Chapter 12

Optimal Design and Scheduling of Batch Processes

12.0 OBJECTIVES

This chapter introduces strategies for designing and scheduling batch processes. It [...] with single equipment items, focusing on methods for achieving the optimal batch ti[...] batch size. Then, reactor–separator processes are examined, where trade-offs exist b[...] the reaction conversion, as it varies with reaction time, the cost of separation, wh[...] creases with conversion, and the batch cycle time. Subsequently, methods of sch[...] batch processes with recipes having numerous tasks and equipment items are consider[...] tially, schedules are considered for plants involving a single product, produced in pro[...] trains that are repeated from batch to batch. The chapter concludes with strategies for [...] ing multiproduct batch plants.

After studying this chapter, the reader should

1. Be knowledgeable about process units executed in batch mode and approaches f[...] mizing their designs and operations.
2. Know how to determine the optimal reaction time for a batch reactor–se[...] process.
3. Be able to schedule recipes for the production of a single chemical product.
4. Understand how to schedule batch plants for the production of multiple products

12.1 INTRODUCTION

Continuous processes are dominant in the chemical process industries for the manufac[...] commodity chemicals, plastics, petroleum products, paper, etc. When production ra[...] low, however—say, in the manufacture of specialty chemicals, pharmaceuticals, an[...] tronic materials—it is difficult to justify the construction of a continuous plant compr[...] small vessels and pipes. In these cases, it is common to design *batch processes* or *se[...] tinuous processes* that are hybrids between batch and continuous processes. The alter[...] are illustrated schematically in Figure 12.1, with a continuous process shown in [...] 12.1a. In the batch process of Figure 12.1b, the chemicals are fed *before* (step 1) [...] products are removed *after* (step 3) the processing (step 2) occurs. *Fed-batch processe[...] bine the first two steps with some or all chemicals being fed continuously during the p[...] ing. Then, when the processing is finished, the products are removed batchwise, as sh[...]
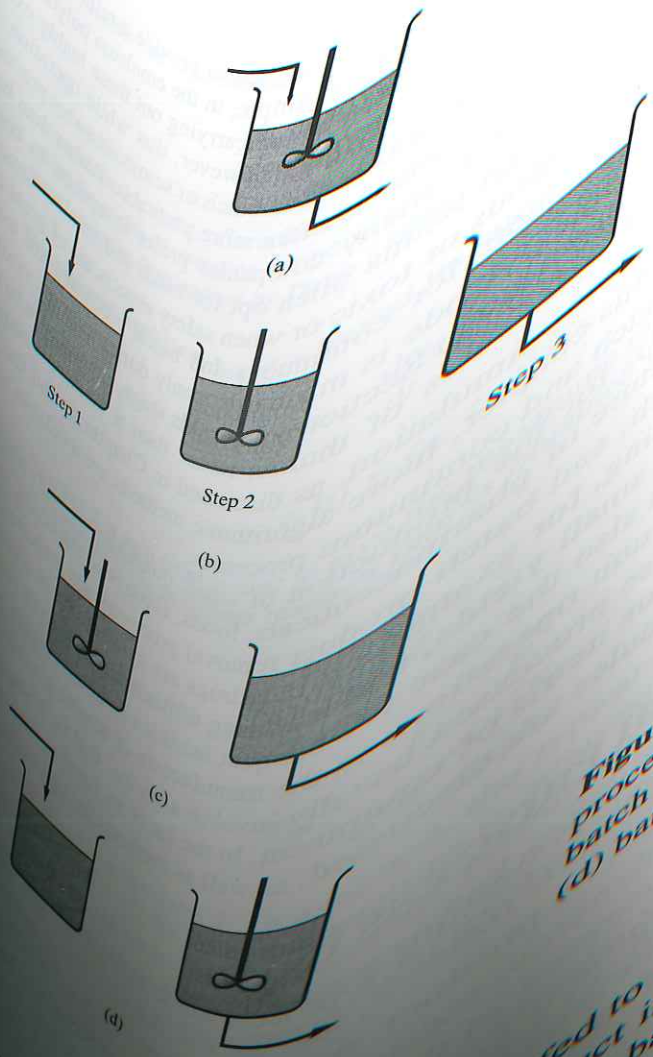
(a)

Step 1

Step 2

Step 3

(b)

(c)

(d)

Figure 12.1 Continuous and batch processes: (a) continuous process; (b) batch process; (c) fed-batch process; (d) batch-product removal process.

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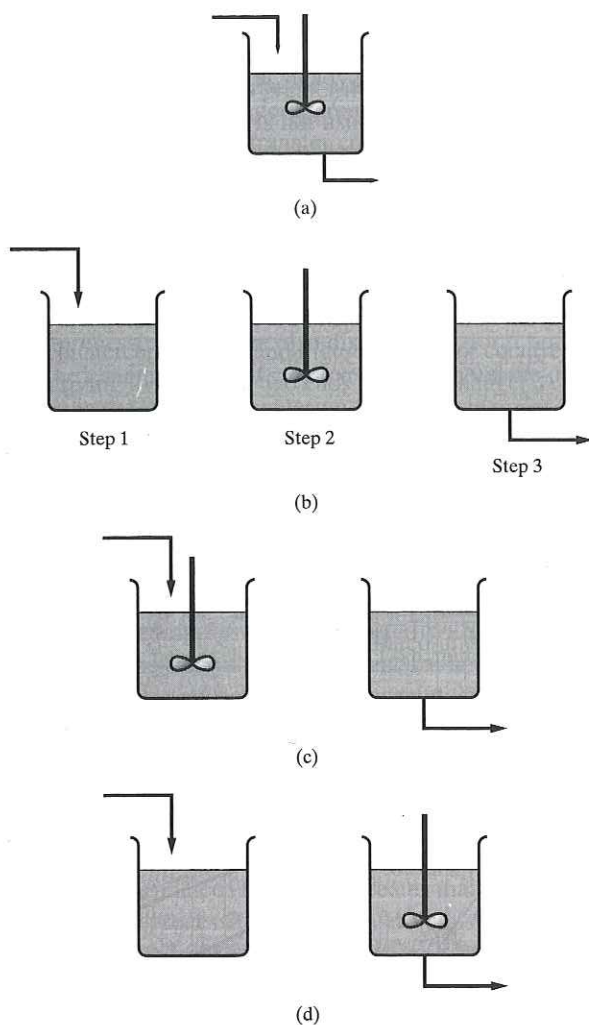
(a)

Step 1   Step 2

Step 3

(b)

(c)

(d)

Figure 12.1 Continuous and batch processes: (a) continuous process; (b) batch process; (c) fed-batch process; (d) batch-product removal process.

Figure 12.1c. In *batch-product removal*, the chemicals are fed to the process before processing begins and steps 2 and 3 are combined; that is, the product is removed continuously as the processing occurs, as shown in Figure 12.1d. In effect, fed-batch and batch-product removal processes are semicontinuous processes.

The challenge in designing a batch, fed-batch, or batch-product removal process is in deciding on the size of the vessel and the processing time. This is complicated for the latter two processes where the flow rate and concentration of the feed stream or the flow rate of the product stream as a function of time strongly influence the performance of the process. Note that the determination of optimal operating profiles is referred to as the solution to the *optimal control problem*. This subject is introduced in the next section.

