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

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

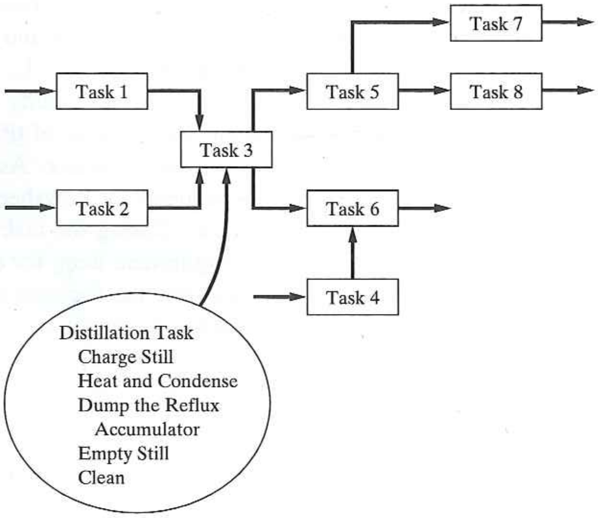
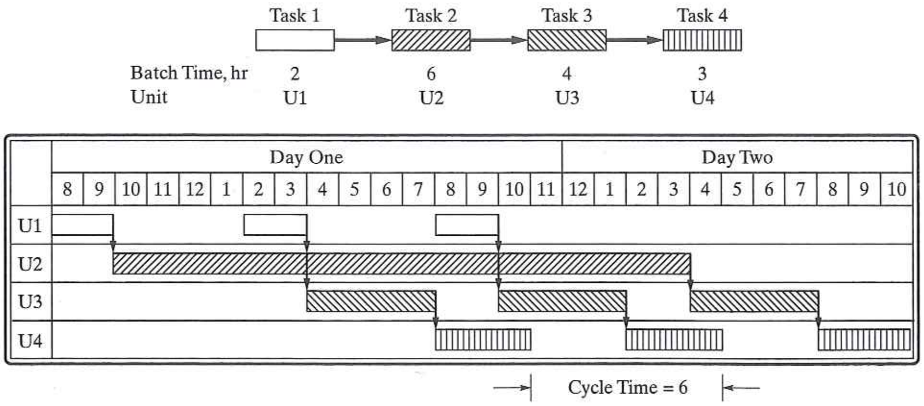
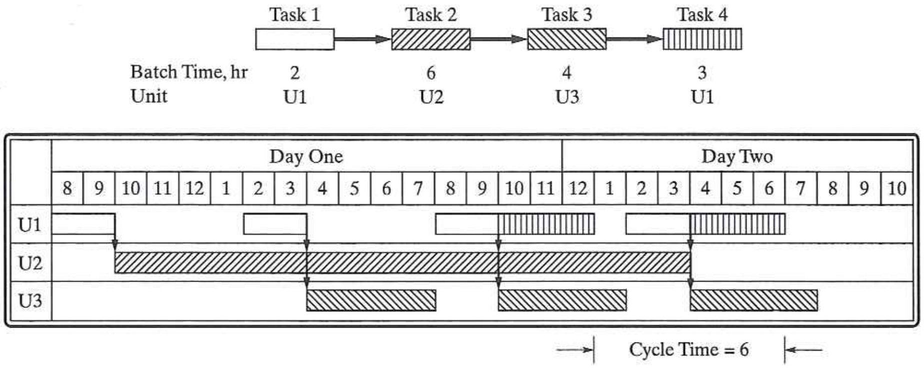


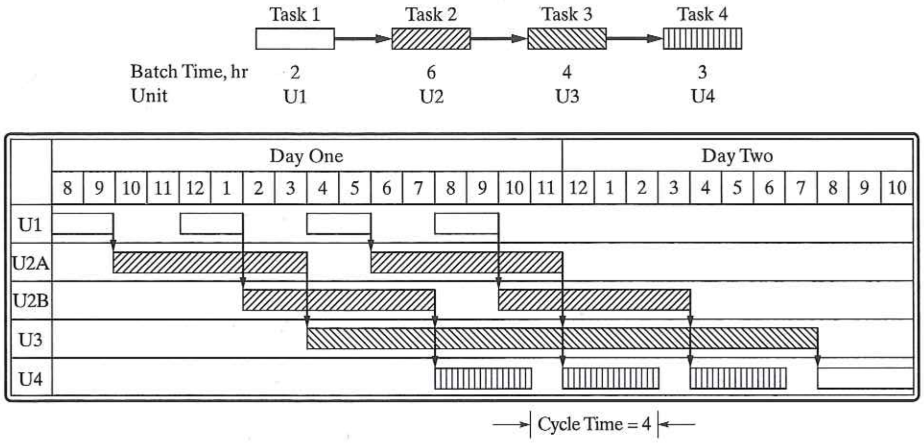
Figure 12.10 Recipes, tasks, and subtasks.



