlled variables. The inequality constraints include upper and lower limits. For example, each manipulated flow rate has an upper limit determined by the pump and control valve characteristics. The lower limit may be zero, or a small positive value, based on safety considerations. Limits on controlled variables reflect equipment constraints (e.g., metallurgical limits) and the operating objectives for the process. For example, a reactor temperature may have an upper limit to avoid undesired side reactions or catalyst degradation, and a lower limit to ensure that the reaction(s) proceed.

The ability to operate a process close to a limiting constraint is an important objective for advanced process control. For many industrial processes, the optimum operating condition occurs at a constraint limit—for example, the maximum allowed impurity level in a product stream. For these situations, the set point should not be the constraint value, because a process disturbance could force the controlled variable beyond the limit. Thus, the set point should be set conservatively, based on the ability of the control system to reduce the effects of disturbances. This situation is illustrated in Fig. 1.9. For (*a*), the variability of the controlled variable is quite high, and consequently, the set point must be specified well below the limit. For (*b*), the improved control strategy has reduced the variability; consequently, the set point can be moved closer to the limit, and the process can be operated closer to the optimum operating condition.

The standard process control techniques of Level 3a may not be adequate for difficult control problems that have serious process interactions and inequality constraints. For these situations, the advanced control techniques of Level 3b, *multivariable control* and *constraint control*, should be considered. In particular, the *model predictive control* (*MPC*) strategy was developed to deal with both process interactions and inequality constraints. MPC is the subject of Chapter 20.

Real-time Optimization (Level 4)

The optimum operating conditions for a plant are determined as part of the process design. But during plant operations, the optimum conditions can change frequently owing to changes in equipment availability, process disturbances, and economic conditions (e.g., raw material costs and product prices). Consequently, it can be very profitable to recalculate the optimum operating conditions on a regular basis. This Level 4 activity, *real-time optimization* (*RTO*), is the subject of Chapter 19. The new optimum conditions are then implemented as set points for controlled variables.

The RTO calculations are based on a steady-state model of the plant and economic data such as costs and product values. A typical objective for the optimization is to minimize operating cost or maximize the operating profit. The RTO calculations can be performed for a single process unit or on a plantwide basis.

The Level 4 activities also include data analysis to ensure that the process model used in the RTO calculations is accurate for the current conditions. Thus, *data reconciliation* techniques can be used to ensure that steady-state mass and energy balances are satisfied. Also, the process model can be updated using parameter estimation techniques and recent plant data (Chapter 7).

Planning and Scheduling (Level 5)

The highest level of the process control hierarchy is concerned with planning and scheduling operations for the entire plant. For continuous processes, the production rates of all products and intermediates must be planned and coordinated, based on equipment constraints, storage capacity, sales projections, and the operation of other plants, sometimes on a global basis. For the intermittent operation of batch and semibatch processes, the production control problem becomes a batch scheduling problem based on similar considerations. Thus, planning and scheduling activities pose difficult optimization problems that are based on both engineering considerations and business projections.

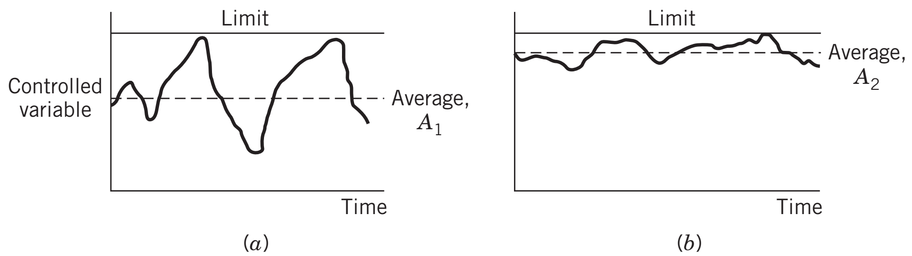

Figure 1.9 Process variability over time: (*a*) before improved process control; (*b*) after.

Summary of the Process Control Hierarchy

The activities of Levels 1, 2, and 3a in Fig. 1.8, are required for all manufacturing plants, while the activities in Levels 3b–5 are optional but can be very profitable. The decision to implement one or more of these higher-level activities depends very much on the application and the company. The decision hinges strongly on economic considerations (e.g., a cost/benefit analysis), and company priorities for their limited resources, both human and financial. The immediacy of the activity decreases from Level 1 to Level 5 in the hierarchy. However, the amount of analysis and the computational requirements increase from the lowest level to the highest level. The process control activities at different levels should be carefully coordinated and require information transfer from one level to the next. The successful implementation of these process control activities is a critical factor in making plant operation as profitable as possible.