Batch and semicontinuous processes are utilized often when production rates are small, residence times are large, and product demand is intermittent, especially when the demand for a chemical is interspersed with the demand for one or more other products and the quantities needed and the timing of the orders are uncertain. Even when the demand is continuous and the production rates are sufficiently large to justify continuous processing, batch and

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

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

Usually, for the production of small quantities of high-priced chemicals, such as manufacture of pharmaceuticals, foods, electronic materials, and specialty chemicals, fed-batch, and batch-product removal processes are preferred. This is often the case i processing, for example, when drugs are synthesized in a series of chemical reactions having small yields, and requiring difficult separations to recover small amounts of pr This is also the case for banquet facilities in hotels, which prepare foods in batches, a many unit operations in the manufacture of semiconductors. As discussed in Chapters 4, these processes usually involve a *recipe*, that is, a sequence of *tasks*, to be carried various items of equipment. In the latter sections of this chapter, variations on batch p 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 dete the *batch time*, τ, and the *size factor*, S, which is usually expressed as the volume p mass of product, that maximize an objective like the amount of product. To accomplis a dynamic model of the process unit is formulated and the degrees of freedom adjusted lustrated in the examples that follow. As will be seen, there are many ways to formula *optimal control problem*. To simplify the discussion, models are presented and studi various input profiles, to see how they affect the objectives. Emphasis is not placed formal methods of optimization.

Batch Processing

For conventional batch processing, with no material transfer to or from the batch, mance is often improved by adjusting the operating variables, such as temperature and tion speed. Through these adjustments, reactor conversion is improved, thereby reduc batch time to achieve the desired conversion. An example is presented next that show 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:

$$n_1A \rightleftharpoons n_2B$$

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, τ_{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:

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

When an upper bound in temperature, T^U, is assigned, the typical solution profile is shown in Figure 12.2. Initially, when $T_{opt} > T^U$, 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.
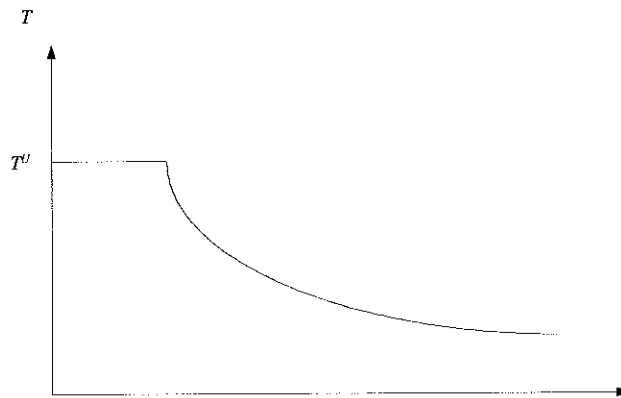

Figure 12.2 Temperature profile to minimize batch reactor time.

EXAMPLE 12.2 *Biosynthesis of Penicillin*

Consider the fed-batch reactor in Figure 12.3. Initially, the reactor is charged with an aqueous $V\{0\}$, containing *E. coli* cells (referred to as biomass) in concentration, $X\{0\}$. Then, an aqueous of sucrose (referred to as the substrate; i.e., the substance being acted on) at a concentration, S_f fed to the reactor at a variable flow rate, $F\{t\}$ (g/hr). The reactor holdup, $V\{t\}$, contains *E. coli* concentration, $X\{t\}$ (g/L), penicillin product in concentration, $P\{t\}$ (g/L), and sucrose in concer $S\{t\}$ (g/L). Using Monod kinetics, the specific growth rate of the cell mass (g cell growth/g cell)

$$\mu = \mu_{max}\left(\frac{S}{K_x X + S}\right)$$

Lim and co-workers (1986) developed the following expressions for the specific rate of penicil duction (g penicillin/g cell):

$$\rho = \rho_{max}\left(\frac{S}{K_p + S(1 + S/K_{in})}\right)$$

and for the specific consumption rate of substrate (g substrate/g cell):

$$s = m_s\left(\frac{S}{K_m + S}\right)$$

Using mass balances for the cell mass, penicillin, and substrate, and the overall mass balance, lowing rate equations can be derived (see Exercise 12.2):

$$\dot{X}\{t\} = \mu\{X, S\}X - \frac{X}{S_f V}F$$

$$\dot{P}\{t\} = \rho\{S\}X - K_{deg}P - \frac{P}{S_f V}F$$

$$\dot{S}\{t\} = -\mu\{X, S\}\frac{X}{Y_{X/S}} - \rho\{S\}\frac{X}{Y_{P/S}} - s\{S\}X + \left(1 - \frac{S}{S_f}\right)\frac{F}{V}$$

$$\dot{V}\{t\} = \frac{F}{S_f}$$

where $Y_{X/S}$ and $Y_{P/S}$ are the yield coefficients which relate the rate of substrate consumption to t of cell growth and penicillin production, respectively.

Using the feed concentration, $S_f = 500$ g S/L, with the kinetic parameters by Lim and co-workers $\mu_{max} = 0.11$ hr^{-1}, $K_x = 0.006$ g S/g X, $K_P = 0.0001$ g S/L, $\rho_{max} = 0.0055$ g P/(g X·hr), $K_{in} = 0.$ $K_{deg} = 0.01$ hr^{-1}, $m_s = 0.029$ g S/(g X·hr), $K_m = 0.0001$ g S/L, $Y_{X/S} = 0.47$ g X/g S, and $Y_{P/S} = 1.2$ for the initial conditions, $V\{0\} = 7$ L, $X\{0\} = 1.5$ g/L, and $P\{0\} = S\{0\} = 0$, and for the constrair

$$0 \le X\{t\} \le 40$$
$$0 \le S\{t\} \le 100$$
$$0 \le V\{t\} \le 10$$
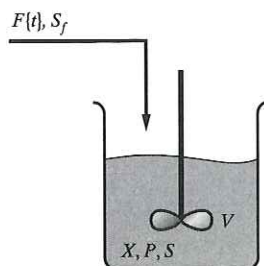$$0 \le F\{t\} \le 50$$
$$72 \le X\{\tau\} \le 200$$

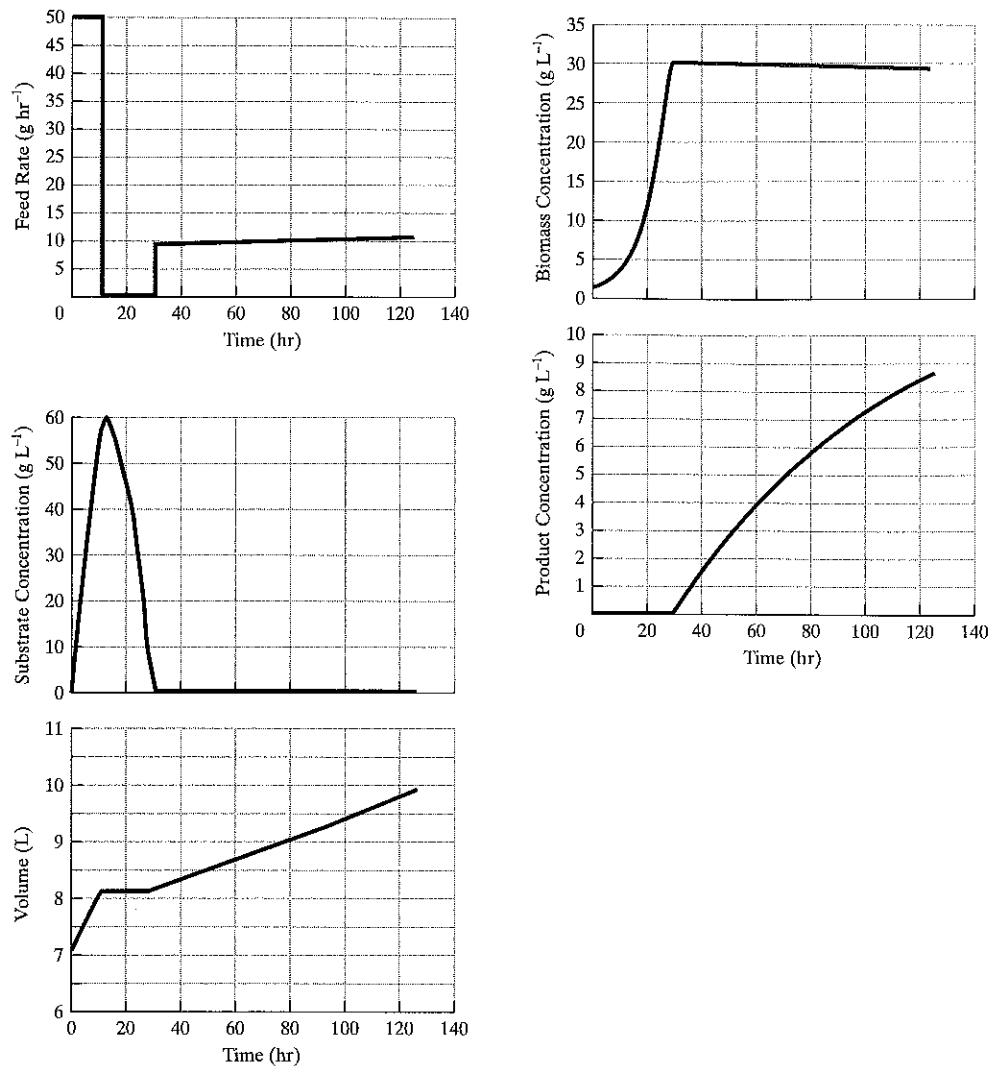**Figure 12.3** Batch penicillin reactor.

