semicontinuous processes are often designed to provide a reliable, though inefficient, route to the production of chemicals. For example, in the emulsion polymerization of resins, large batch reactors are installed often to avoid carrying out these highly exothermic reactions in continuous stirred-tank reactors. Note, however, that while operation at a low-conversion steady state is often less profitable than batch or semicontinuous processing, operation at an open-loop unstable steady state is often more profitable. Rather than install a control system to stabilize the operation, many companies prefer to operate in batch or semicontinuous mode. Similarly, design teams often opt for batch and semicontinuous processes when the chemicals are hazardous or toxic or when safety aspects are of great concern.

Because the designs for continuous and batch processes are usually very different, the choice of processing mode is made commonly during process synthesis, in the task integration step, as discussed in Section 3.4. At this stage, the decision to reject continuous processing is based upon rules of thumb, rather than a detailed comparison of the alternatives. Through process simulation, as discussed in Chapter 4, and the optimization methods presented in this chapter, more algorithmic methods are available for selecting from among the various batch and continuous processes.

Usually, for the production of small quantities of high-priced chemicals, such as in the manufacture of pharmaceuticals, foods, electronic materials, and specialty chemicals, batch, fed-batch, and batch-product removal processes are preferred. This is often the case in bioprocessing, for example, when drugs are synthesized in a series of chemical reactions, each having small yields, and requiring difficult separations to recover small amounts of product. This is also the case for banquet facilities in hotels, which prepare foods in batches, and for many unit operations in the manufacture of semiconductors. As discussed in Chapters 3 and 4, these processes usually involve a *recipe*, that is, a sequence of *tasks*, to be carried out in various items of equipment. In the latter sections of this chapter, variations on batch process schedules are discussed, as well as methods for optimizing the schedules.

12.2 DESIGN OF BATCH PROCESS UNITS

When designing a process unit to operate in batch mode, it is usually desired to determine the *batch time*, τ, and the *size factor*, S, which is usually expressed as the volume per unit mass of product, that maximize an objective like the amount of product. To accomplish this, a dynamic model of the process unit is formulated and the degrees of freedom adjusted, as illustrated in the examples that follow. As will be seen, there are many ways to formulate this *optimal control problem*. To simplify the discussion, models are presented and studied for various input profiles, to see how they affect the objectives. Emphasis is not placed on the formal methods of optimization.

Batch Processing

For conventional batch processing, with no material transfer to or from the batch, performance is often improved by adjusting the operating variables, such as temperature and agitation speed. Through these adjustments, reactor conversion is improved, thereby reducing the batch time to achieve the desired conversion. An example is presented next that shows how to achieve this objective by optimizing the temperature during batch processing.

EXAMPLE 12.1 *Exothermic Batch Reactor*

Consider a batch reactor to carry out the exothermic reversible reaction:

$$n_1\text{A} \rightleftharpoons n_2\text{B}$$

where the rate of consumption of A is:

$$r\{c_A, c_B, t\} = c_A^{n_1} k_1^\circ e^{\frac{-E_1}{RT}} - c_B^{n_2} k_2^\circ e^{\frac{-E_2}{RT}} \tag{12.1}$$

and where $E_1 < E_2$ for the exothermic reaction. The reaction is charged initially with A and B at concentrations, c_{A_o} and c_{B_o}. To achieve a specified fractional conversion of A, $X = (c_{A_o} - c_A)/c_{A_o}$, determine the profile of operating temperature in time that gives the minimum batch time. This example is based upon the development by Denn (1969).

SOLUTION

The minimum batch time, $\tau_{\min}$, is achieved by integrating the mass balances:

$$\frac{dc_A}{dt} = -r\{c_A, c_B, t\} \tag{12.2}$$

$$c_B\{t\} = c_{B_o} + \frac{n_1}{n_2}[c_{A_o} - c_A\{t\}] \tag{12.3}$$

while adjusting T at each point in time to give the maximum reaction rate.

The temperature at the maximum reaction rate is obtained by differentiation of Eq. (12.1) with respect to T:

$$\frac{dr}{dT} = 0 \tag{12.4}$$

Rearranging:

$$T_{\text{opt}} = \frac{E_2 - E_1}{R \ln \dfrac{c_B^{n_2} k_2^\circ E_2}{c_A^{n_1} k_1^\circ E_1}} \tag{12.5}$$

When an upper bound in temperature, T^U, is assigned, the typical solution profile is shown in Figure 12.2. Initially, when $T_{\text{opt}} > T^U$, the reactor temperature is adjusted to the upper bound, T^U. Then, as conversion increases, the reactor temperature decreases, leveling off to the equilibrium conversion. In practice, this optimal temperature trajectory is approached using feedback control, with the coolant flow rate adjusted to give temperature measurements that track the optimal temperature trajectory. ■

Fed-Batch Processing

Fermentation processes for the production of drugs are usually carried out in fed-batch reactors. In these reactors, it is desirable to find the best profile for feeding substrate into the fermenting broth, as illustrated in the next example.

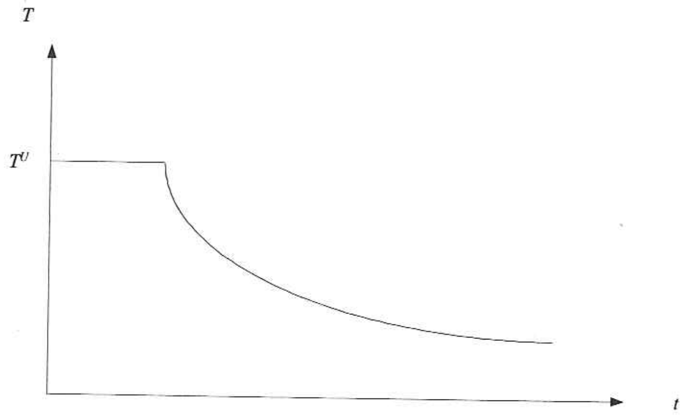

Figure 12.2 Temperature profile to minimize batch reactor time.