1.6 AN OVERVIEW OF CONTROL SYSTEM DESIGN

In this section, we introduce some important aspects of control system design. However, it is appropriate first to describe the relationship between process design and process control.

Historically, process design and control system design have been separate engineering activities. Thus, in the traditional approach, control system design is not initiated until after plant design is well underway, and major pieces of equipment may even have been ordered. This approach has serious limitations because the plant design determines the process dynamics as well as the operability of the plant. In extreme situations, the process may be uncontrollable, even though the design appears satisfactory from a steady-state perspective. A better approach is to consider process dynamics and control issues early in the process design. The interaction between process design and control is analyzed in more detail in Chapter 13 and Appendices G, H and I.

Next, we consider two general approaches to control system design:

1. ***Traditional Approach.*** The control strategy and control system hardware are selected based on knowledge of the process, experience, and insight. After the control system is installed in the plant, the controller settings (such as controller gain K_c in Eq. 1-4) are adjusted. This activity is referred to as *controller tuning*.
2. ***Model-Based Approach.*** A dynamic model of the process is first developed that can be helpful in at least three ways: (i) it can be used as the basis for model-based controller design methods (Chapters 12 and 14), (ii) the dynamic model can be incorporated directly in the control law (e.g., model predictive control), and (iii) the model can be used in a computer simulation to evaluate alternative control strategies and to determine preliminary values of the controller settings.

In this book, we advocate the philosophy that for complex processes, a dynamic model of the process should be developed so that the control system can be properly designed. Of course, for many simple process control problems, controller specification is relatively straightforward and a detailed analysis or an explicit model is not required. For complex processes, however, a process model is invaluable both for control system design and for an improved understanding of the process. As mentioned earlier, process control should be based on process understanding.

The major steps involved in designing and installing a control system using the model-based approach are shown in the flow chart of Fig. 1.10. The first step, formulation of the control objectives, is a critical decision. The formulation is based on the operating objectives for the plants and the process constraints. For example, in the distillation column control problem, the objective might be to regulate a key component in the distillate stream, the bottoms stream, or key components in both streams. An alternative would be to minimize energy consumption (e.g., reboiler heat duty) while meeting product quality specifications on one or both product streams. The inequality constraints should include upper and lower limits on manipulated variables, conditions that lead to flooding or weeping in the column, and product impurity levels.

After the control objectives have been formulated, a dynamic model of the process is developed. The dynamic model can have a theoretical basis, for example, physical and chemical principles such as conservation laws and rates of reactions (Chapter 2), or the model can be developed empirically from experimental data (Chapter 7). If experimental data are available, the dynamic model should be validated, and the model accuracy is characterized. This latter information is useful for control system design and tuning.

The next step in the control system design is to devise an appropriate control strategy that will meet the control objectives while satisfying process constraints. As indicated in Fig. 1.10, this design activity is both an art and a science. Process understanding and the experience and preferences of the design team are key factors. Computer simulation of the controlled process is used to screen alternative control strategies and to provide preliminary estimates of appropriate controller settings.