Figure 12.4 Optimal profiles for the penicillin reactor.

Cuthrell and Biegler (1989) maximize the production of penicillin, $P\{\tau\}V\{\tau\}$, where τ is the batch time, using variational calculus (Pontryagin maximum principle) to obtain the solution in Figure 12.4. As seen, at the optimum, the batch time is 124.9 hr, with the production of 87.05 g of penicillin. It is notable that the optimal feed flow rate is 50 g/hr for the first 11.21 hr, after which the feed stream is turned off until 28.79 hr, when it is held constant at 10 g/hr. This "on–off" control strategy is commonly referred to as *bang–bang control*. To confirm the cell mass, penicillin, and substrate concentration profiles, the differential equations can be integrated using a mathematical software package such as MATLAB. Furthermore, Cuthrell and Biegler (1989) show how to solve numerically for the optimal solution, which is often referred to as the "optimal control profile," using orthogonal collocation on finite elements, to discretize the differential equations, and successive quadratic programming (SQP). ■

Batch-Product Removal

When distillations are carried out in batch mode, the still is charged with the feed mixture and the heat is turned on in the reboiler. The lightest species concentrate in the distillate, which is condensed and recovered in *batch-product removal* mode. As the light species is

recovered, it is accompanied by increasing fractions of the heavier species unless a s
is applied to maintain a high concentration of light species.

For multicomponent separations, to simplify operation it is often satisfactory to adj
reflux rate once or twice while recovering each species. When the purity of a species,
is being collected in the product accumulator, drops below its specification, the cont
the product accumulator are dumped into its product receiver, and the reflux rate is ad
Stated differently, the reflux rate is increased as the difficulty of the separation betw
light and heavy key components increases. This is illustrated in the next example.

EXAMPLE 12.3 Batch Distillation

A 100 lbmole mixture of methanol, water, and propylene glycol, with mole fractions, 0.33, 0.
0.34, is separated using a 15-tray batch distillation operation, as shown in Figure 12.5. Assume
tion at a nominal pressure of 1 atm, realizing that the pressure in the still will have to be so
higher than this to avoid a vacuum in the reflux accumulator. The tray and condenser liquid hol
0.1 ft³/tray and 1.0 ft³, respectively.

In an attempt to devise a satisfactory operating strategy, the following recipe (also called a ca
was proposed:

Methanol Recovery

1. Bring the column to total reflux operation, with the distillate valve closed.
2. Using a reflux ratio of 3, send 5 lbmol/hr of distillate continuously to the product accu
   Continue until the mole fraction of water in the instantaneous distillate reaches 0.001.
3. Bring the column to total reflux.
4. Using a reflux ratio of 5, send 2.5 lbmol/hr of distillate continuously to the product accu
   Continue until the mole fraction of water in the instantaneous distillate reaches 0.001, a
   point the distillate valve is closed. Dump the contents of the product accumulator into the n
   product receiver.

Propylene Glycol Recovery

5. The column is now at total reflux.
6. Using a reflux ratio of 3, send 20 lbmol/hr of distillate continuously to the product accu
   Continue until the mole fraction of propylene glycol in the instantaneous distillate reache
   Dump the contents of the product accumulator into the water product receiver.
7. Pump the contents of the still pot into the propylene glycol product receiver.

To examine the performance of this recipe, it is helpful to use a batch distillation progr
process simulator, such as BATCHFRAC by Aspen Technology, Inc. (Boston et al., 1981).

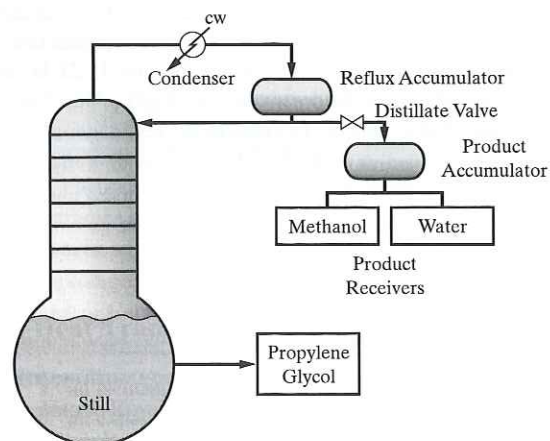**Figure 12.5** Batch distillation oper

processing objective can be specified (such as minimum batch time, energy consumption, or reject chemicals, or some combination of these) and variations on the recipe can be explored in an effort to achieve more optimal operation, as in Exercise 12.3.

SOLUTION

Using the BATCHFRAC simulator, the results are as follows, where Distil. and Accum. refer to the instantaneous distillate and product accumulator, respectively:

After Step		Methanol	Water	Propylene Glycol	Total Amount (lbmol)	Step Time (hr)	Total Time (hr)
1	Charge	0.3300	0.3300	0.3400	100		0
2	Distil.	0.9990	0.0010	—	—	5.63	5.63
	Accum.	0.9999	0.0001	—	28.14		
	Still^x	0.0676	0.4592	0.4732	71.86		
3	Total reflux						
4*	Distil.	0.9990	0.0010	—	—	0.69	6.32
	Accum.	0.9999	0.0001	—	29.88		
	Still^x	0.0446	0.4705	0.4849	70.12		
5	Total reflux						
6*	Distil.	—	0.9990	0.0010	—	1.65	7.97
	Accum.^{x}	0.0947	0.9053	—	33.03		
	Still	—	0.0836	0.9164	37.09		

*Before the reflux accumulator is dumped.
^{x}Includes tray and condenser liquid holdups

As can be seen, the total batch time is nearly 8 hr, the amounts of 99.9 mol% methanol and 91.64 mol% propylene glycol products are 29.88 lbmol and 37.09 lbmol, respectively. Note that after step 4 the methanol product accumulator contains $0.999 \times 29.88 = 29.85$ lbmol methanol. The remainder, $33.33 - 29.85 = 3.48$ lbmol methanol is recovered initially in the water product accumulator during step 6. Hence, the water product accumulator contains a "slop cut" of water. Nearly all of the propylene glycol is recovered in the still. These results can be reproduced using the BATCHFRAC file, EXAM12–3.bkp, on the multimedia CD-ROM. ∎

12.3 DESIGN OF REACTOR–SEPARATOR PROCESSES

In this section, an approach to solving the optimal control problem is introduced for reactor–separator processes. The approach involves the simultaneous determination of the batch times and size factors for both of the process units. Furthermore, the interplay between the two units involves trade-offs between them that are adjusted in the optimization. It should be noted that simpler models, than in normal practice, are used here to demonstrate the concept and, in the first example, provide an analytical solution that is obtained with relative ease.