(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 batch times, $\tau_j, j = 1, \ldots, M$:

$$CT = \max_{j=1,\ldots,M} \tau_j \tag{12.12}$$

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

$$CT = \max_{j=1,\ldots,M} \frac{\tau_j}{n_j} \tag{12.13}$$

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

$$CT = \max_{j=1,\ldots,M} \frac{\tau_j}{n_j} = \max\{2, \tfrac{6}{2}, 4, 3\} = 4 \text{ hr} \tag{12.14}$$

Intermediate Storage

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

Batch Size

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

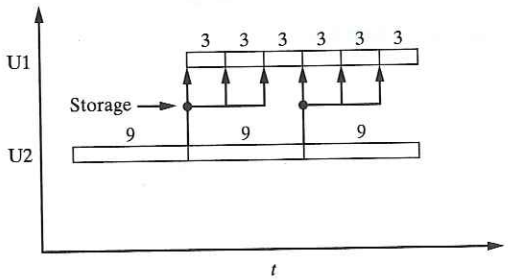


Figure 12.12 Gantt chart with unlimited intermediate storage (UIS).

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

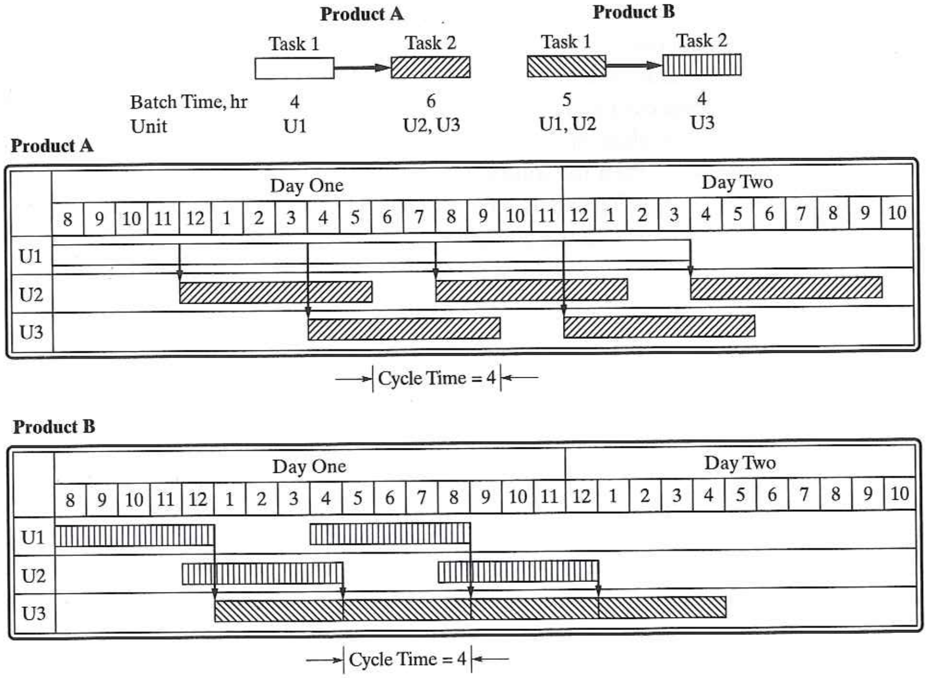


Figure 12.13 Gantt charts for a multipurpose plant.

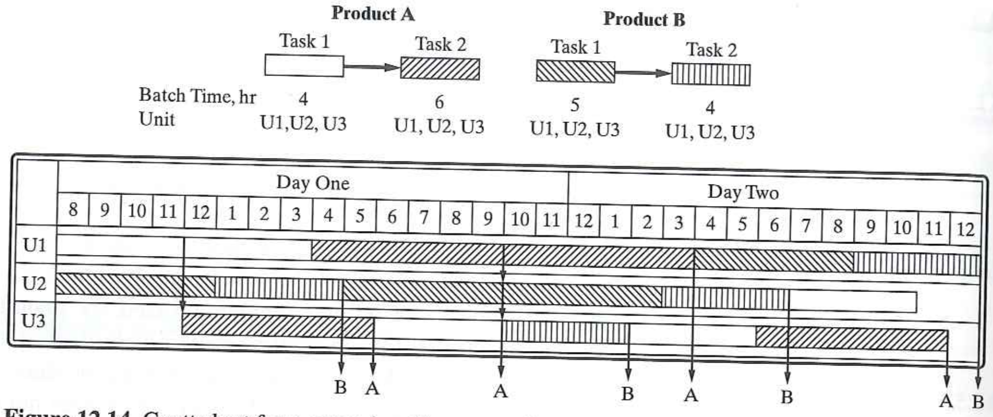


Figure 12.14 Gantt chart for a general multipurpose plant.

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.