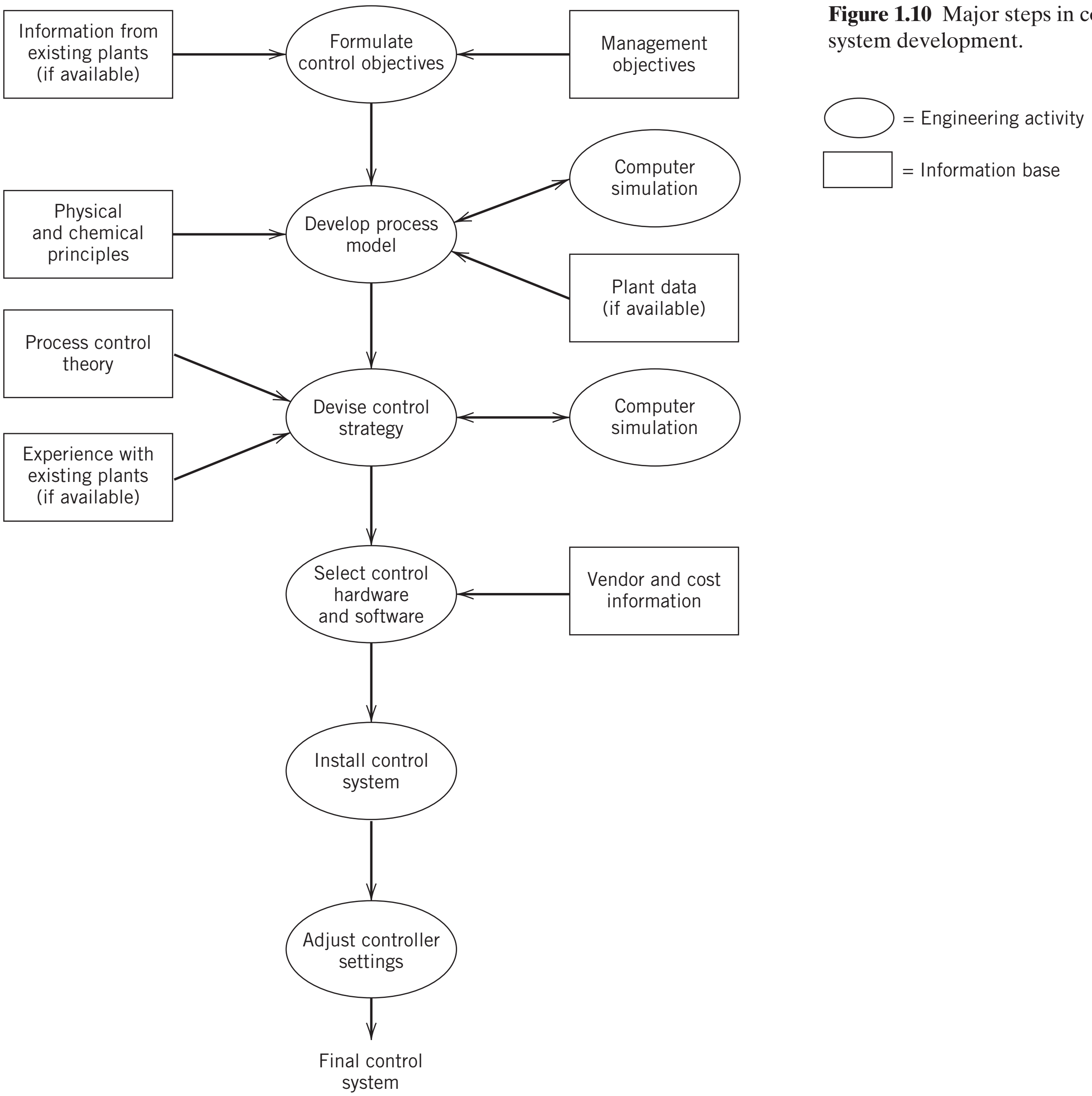

Figure 1.10 Major steps in control system development.

Finally, the control system hardware and instrumentation are selected, ordered, and installed in the plant. Then the control system is tuned in the plant using the preliminary estimates from the design step as a starting point. Controller tuning usually involves trial-and-error procedures, as described in Chapter 12.

SUMMARY

In this chapter, we have introduced the basic concepts of process dynamics and process control. The process dynamics determine how a process responds during transient conditions, such as plant start-ups and shutdowns, grade changes, and unusual disturbances. Process control enables the process to be maintained at the desired operating conditions, safely and economically, while satisfying environmental and product quality requirements. Without effective process control, it would be impossible to operate large-scale industrial plants.

Two physical examples, a continuous blending system and a distillation column, have been used to introduce basic control concepts, notably, feedback and feedforward control. We also motivated the need for a systematic approach for the design of control systems for complex processes. Control system development consists of a number of separate activities that are shown in Fig. 1.10. In this book, we advocate the design philosophy that for complex processes, a dynamic model of the process should be developed so that the control system can be properly designed.

A hierarchy of process control activities was presented in Fig. 1.8. Process control plays a key role in ensuring process safety and protecting personnel, equipment, and the environment. Controlled variables are maintained near their set points by the application of regulatory control techniques and advanced control techniques such as multivariable and constraint control. Real-time optimization can be employed to determine the optimum controller set points for current operating conditions and constraints. The highest level of the process control hierarchy is concerned with planning and scheduling operations for the entire plant. The different levels of process control activity in the hierarchy are related and should be carefully coordinated.

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EXERCISES

1.1 Which of the following statements are true? For the false statements, explain why you think they are false:

(a) Feedforward and feedback control require a measured variable.

(b) For feedforward control, the measured variable is the variable to be controlled.

(c) Feedback control theoretically can provide perfect control (i.e., no deviations from set point) if the process model used to design the control system is perfect.

(d) Feedback control takes corrective action for all types of process disturbances, both known and unknown.

(e) Feedback control is superior to feedforward control.

1.2 Consider a home heating system consisting of a natural gas-fired furnace and a thermostat. In this case, the *process* consists of the interior space to be heated. The thermostat contains both the temperature sensor and the controller. The furnace is either on (heating) or off. Draw a schematic diagram for this control system. On your diagram, identify the controlled variables, manipulated variables, and disturbance variables. Be sure to include several possible sources of disturbances that can affect room temperature.

1.3 In addition to a thermostatically operated home heating system, identify two other feedback control systems that can be found in most residences. Describe briefly how each of them works; include sensor, actuator, and controller information.