EXAMPLE 12.4

Consider the batch reactor–separator combination in Figure 12.6, initially presented by Rudd and Watson (1968). In the reactor, the isothermal, irreversible reaction, A → B, is carried out. The separator recovers the product B from unreacted A. The rate constant for the reaction is $k = 0.534$ day^{-1}. It is assumed that the cost of A is negligible compared to the value of the product, B, $C_B =$ \$2.00/lb, that the operating costs of the reactor are proportional to the batch time (that is, $C_O = \alpha t$, where $\alpha =$ \$100/day), and that the cost of separation per batch, C_S, is inversely proportional to the conversion of A in the reactor, X (that is, $C_S = KV/X$), where K is the proportionality constant and V is the holdup volume in the reactor. Find the batch time for the reactor when the gross profit in \$/day is maximized. Let $c_{Ao} = 10$ lb/ft^3, $V = 100$ ft^3, and $K = 1.0$ \$/(ft^3·batch). Note that as the conversion of A to product B increases, the cost of separation decreases, as shown in Figure 12.7b.
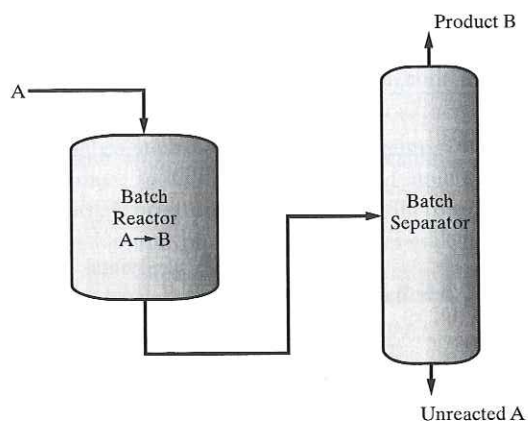
Unreacted A   **Figure 12.6** Reactor–separator process

SOLUTION

For the first-order reaction, it can be shown (Exercise 12.4) that:

$$X = 1 - e^{-kt}$$

as illustrated in Figure 12.7a, and

$$c_B = c_{Ao}X$$

It is desired to maximize the gross profit, GP, in \$/day; that is,

$$\max_t \text{GP} = \frac{1}{t}[C_B V c_B\{t\} - C_O\{t\} - C_S\{X\{t\}\}]$$

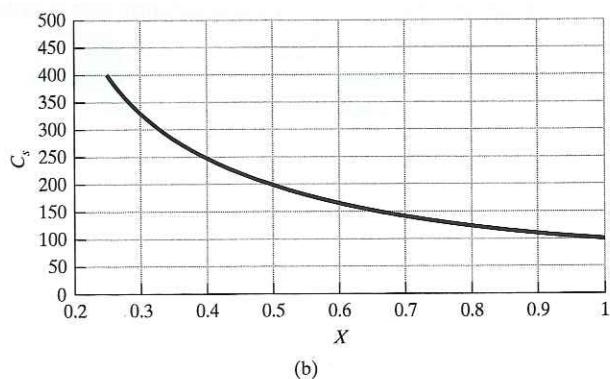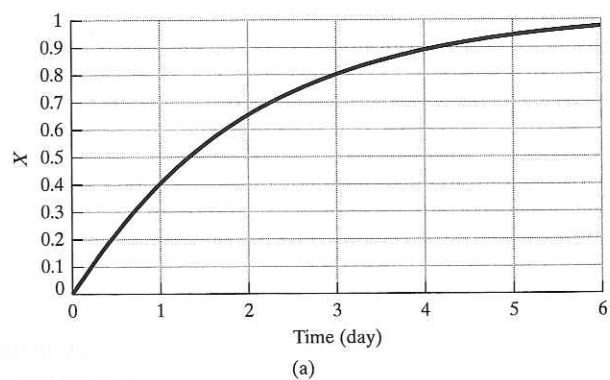
(a)

(b)

Figure 12.7 Conversion and separation. (a) First-order r of conversion; (b) cost of se as a function of conversion.

To locate the maximum, substitute the equations above and differentiate:

$$\frac{dGP}{dt} = 0$$

It can be shown (Exercise 12.4) that at the maximum, the reactor batch time is $\tau_{opt} = 1.35$ day, with a fractional conversion, x_{opt}, of 0.514. At longer times, while the revenues increase due to increased conversion and the separation costs decrease, the gross profit decreases due to the increase in the batch time in the denominator of Eq. (12.8). At shorter times, the revenues decrease due to smaller conversion and separation costs increase due to a more difficult separation, more than countering the decrease in the denominator and leading to smaller gross profit. At the maximum, $GP_{opt} = \$516.8/\text{day}$. Note that $GP < 0$ when $t < 0.507$ day. ■

EXAMPLE 12.5

Figure 12.8 shows an isothermal batch reactor, in which the irreversible reactions, A → B → C, take place, with B the desired product and C an undesired byproduct. The reactions are irreversible and first-order in the reactants. The reaction rate constants are $k_1 = 0.628 \text{ hr}^{-1}$ and $k_2 = 0.314 \text{ hr}^{-1}$. The reactor products are fed from an intermediate storage tank (not shown) to a batch distillation column, from which the most volatile species, A, is removed first in the distillate, followed by the product B, which is the intermediate boiler. For specified reactor volume, V_r, and column volume, V_c, it is desired to determine the batch times for the reactor and column that minimize the cost of producing the desired amount of product B, B_{tot}, moles, in a single campaign. Following Barrera and Evans (1989), the analysis is simplified by assuming that the distillation column produces pure A until it is depleted from the still, followed by pure B. Furthermore, specifications include the total molar concentration in the reactor, C, the distillate flow rate, F_d, the time horizon within which the campaign must be completed, τ_{hor}, and the cleaning times between batches for the reactor and distillation column, t_{cr} and t_{cc}. In addition, several cost coefficients are specified, including the cost of fresh feed, P_A ($/mol), recycling credit for A, P_{rA}, cost or credit for the byproduct C, P_C; the rental rates of the reactor, r_r ($/hr), intermediate storage, r_s, and distillation column, r_c; the costs of cleaning the reactor, C_{clr} ($/batch), and distillation column, C_{clc}; and the utility cost per mole of distillate, P_u. These specifications are given in Table 12.1.

SOLUTION

By integration of the kinetic rate equations, it can be shown (Exercise 12.5) that the mole fraction profiles in time are given by:

$$x_A = e^{-k_1 t_r} \tag{12.9}$$

$$x_B = \frac{k_1(e^{-k_1 t_r} - e^{-k_2 t_r})}{k_2 - k_1} \tag{12.10}$$

$$x_C = 1 - x_A - x_B \tag{12.11}$$
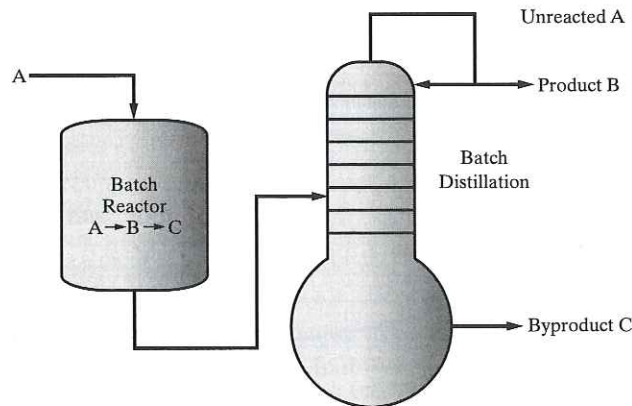
These profiles are graphed in Figure 12.9.