1.4 Does a typical microwave oven utilize feedback control to set the cooking temperature or to determine if the food is "cooked"? If not, what technique is used? Can you think of any disadvantages to this approach, for example, in thawing and cooking foods?

1.5 Driving an automobile safely requires considerable skill. Even if not generally recognized, the driver needs an intuitive ability to utilize feedforward and feedback control methods.

(a) In the process of steering a car, one objective is to keep the vehicle generally centered in the proper traffic lane. Thus, the controlled variable is some measure of that distance. If so, how is feedback control used to accomplish this objective? Identify the sensor(s), the actuator, how the appropriate control action is determined, and some likely disturbances.

(b) The process of braking or accelerating an automobile is highly complex, requiring the skillful use of both feedback and feedforward mechanisms to drive safely. For feedback control, the driver normally uses distance to the vehicle ahead as the measured variable. This "set point" is often recommended to be some distance related to speed, for example, one car length separation for each 10 mph. If this recommendation is used, how does feedforward control come into the accelerating/braking process when one is attempting to drive in traffic at a constant speed? In other words, what other information—in addition to distance separating the two vehicles—does the driver utilize to avoid colliding with the car ahead?

1.6 The human body contains numerous feedback control loops that are essential for regulating key physiological variables. For example, body temperature in a healthy person must be closely regulated within a narrow range.

(a) Briefly describe one or more ways in which body temperature is regulated by the body using feedback control.

(b) Briefly describe a feedback control system for the regulation of another important physiological variable.

1.7 The distillation column shown in Fig. E1.7 is used to distill a binary mixture. Symbols x, y, and z denote mole fractions of the more volatile component, while B, D, R, and F represent molar flow rates. It is desired to control distillate composition y despite disturbances in feed flow rate F. All flow rates can be measured and manipulated with the exception of F, which can only be measured. A composition analyzer provides measurements of y.

(a) Propose a feedback control method and sketch the schematic diagram.

(b) Suggest a feedforward control method and sketch the schematic diagram.

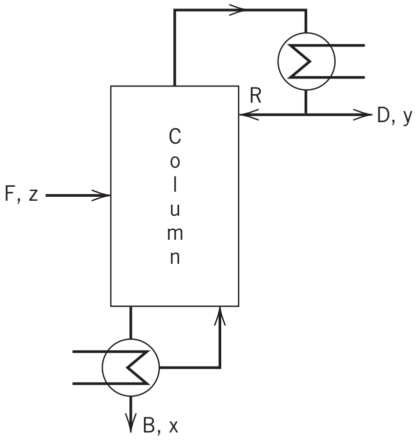

Figure E1.7

1.8 Describe how a bicycle rider utilizes concepts from both feedforward control and feedback control while riding a bicycle.

1.9 Two flow control loops are shown in Fig. E1.9. Indicate whether each system is either a feedback or a feedforward control system. Justify your answer. It can be assumed that the distance between the flow transmitter (FT) and the control valve is quite small in each system.

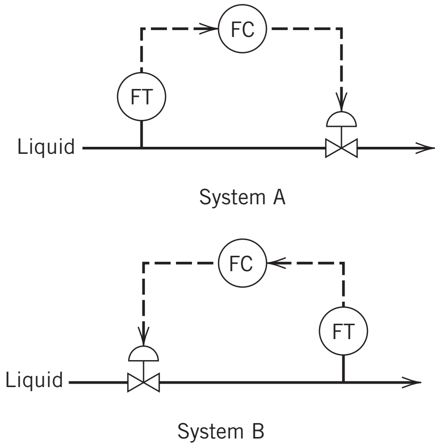

Figure E1.9

1.10 In a thermostat control system for a home heating system,

(a) Identify the manipulated variable

(b) Identify the controlled variable

(c) How is the manipulated variable adjusted?

(d) Name one important disturbance (it must change with respect to time).

1.11 Identify and describe three automatic control systems in a modern automobile (besides cruise control).

1.12 In Figure 1.1(d), identify the controlled, manipulated, and disturbance variables (there may be more than one of each type). How does the length of time for the dialysis treatment affect the waste concentration?

Chapter 2

Theoretical Models of Chemical Processes

CHAPTER CONTENTS

In this chapter we consider the derivation of unsteady-state models of chemical processes from physical and chemical principles. Unsteady-state models are also referred to as *dynamic models*. We first consider the rationale for dynamic models and then present a general strategy for deriving them from first principles such as conservation laws. Then dynamic models are developed for several representative processes. Finally, we describe how dynamic models that consist of sets of ordinary differential equations and algebraic relations can be solved numerically using computer simulation.