Figure 12.8 Reactor–distillation process.

Table 12.1 Specifications for Example 12.5

$V_r = 3{,}503$ L, $V_c = 784$ L
$B_{tot} = 800$ mol
$C = 0.5$ mol/L
$F_d = 206.2$ mol/hr
$\tau_{hor} \le 24$ hr
$t_{cr} = 0.8$ hr, $t_{cc} = 0.5$ hr
$P_A = 1$ \$/mol, $P_{rA} = 0.2$ \$/mol, $P_C = 0.4$ \$/mol
$r_r = 100$ \$/hr, $r_s = 20$ \$/hr, $r_c = 100$ \$/hr
$C_{clr} = 100$ \$/batch, $C_{clc} = 100$ \$/batch
$P_u = 0.45$ \$/mol

The minimization of the campaign costs is expressed as:

$$\min_{t_r, \tau_c} \phi = \phi_{rm} + \phi_{eq} + \phi_{cl} + \phi_u$$

where t_r is the reaction time (reactor operating time), τ_c is the batch time for the distillation colu
the campaign costs for the raw materials, equipment rental, cleaning, and utilities, are

$$\phi_{rm} = CV_r[P_A + P_{rA}x_A + P_C x_C]\tau_{tot}/\tau_r$$
$$\phi_{eq} = [r_r + r_s + r_c]\tau_{tot}$$
$$\phi_{cl} = [C_{clr}/\tau_r + C_{clc}/\tau_c]\tau_{tot}$$
$$\phi_u = P_u F_d t_c \tau_{tot}/\tau_c$$

Note that the quantity $P_u F_d$ is \$/hr charge for utilities, t_c/τ_c is the fraction of column batch tim
which the column is operational (and using utilities), and τ_{tot} is the total batch time. These quan
multiplied to give ϕ_u, the cost of utilities per batch. This assumes that the utilities are applied
t_c/τ_c fraction of the reactor operation. The minimization is carried out subject to a mass balanc
reactor:

$$B_{tot} = CV_r x_B \tau_{tot}/\tau_r,$$

an equation that assures periodicity in the storage tank (i.e., equal volumes processed per unit t

$$\frac{V_r}{\tau_r} = \frac{V_c}{\tau_c},$$

a mass balance for the distillation column:

$$t_c = V_r C(1 - x_C)/F_d$$

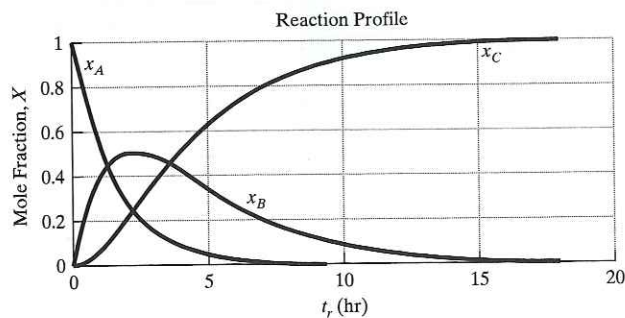and the total campaign time:

$$\tau_{tot} = \tau_r + \tau_c$$

Figure 12.9 Mole fractio
for batch reactions: $k_1 = ($
and $k_2 = 0.314$ hr^{-1}.

where τ_r is the batch time for the reactor and t_c is the column operating time. In addition, as the optimization proceeds, it is necessary to satisfy the following inequality constraints:

$$\tau_{tot} \leq \tau_{hor}$$
$$\tau_r - (t_r + t_{cr}) \geq 0$$
$$\tau_c - (t_c + t_{cc}) \geq 0$$

For the specifications in Table 12.1, the following solution was obtained using successive quadratic programming (SQP) in GAMS (see Section 18.6). The reactor operates for $t_r = 4.44$ hr to produce a product containing 0.062, 0.373, and 0.565 mole fractions of A, B, and C. For periodic cycling, its batch time, $\tau_r = 18.74$ hr, which exceeds the total of the reactions and cleaning times. The distillation column operates for $t_c = 3.69$ hr, which together with its cleaning time, $t_{cc} = 0.5$ hr, gives a batch time for the column, $\tau_c = 4.19$ hr. The total time, or cycle time, is $\tau_{tot} = 22.93$ hr, which falls within the horizon time specified, $\tau_{hor} = 24$ hr. These times correspond to the minimum cost, $\phi = \$10,240$. By varying t_r, it can be shown that this is the minimum cost. ∎

12.4 DESIGN OF SINGLE PRODUCT PROCESSING SEQUENCES

Having examined small optimal control problems for batch process units in Section 12.2 and for reactor–separator sequences in Section 12.3, it should be clear that the determination of optimal batch times, given batch sizes expressed as batch volumes per unit mass of product, can be demanding computationally. Since most processes, in practice, have recipes with numerous tasks and a comparable number of processing units (e.g., the tPA process in Chapters 3 and 4), it is normally not practical to optimize the batch times for the individual processing units when preparing a schedule of tasks and equipment items for the manufacture of a product. Consequently, when preparing a schedule of tasks and equipment items, it is common to specify batch times for tasks to be performed in specific units, usually with batch sizes, and to optimize cycle times for a specific recipe. In some cases, using the rates of production and yields, the vessels are designed as well; that is, vessel sizes are determined to minimize the cost of the plant while determining the cycle times for a specific recipe. In this section, schedules are determined for the batch processes that involve only single products. In the next section, the methodology is extended for multi-product batch processes.

Batch process design begins with the specification of a *recipe* of *tasks* to produce a product. In continuous processing, each task is carried out in a specific equipment item, with one-to-one correspondence between them, shown on a flowsheet that remains fixed in time. Similarly, in batch processes, the tasks are assigned to equipment items, but over specific intervals of time, which vary with batch size, which is often determined by the available equipment sizes. For example, in the tPA process in Sections 3.4 and 4.5, given the rate of tPA production [50 pg tPA/(cell-day), where pg are picograms $= 10^{-12}$] and the cell concentration (between 0.225×10^6 and 3×10^6 cell/mL), the availability of a 5,000-L cultivator determines the 14-day batch time and the batch size (2.24 kg of tPA, produced in 4,000 L of medium, yielding 1.6 kg of final product) for the cultivator. As discussed in Section 3.4, process synthesis involves the creation of a sequence or flowsheet of operations, which can be referred to as a *recipe* of operations or tasks. During the *task integration* step, tasks are often combined to be carried out in a single equipment item; for example, heating and reaction in a pyrolysis furnace. Also, during this step, the decision to use continuous or batch processing is made. At this point, the available equipment sizes often determine the batch sizes and times.

Batch Cycle Times

When scheduling and designing batch processes, several formalisms are widely used, as reviewed by Reklaitis (1995). In this section, and those that follow, portions of the presentation are derived from his article.