2.1 THE RATIONALE FOR DYNAMIC PROCESS MODELS

Dynamic models play a central role in the subject of process dynamics and control. The models can be used to:

1. ***Improve understanding of the process.*** Dynamic models and computer simulation allow transient process behavior to be investigated without having to disturb the process. Computer simulation allows valuable information about dynamic and steady-state process behavior to be acquired, even before the plant is constructed.

2. ***Train plant operating personnel.*** Process simulators play a critical role in training plant operators to run complex units and to deal with dangerous situations or emergency scenarios. By interfacing a process simulator to standard process control equipment, a realistic training environment is created. This role is analogous to flight training simulators used in the aerospace industry.
3. ***Develop a control strategy for a new process.*** A dynamic model of the process allows alternative control strategies to be evaluated. For example, a dynamic model can help identify the process variables that should be controlled and those that should be manipulated (Chapter 13). Preliminary controller tuning may be derived using a model, prior to plant start-up using empirical models (Chapter 12). For model-based control strategies (Chapters 12, 16 and 20), the process model is an explicit element of the control law.
4. ***Optimize process operating conditions.*** It can be advantageous to recalculate the optimum operating conditions periodically in order to maximize profit or minimize cost. A steady-state process model and economic information can be used to determine the most profitable operating conditions (see Chapter 19).

For many of the examples cited above—particularly where new, hazardous, or difficult-to-operate processes are involved—development of a suitable process model can be crucial to success. Models can be classified based on how they are obtained:

(a) *Theoretical models* are developed using the principles of chemistry, physics, and biology.

(b) *Empirical models* are obtained by fitting experimental data (more in Chapter 7).

(c) *Semi-empirical models* are a combination of the models in categories (a) and (b); the numerical values of one or more of the parameters in a theoretical model are calculated from experimental data.

Theoretical models offer two very important advantages: they provide physical insight into process behavior, and they are applicable over wide ranges of conditions. However, there are disadvantages associated with theoretical models. They tend to be expensive and time-consuming to develop. In addition, theoretical models of complex processes typically include some model parameters that are not readily available, such as reaction rate coefficients, physical properties, or heat transfer coefficients.

Although empirical models are easier to develop and to use in controller design than theoretical models, they have a serious disadvantage: *empirical models typically do not extrapolate well*. More specifically, empirical models should be used with caution for operating conditions that were not included in the experimental data used to fit the model. The range of the data is typically quite small compared to the full range of process operating conditions.

Semi-empirical models have three inherent advantages: (i) they incorporate theoretical knowledge, (ii) they can be extrapolated over a wider range of operating conditions than purely empirical models, and (iii) they require less development effort than theoretical models. Consequently, semi-empirical models are widely used in industry.

This chapter is concerned with the development of theoretical models from first principles such as conservation laws.

2.1.1 An Illustrative Example: A Blending Process

In Chapter 1 we developed a steady-state model for a stirred-tank blending system based on mass and component balances. Now we develop an unsteady-state model that will allow us to analyze the more general situation where process variables vary with time and accumulation terms must be included.

As an illustrative example, we consider the isothermal stirred-tank blending system in Fig. 2.1. It is a more general version of the blending system in Fig. 1.3 because the overflow line has been omitted and inlet stream 2 is not necessarily pure A (that is, $x_2 \neq 1$). Now the volume of liquid in the tank V can vary with time, and the exit flow rate is not necessarily equal to the sum of the inlet flow rates. An unsteady-state mass balance for the blending system in Fig. 2.1 has the form

$$\left\{\begin{matrix}\text{rate of accumulation}\\ \text{of mass in the tank}\end{matrix}\right\} = \left\{\begin{matrix}\text{rate of}\\ \text{mass in}\end{matrix}\right\} - \left\{\begin{matrix}\text{rate of}\\ \text{mass out}\end{matrix}\right\} \tag{2-1}$$

The mass of liquid in the tank can be expressed as the product of the liquid volume V and the density ρ.

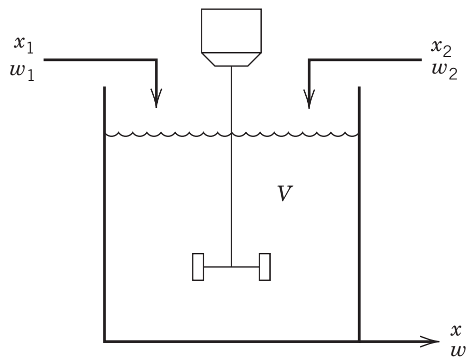

Figure 2.1 Stirred-tank blending process.

Consequently, the rate of mass accumulation is simply $d(V\rho)/dt$, and Eq. 2-1 can be written as

$$\frac{d(V\rho)}{dt} = w_1 + w_2 - w \tag{2-2}$$

where w_1, w_2, and w are mass flow rates.

The unsteady-state material balance for component A can be derived in an analogous manner. We assume that the blending tank is perfectly mixed. This assumption has two important implications: (i) there are no concentration gradients in the tank contents and (ii) the composition of the exit stream is equal to the tank composition. The perfect mixing assumption is valid for low-viscosity liquids that receive an adequate degree of agitation. In contrast, the assumption is less likely to be valid for high-viscosity liquids such as polymers or molten metals. Nonideal mixing is modeled in books on reactor analysis (e.g., Fogler, 2006).

For the perfect mixing assumption, the rate of accumulation of component A is $d(V\rho x)/dt$, where x is the mass fraction of A. The unsteady-state component balance is

$$\frac{d(V\rho x)}{dt} = w_1 x_1 + w_2 x_2 - wx \tag{2-3}$$

Equations 2-2 and 2-3 provide an unsteady-state model for the blending system. The corresponding steady-state model was derived in Chapter 1 (cf. Eqs. 1-1 and 1-2). It also can be obtained by setting the accumulation terms in Eqs. 2-2 and 2-3 equal to zero,

$$0 = \overline{w}_1 + \overline{w}_2 - \overline{w} \tag{2-4}$$

$$0 = \overline{w}_1 \overline{x}_1 + \overline{w}_2 \overline{x}_2 - \overline{w}\,\overline{x} \tag{2-5}$$

where the nominal steady-state conditions are denoted by $\overline{x}$ and $\overline{w}$ and so on. In general, a steady-state model is a special case of an unsteady-state model that can be derived by setting accumulation terms equal to zero.

A dynamic model can be used to characterize the transient behavior of a process for a wide variety of conditions. For example, some relevant concerns for the blending process: How would the exit composition change after a sudden increase in an inlet flow rate or after a gradual decrease in an inlet composition? Would these transient responses be very different if the volume of liquid in the tank is quite small, or quite large, when an inlet change begins? These questions can be answered by solving the ordinary differential equations (ODE) in Eqs. 2-2 and 2-3 for specific initial conditions and for particular changes in inlet flow rates or compositions. The solution of dynamic models is considered further in this chapter and in Chapters 3–6.

Before exploring the blending example in more detail, we first present general principles for the development of dynamic models.

2.2 GENERAL MODELING PRINCIPLES

It is important to remember that a process model is nothing more than a mathematical abstraction of a real process. The model equations are at best an approximation to the real process as expressed by the adage that "all models are wrong, but some are useful." Consequently, the model cannot incorporate all of the features, whether macroscopic or microscopic, of the real process. Modeling inherently involves a compromise between model accuracy and complexity on one hand, and the cost and effort required to develop the model and verify it on the other hand. The required compromise should consider a number of factors, including the modeling objectives, the expected benefits from use of the model, and the background of the intended users of the model (e.g., research chemists versus plant engineers).

Process modeling is both an art and a science. Creativity is required to make simplifying assumptions that result in an appropriate model. Consequently, careful enumeration of all the assumptions that are invoked in building a model is crucial for its final evaluation. The model should incorporate all of the important dynamic behavior while being no more complex than is necessary. Thus, less important phenomena are omitted in order to keep the number of model equations, variables, and parameters at reasonable levels. The failure to choose an appropriate set of simplifying assumptions invariably leads to either (1) rigorous but excessively complicated models or (2) overly simplistic models. Both extremes should be avoided. Fortunately, modeling is also a science, and predictions of process behavior from alternative models can be compared, both qualitatively and quantitatively. This chapter provides an introduction to the subject of theoretical dynamic models and shows how they can be developed from first principles such as conservation laws. Additional information is available in the books by Bequette (1998), Aris (1999), Elnashaie and Garhyan (2003), and Cameron and Gani (2011).

A systematic procedure for developing dynamic models from first principles is summarized in Table 2.1. Most of the steps in Table 2.1 are self-explanatory, with the possible exception of Step 7. The *degrees of freedom analysis* in Step 7 is required in model development for complex processes. Because these models typically contain large numbers of variables and equations, it is not obvious whether the model can be solved, or whether it has a unique solution. Consequently, we consider the degrees of freedom analysis in Sections 2.3 and 13.1.