In batch processes, it is common for a task to consist of a sequence of *steps* to be ca
out in the same equipment unit. For example, Figure 12.10 shows a typical recipe wi
tasks and steps. Note that each step involves a *batch time*, which is determined by the
cessing rates and the *batch size*; that is, the amount of the *final* product manufactured i
batch. Furthermore, a *production line* is a set of equipment items assigned to the tasks
recipe to produce a product. When a production line is used to produce a sequence of id
cal batches, the *cycle time* is the time between the completions of batches. To better visu
the schedule of production, an equipment occupation diagram, known as a *Gantt cha*
prepared, showing the periods of time during which each equipment item is utilize
shown in Figure 12.11a. Note that the unit having the longest batch time (6 hr), U2, i
bottleneck unit, as it is always in operation. Note also that the second batch is begun in
to produce the feed to the unit, U2, when the latter becomes available after processin
first batch. In this diagram, the batches are transferred from unit-to-unit immediately
called *zero-wait* strategy, with no intermediate storage utilized). Clearly, the cycle time,
is the batch time of U2.

In the schedule in Figure 12.11a, the serial process has a distinct task assigned to
equipment item. Often, to utilize the equipment more efficiently, it is possible to u
equipment item to carry out two or more tasks. Note that this may not be possible when
ufacturing specialty chemicals that are very sensitive to contamination, as in the manufa
of pharmaceuticals. Returning to the schedule in Figure 12.11a, when the fourth task c
carried out in U1, this unit is better utilized and U4 can be released for production else
in the batch plant, as shown in Figure 12.11b. Note that to achieve this schedule, wi
adding intermediate storage, it is necessary to retain the batch within U3 until U1 bec
available. Furthermore, to increase the efficiency of the schedule, that is, reduce the
time, it is common to add one or more units in parallel. When in phase, it is clear th
batch time for the unit is reduced to τ_j/n_j, where n_j is the number of units in parallel for t
For example, when two U2 units, each half-size, are installed in parallel, the effective
time for unit U2 is reduced to 3 hr, and the cycle time is reduced to 4 hr, with U3 the b
neck unit. Alternatively, the parallel units can be sequenced out-of-phase, without al
their batch time, as shown in Figure 12.11c. In both cases, the U2 bottleneck is elimi
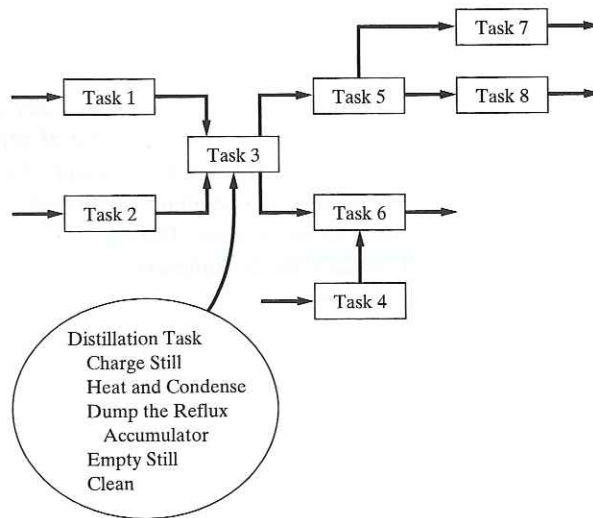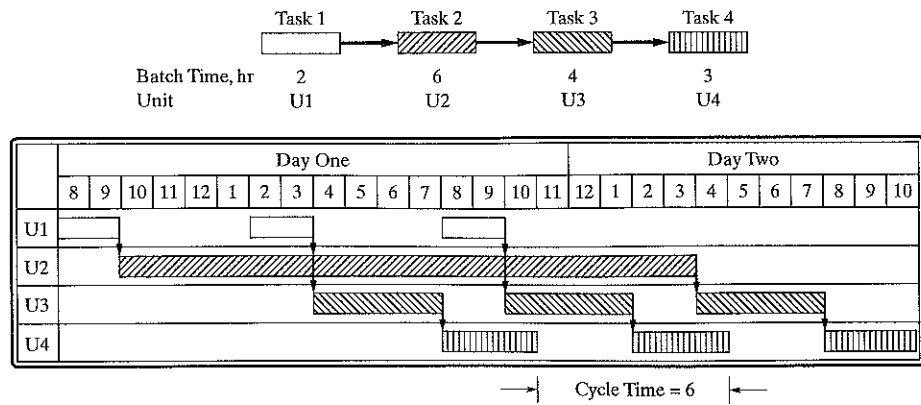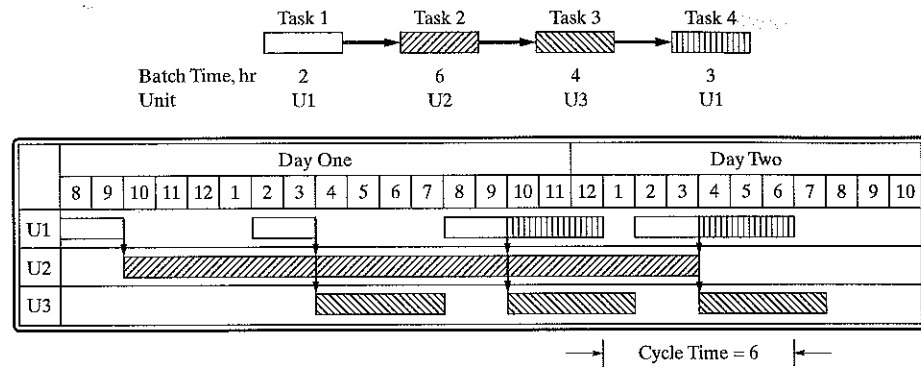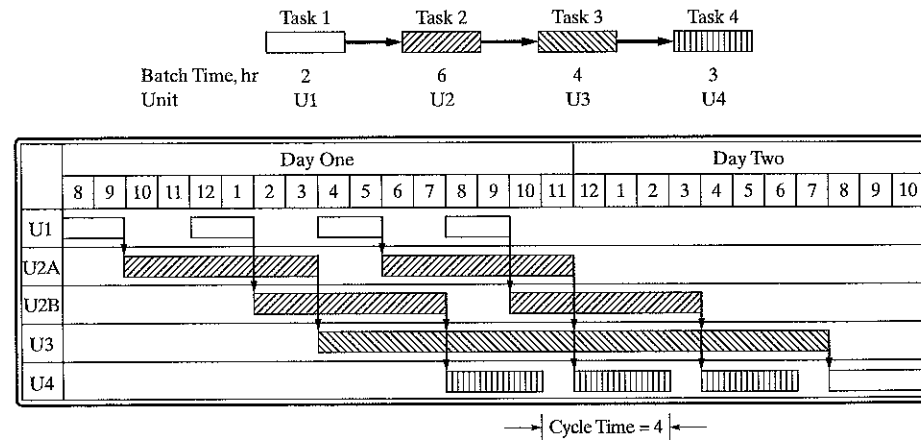and the cycle time is reduced to 4 hr.

Figure 12.10 Recipes, tasks
subtasks.

(a) Distinct Task Assigned to Each Unit

(b) Multiple Tasks Assigned to Same Unit

(c) Parallel Units

Figure 12.11 Serial recipe and Gantt charts.