Dynamic models of chemical processes consist of ODE and/or partial differential equations (PDE), plus related algebraic equations. In this book we will restrict our discussion to ODE models. Additional details about PDE models for reaction engineering can be found in Fogler (2006) and numerical procedures for solving such models are available in, for example,

Table 2.1 A Systematic Approach for Developing Dynamic Models

1. State the modeling objectives and the end use of the model. Then determine the required levels of model detail and model accuracy.
2. Draw a schematic diagram of the process and label all process variables.
3. List all of the assumptions involved in developing the model. Try to be parsimonious: the model should be no more complicated than necessary to meet the modeling objectives.
4. Determine whether spatial variations of process variables are important. If so, a partial differential equation model will be required.
5. Write appropriate conservation equations (mass, component, energy, and so forth).
6. Introduce equilibrium relations and other algebraic equations (from thermodynamics, transport phenomena, chemical kinetics, equipment geometry, etc.).
7. Perform a degrees of freedom analysis (Section 2.3) to ensure that the model equations can be solved.
8. Simplify the model. It is often possible to arrange the equations so that the output variables appear on the left side and the input variables appear on the right side. This model form is convenient for computer simulation and subsequent analysis.
9. Classify inputs as disturbance variables or as manipulated variables.

Chapra and Canale (2014). For process control problems, dynamic models are derived using unsteady-state conservation laws. In this section, we first review general modeling principles, emphasizing the importance of the mass and energy conservation laws. Force–momentum balances are employed less often. For processes with momentum effects that cannot be neglected (e.g., some fluid and solid transport systems), such balances should be considered. The process model often also includes algebraic relations that arise from thermodynamics, transport phenomena, physical properties, and chemical kinetics. Vapor–liquid equilibria, heat transfer correlations, and reaction rate expressions are typical examples of such algebraic equations.

2.2.1 Conservation Laws

Theoretical models of chemical processes are based on conservation laws such as the conservation of mass and energy. Consequently, we now consider important conservation laws and use them to develop dynamic models for representative processes.

Conservation of Mass

$$\left\{\begin{matrix}\text{rate of mass}\\\text{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\text{rate of}\\\text{mass in}\end{matrix}\right\} - \left\{\begin{matrix}\text{rate of}\\\text{mass out}\end{matrix}\right\} \tag{2-6}$$

Conservation of Component i

$$\left\{\begin{matrix}\text{rate of component } i\\\text{accumulation}\end{matrix}\right\} = \left\{\begin{matrix}\text{rate of component } i\\\text{in}\end{matrix}\right\} - \left\{\begin{matrix}\text{rate of component } i\\\text{out}\end{matrix}\right\} + \left\{\begin{matrix}\text{rate of component } i\\\text{produced}\end{matrix}\right\} \tag{2-7}$$

The last term on the right-hand side of Eq. 2-7 represents the rate of generation (or consumption) of component i as a result of chemical reactions. Conservation equations can also be written in terms of molar quantities, atomic species, and molecular species (Felder and Rousseau, 2015).

Conservation of Energy

The general law of energy conservation is also called the First Law of Thermodynamics (Sandler, 2006). It can be expressed as

$$\begin{aligned}\left\{\begin{matrix}\text{rate of energy}\\\text{accumulation}\end{matrix}\right\} = &\left\{\begin{matrix}\text{rate of energy in}\\\text{by convection}\end{matrix}\right\} - \left\{\begin{matrix}\text{rate of energy out}\\\text{by convection}\end{matrix}\right\}\\ &+ \left\{\begin{matrix}\text{net rate of heat addition}\\\text{to the system from}\\\text{the surroundings}\end{matrix}\right\} + \left\{\begin{matrix}\text{net rate of work}\\\text{performed on the system}\\\text{by the surroundings}\end{matrix}\right\}\end{aligned} \tag{2-8}$$

The total energy of a thermodynamic system, U_{tot}, is the sum of its internal energy, kinetic energy, and potential energy:

$$U_{\text{tot}} = U_{\text{int}} + U_{KE} + U_{PE} \tag{2-9}$$

For the processes and examples considered in this book, it is appropriate to make two assumptions:

1. Changes in potential energy and kinetic energy can be neglected, because they are small in comparison with changes in internal energy.
2. The net rate of work can be neglected, because it is small compared to the rates of heat transfer and convection.

For these reasonable assumptions, the energy balance in Eq. 2-8 can be written as (Bird et al., 2002)

$$\frac{dU_{\text{int}}}{dt} = -\Delta(w\hat{H}) + Q \tag{2-10}$$

where U_{int} is the internal energy of the system, $\hat{H}$ is the enthalpy per unit mass, w is the mass flow rate, and Q is the rate of heat transfer to the system. The Δ operator denotes the difference between outlet conditions and inlet conditions of the flowing streams. Consequently, the $-\Delta(w\hat{H})$ term represents the enthalpy of the inlet stream(s) minus the enthalpy of the outlet stream(s). The analogous equation for molar quantities is

$$\frac{dU_{\text{int}}}{dt} = -\Delta(\tilde{w}\tilde{H}) + Q \tag{2-11}$$

where $\tilde{H}$ is the enthalpy per mole and $\tilde{w}$ is the molar flow rate.