Clearly, without parallel operation, the batch cycle time, CT, is the maximum of the b
times, $\tau_j, j = 1, \ldots, M$:

$$CT = \max_{j=1,\ldots,M} \tau_j \qquad (12$$

where M is the number of unique equipment units. With n_j units in parallel and in phase
cycle time is given by:

$$CT = \max_{j=1,\ldots,M} \frac{\tau_j}{n_j} \qquad (12$$

Returning to the example, when two units U2 are installed in parallel to perform task 2:

$$CT = \max_{j=1,\ldots,M} \frac{\tau_j}{n_j} = \max\left\{2, \tfrac{6}{2}, 4, 3\right\} = 4 \text{ hr} \qquad (12$$

Intermediate Storage

Thus far, two storage options have been illustrated. No storage is used in the schedul
Figures 12.11a and 12.11c, with the contents of each unit transferred immediately to the
unit, experiencing no delay after its task has been completed. As mentioned above, this i
so-called *zero-wait* (ZW) strategy. In the schedule of Figure 12.11b, U3 provides intern
ate storage until U1 becomes available. Hence, a zero-wait strategy is implemented,
some intermediate storage when necessary. This is referred to as an *intermediate storage*
strategy. The third strategy involves unlimited intermediate storage (UIS), sufficient to
the contents of the products from a unit having a lengthy batch time, to be used repeated
a unit having half the batch time or less, as illustrated in Figure 12.12. Here, U1 is util
at all times and the cycle time is reduced from 9 to 3 hr. To produce a specified amou
product, the batch size is reduced by a factor of one-third since the cycle time is div
by three.

Batch Size

It is convenient to define the size factor, S_j, for task j, as the capacity required per un
product. Commonly, it is defined as the volume required to produce a unit mass of pro
For example, for the third cultivator in the tPA process of Sections 3.4 and 4.5, 4,000
medium yields 2.24 kg of tPA, which eventually yields 1.6 kg of final tPA product. Co
quently, its size factor is 4,000 L/ 1.6 kg = 2,500 L/kg tPA product. Size factors can be
puted for each task in a recipe. Normally, equipment vessel sizes are selected that ex
batch volume by 10 to 20%. Clearly, the batch factor in volume/mass produced is d
mined by the rate of processing the batch (e.g., kg/hr) multiplied by the batch time (hr)
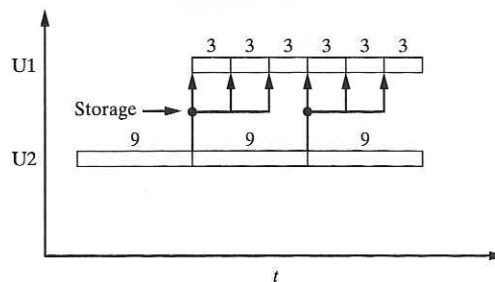divided by the density of the batch (kg/L) and the mass of product produced (kg).

Figure 12.12 Gantt chart with unli
intermediate storage (UIS).

12.5   DESIGN OF MULTIPRODUCT PROCESSING SEQUENCES

A *multiproduct batch plant* produces a set of products whose recipe structures are the same, or nearly identical. One example is a foundry that manufactures integrated circuit (IC) chips in which several different devices are produced simultaneously, each involving hundreds of tasks and utilizing several equipment items. In these plants, each product is produced in the same production line, with multiple processing tasks carried out using the same equipment items. The recipes are expressed in serial campaigns for each product. Figure 12.13 shows schedules in which a campaign of two batches to produce product A is followed by a campaign of two batches to produce product B. It should be noted, however, that because the tasks for products A and B differ in equipment utilized, the plant is not a multiproduct batch plant; instead, it is referred to as a *multipurpose batch plant*. Although the cycle times for both products are identical (4 hr), it is common for the product cycle times to be unequal. The use of alternating product cycles is a limitation that does not apply to *general multipurpose plants* in which there are no well-defined production lines and no cyclic patterns of batch completion, as shown in Figure 12.14. Such plants are more flexible and effective for a large number of products that are produced in small volumes, where their vessels are cleaned easily and the presence of trace contaminants in the products is not a concern. Their equipment items are utilized more completely, without the idle-time gaps in plants with cyclic campaigns for each product. Consequently, multiproduct batch plants are used for larger volume products having similar recipes, as is often the case for plants that produce a family of grades of a specific product.

Scheduling and Designing Multiproduct Plants

For an existing plant, the scheduling problem involves a specification of the: (1) product orders and recipes, (2) number and capacity of the equipment items, (3) a listing of the equipment items available for each task, (4) limitations on the shared resources (e.g., involving the usage of utilities and manpower), and (5) restrictions on the use of equipment due to operating or
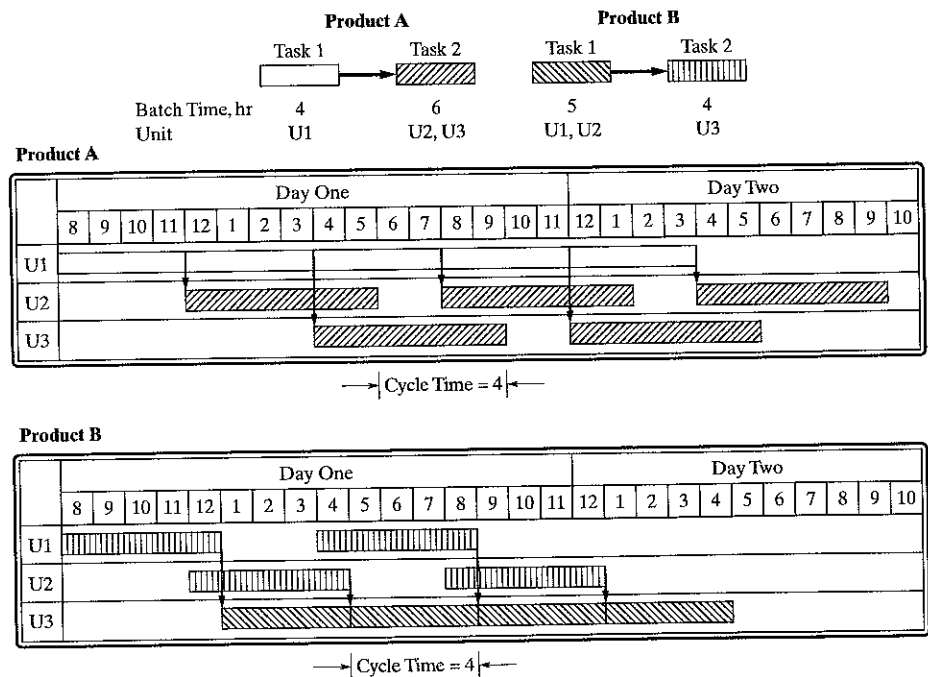

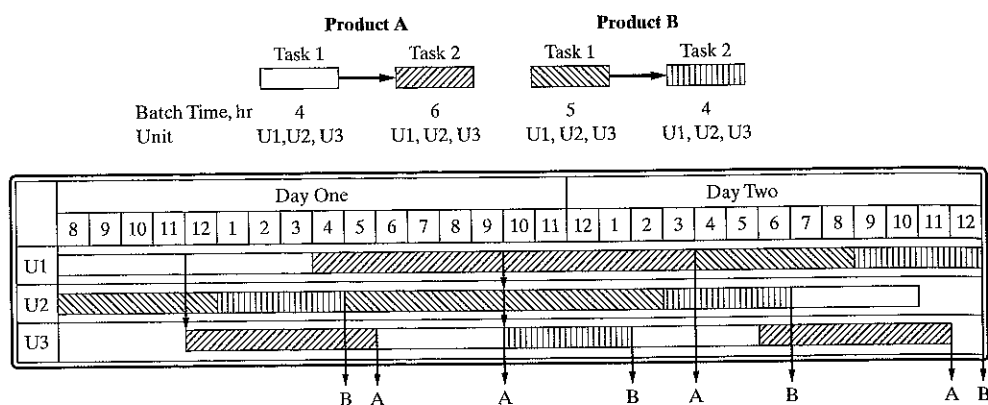Figure 12.13   Gantt charts for a multipurpose plant.

Figure 12.14 Gantt chart for a general multipurpose plant.

safety considerations. In solving the problem, that is, determining an optimal schedule, the order in which tasks use the equipment and resources is determined, with specific timings of the tasks provided, that optimize the plant performance (which can be specified in many ways, e.g., to maximize the gross profit).