Note that the conservation laws of this section are valid for batch and semibatch processes, as well as for continuous processes. For example, in batch processes, there are no inlet and outlet flow rates. Thus, $w = 0$ and $\tilde{w} = 0$ in Eqs. 2-10 and 2-11.

In order to derive dynamic models of processes from the general energy balances in Eqs. 2-10 and 2-11, expressions for U_{int} and $\hat{H}$ or $\tilde{H}$ are required, which can be derived from thermodynamics. These derivations and a review of related thermodynamics concepts are included in Appendix B.

2.2.2 The Blending Process Revisited

Next, we show that the dynamic model of the blending process in Eqs. 2-2 and 2-3 can be simplified and expressed in a more appropriate form for computer simulation. For this analysis, we introduce the additional assumption that the density of the liquid, ρ, is a constant. This assumption is reasonable because often the density has only a weak dependence on composition. For constant ρ, Eqs. 2-2 and 2-3 become

$$\rho\frac{dV}{dt} = w_1 + w_2 - w \tag{2-12}$$

$$\rho\frac{d(Vx)}{dt} = w_1x_1 + w_2x_2 - wx \tag{2-13}$$

Equation 2-13 can be further simplified by expanding the accumulation term using the "chain rule" for differentiation of a product:

$$\rho\frac{d(Vx)}{dt} = \rho V\frac{dx}{dt} + \rho x\frac{dV}{dt} \tag{2-14}$$

Substitution of Eq. 2-14 into Eq. 2-13 gives

$$\rho V\frac{dx}{dt} + \rho x\frac{dV}{dt} = w_1x_1 + w_2x_2 - wx \tag{2-15}$$

Substitution of the mass balance in Eq. 2-12 for $\rho dV/dt$ in Eq. 2-15 gives

$$\rho V\frac{dx}{dt} + x(w_1 + w_2 - w) = w_1x_1 + w_2x_2 - wx \tag{2-16}$$

After canceling common terms and rearranging Eqs. 2-12 and 2-16, a more convenient model form (the so-called "state-space" form) is obtained:

$$\frac{dV}{dt} = \frac{1}{\rho}(w_1 + w_2 - w) \tag{2-17}$$

$$\frac{dx}{dt} = \frac{w_1}{V\rho}(x_1 - x) + \frac{w_2}{V\rho}(x_2 - x) \tag{2-18}$$

The dynamic model in Eqs. 2-17 and 2-18 is quite general and is based on only two assumptions: perfect mixing and constant density. For special situations, the liquid volume V is constant (i.e., $dV/dt = 0$), and the exit flow rate equals the sum of the inlet flow rates, $w = w_1 + w_2$. These conditions might occur when

1. An overflow line is used in the tank as shown in Fig. 1.3.
2. The tank is closed and filled to capacity.
3. A liquid-level controller keeps V essentially constant by adjusting a flow rate.

In all three cases, Eq. 2-17 reduces to the same form as Eq. 2-4, not because each flow rate is constant, but because $w = w_1 + w_2$ at all times.

The dynamic model in Eqs. 2-17 and 2-18 is in a convenient form for subsequent investigation based on analytical or numerical techniques. In order to obtain a solution to the ODE model, we must specify the inlet compositions (x_1 and x_2) and the flow rates (w_1, w_2, and w) as functions of time. After specifying initial conditions for the dependent variables, $V(0)$ and $x(0)$, we can determine the transient responses, $V(t)$ and $x(t)$. The derivation of an analytical expression for $x(t)$ when V is constant is illustrated in Example 2.1.

EXAMPLE 2.1

A stirred-tank blending process with a constant liquid holdup of 2 m^3 is used to blend two streams whose densities are both approximately 900 kg/m^3. The density does not change during mixing.

(a) Assume that the process has been operating for a long period of time with flow rates of $w_1 = 500$ kg/min and $w_2 = 200$ kg/min, and feed compositions (mass fractions) of $x_1 = 0.4$ and $x_2 = 0.75$. What is the steady-state value of x?

(b) Suppose that w_1 changes suddenly from 500 to 400 kg/min and remains at the new value. Determine an expression for $x(t)$ and plot it.

(c) Repeat part (**b**) for the case where w_2 (instead of w_1) changes suddenly from 200 to 100 kg/min and remains there.

(d) Repeat part (**c**) for the case where x_1 suddenly changes from 0.4 to 0.6 (in addition to the change in w_2).

(e) For parts (**b**) through (**d**), plot the normalized response $x_N(t)$,

$$x_N(t) = \frac{x(t) - x(0)}{x(\infty) - x(0)}$$