When the plant does not exist, that is, when a new plant is to be designed, the product orders are usually not well defined. Otherwise, the specifications are identical. In fact, the design problem encompasses the scheduling problem in that its solution involves determining the number and capacity of the equipment items in addition to the optimal schedule. For the design problem, these are determined to optimize an objective that includes the investment costs of the equipment, such as the annualized cost. Because the product orders are not as well known during the design stage, it is common to solve the scheduling problem less rigorously.

As mentioned earlier, it is common to specify size factors and input/output ratios as known constants when defining recipes. Also, batch times for each task are often specified as constant, or as known functions of the batch size. These can be determined by optimizing the operation of each equipment item, as discussed in Section 12.2.

It is common to formulate the design problem for a multiproduct batch plant involving the processing of batch campaigns in series (i.e., one-at-a-time—commonly referred to as a *Flowshop plant*) as a mixed-integer nonlinear program (MINLP). Then, the formulation is simplified for solution using strategies that are beyond the scope of this book (Biegler et al., 1998). Herein, as an introduction, a typical formulation is presented without simplification. It begins with the objective, that is, to minimize the total investment cost, C:

$$\min C = \sum_{j=1}^{M} m_j a_j V_j^{\alpha_j}$$

where m_j is the number of out-of-phase units assigned to task j (integer variables), M is the number of tasks, and V_j is the size of the unit assigned to task j (usually in L; a_j and α_j are cost coefficients). This objective is minimized commonly subject to inequalities that involve the vessel size:

$$V_j \geq B_i S_{ij}$$

where B_i is the batch size of product i (i.e., the final product size, typically in kg), and S_{ij} is the size factor for task j in producing product i (typically in L/kg). This inequality insures that the unit size exceeds the smallest size required to produce all of the products. In addition, lower and upper bounds are specified on the equipment sizes in accordance with manufacturing limitations:

$$V_j^L \leq V_j \leq V_j^U$$

Inequalities are associated also with the cycle time and time horizon:

$$CT_i \geq \tau_{ij}/m_j$$

$$\sum_{i=1}^{N} \frac{Q_i}{B_i} CT_i \leq H$$

where CT_i is the cycle time for producing product i [which can be determined using Eqs. (12.12) and (12.13)], τ_{ij} is the batch time for task j in producing product i, Q_i is the annual demand for product i (typically, in kg/yr), and H is the production hours available annually.

12.6 SUMMARY

Initially, this chapter focuses on the optimal control of batch processing units, with emphasis on reducing the batch time and batch size. Then, the batch times for reactor–separator processes are optimized with emphasis on the interactions between the process units and the trade-offs in adjusting their batch times. Finally, the problem of determining operating schedules for single- and multiproduct batch plants, involving the possibility of intermediate storage and complex recipes with numerous tasks in numerous process units is examined.

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EXERCISES

12.1 In Example 12.2, derive the mass balances for the cell mass, penicillin, and substrate, and the overall mass balance.

12.2 For the penicillin reactor in Example 12.2, using repeated simulations search for the optimal feed profile to maximize:

$$0.025P\{\tau\}V\{\tau\} - 1.68\tau - 0.00085 \int_0^\tau F\{t\}\, dt$$

where τ is the batch time. This objective function maximizes the penicillin produced while penalizing long batch times and the cost of the substrate feed stream. Indicate how the penalty terms affect the feed rate profile.

12.3 For the batch distillation column in Example 12.3, devise a recipe that will decrease the batch time without reducing the amount of product recovered. Estimate the increase in the utility usage.

12.4 In Example 12.4, derive Eqs. (12.6) and (12.7). Then, graph the gross profit as a function of the reactor batch time for various values of the rate constant, k, over the range 0.4–0.6 day^{-1}.

12.5 In Example 12.5, derive Eqs. (12.9)–(12.11).

12.6 For the reactor–distillation process in Example 12.5, recompute the solution when the reactor and column volumes are decreased by 20%.

12.7 Construct a Gantt chart for the general multipurpose plant in Figure 12.14, but with the unit assignments specified in Figure 12.13.

12.8 A batch process requires the following operations to be completed in sequence: 3 hr of mixing, 5 hr of heating, 4 hr of reaction, 7 hr of purification, and 2 hr of transfer.

a. When the five operations are carried out in vessels U1, U2, U3, U4, and U5, respectively, determine the cycle times, and construct Gantt charts corresponding to the zero-wait, intermediate storage, and unlimited intermediate storage inventory strategies.

b. When a new purification vessel U4A is purchased, so that two 7-hr purifications can take place in parallel, determine the system bottleneck using the intermediate storage, inventory strategy.

Potential Opportunity

Part I
Create and Assess Primitive Problem

No ◁ Is the Chemical Structure Known? ▷ Yes

Part I
Find Chemicals or Chemical Mixtures That Have the Desired Properties and Performance

No ◁ Is a Process Required to Produce the Chemicals?

Yes

Part I
Process Creation

Is the Gross Profit Favorable? — No → Reject

Yes

Part I	Part II
Development of Base Case	Detailed Process Synthesis—Algorithmic Methods

No ◁ Is the Process Still Promising?

Yes

Plantwide Par
Controllabilit
Assessment

Detailed Design, Equipment Sizing, and Optimization — Part III

Is the Final Product a:

— Commodity Chemical

— Specialty Chemical

— Configured Consumer or Industrial Product (that uses the Chemicals or Chemical Mixtures Produced)?

Startup
Assessmen

Reliability a
Safety Assessm

Equipment Sizing
Heat Exchanger Design
Tower Design
Pump & Compressor Design

Product Design

Capital Cost Estimation

Profitability Analysis

Optimization

Written Design R
and Oral Present

Yes ◁ Is the Process and/or Product Still Promising? ◁ No — Is the Process and/or Product Feasible?

Yes

No

Reject

Plant Desig
Construction
Startup, and
Operation

Part Three

DETAILED DESIGN, EQUIPMENT SIZING, AND OPTIMIZATION - CONFIGURED PRODUCT DESIGN

This part concentrates on the steps carried out approximately during process creation and more rigorously after a base-case design(s) has been developed, as discussed in Part One. It covers the steps of detailed design in (1) determining equipment sizes, (2) carrying out economic calculations, and (3) optimization. In all of the discussions, approximate and rigorous methods are presented. The approximate methods are used throughout the steps of process creation covered in Part One and the algorithmic methods for process synthesis covered in Part Two. They are referred to repeatedly in those parts and, consequently, this part of the book should be used long before Parts One and Two are completed.

In addition, Chapter 19 introduces the steps in configured product design. These are illustrated using several case studies.

Chapter 13, on the design of heat exchangers, contains some basic introductory material that may be helpful before or during the study of Chapter 10 on heat and power integration. As mentioned therein, the emphasis in that chapter is on the design of an energy-efficient heat exchanger network (HEN) and not on the details of the individual heat exchangers. This is the subject of Chapter 13. Students who have had a strong course in heat transfer are likely to find much of this material a review. They should, however, find the many recommendations for design helpful, including the selection of heating and cooling media, avoidance of temperature crossovers, and the frequent need for multiple shell and tube passes in heat exchangers.

Chapters 14 and 15 provide similar coverage on the details of the design of multistage and packed towers, and of pumps, compressors, and expanders, respectively. While some of this material may be a review for students, the recommendations for equipment design should be helpful.

Chapters 16 and 17, on cost accounting and capital cost estimation, and profitability analysis, respectively, provide a comprehensive treatment of these subjects. Both approximate and rigorous methods are presented. Equations are provided for estimating the purchase cost of a