Chapter 19

Real-Time Optimization

Previous chapters have considered the development of process models and the design of controllers from an unsteady-state point of view. Such an approach focuses on obtaining reasonable closed-loop responses for set-point changes and disturbances. Up to this point, we have only peripherally mentioned how set points should be specified for the process. The on-line calculation of optimal set points, also called *real-time optimization* (RTO), allows the profits from the process to be maximized (or costs to be minimized) while satisfying operating constraints. The appropriate optimization techniques are implemented in the computer control system. Steady-state models are normally used, rather than dynamic models, because the process is intended to be operated at steady state except when the set point is changed.

This chapter first discusses basic RTO concepts and then describe typical applications to process control. Guidelines for determining when RTO can be advantageous are also presented. Subsequently, set-point selection is formulated as an optimization problem, involving economic information and a steady-state process model. Optimization techniques that are used in the process industries are briefly described. For more information, see textbooks on optimization methodology (Ravindran et al., 2006; Griva et al., 2008; Edgar et al., 2001).

Figure 19.1 is a detailed version of Fig. 1.7, which shows the five levels in the process control hierarchy where various optimization, control, monitoring, and data acquisition activities are employed. The relative position of each block in Fig. 19.1 is intended to be conceptual, because there can be overlap in the functions carried out, and often several levels may utilize the same computing platform. The relative time scale for each level's activity is also shown. Process data (flows, temperatures, pressures, compositions, etc.) as well as *enterprise data*, consisting of commercial and financial information, are used with the methodologies

shown to make decisions in a timely fashion. The highest level (planning and scheduling) sets production goals to meet supply and logistics constraints and addresses time-varying capacity and manpower utilization decisions. This *enterprise resource planning* (ERP) and the *supply chain management* in Level 5 refer to the links in a web of relationships involving retailing (sales), distribution, transportation, and manufacturing (Bryant, 1993). Planning and scheduling usually operate over relatively long time scales and tend to be decoupled from the rest of the activities in lower levels (Geddes and Kubera, 2000). For example, Baker (1993) and Shobrys and White (2002) indicate that all of the refineries owned by an oil company are usually included in a comprehensive planning and scheduling model. This model can be optimized to obtain target levels and prices for inter-refinery transfers, crude oil and product allocations to each refinery, production targets, inventory targets, optimal operating conditions, stream allocations, and blends for each refinery.

In Level 4, RTO is utilized to coordinate the network of process units and to provide optimal set points for each unit, which is called *supervisory control*. For multivariable control or processes with active constraints, set-point changes are performed in Level 3b (e.g., model predictive control discussed in Chapter 20). For single-loop or multiloop control the regulatory control is performed at Level 3a. Level 2 (safety and environmental/equipment protection) includes activities such as alarm management and emergency shutdowns. Although software implements the tasks shown, there is also a separate hard-wired safety system for the plant, as discussed in Chapter 9. Level 1 (process measurement and actuation) provides data acquisition and on-line analysis and actuation functions, including some sensor validation. Ideally, there is bidirectional communication between levels, with higher levels setting goals for
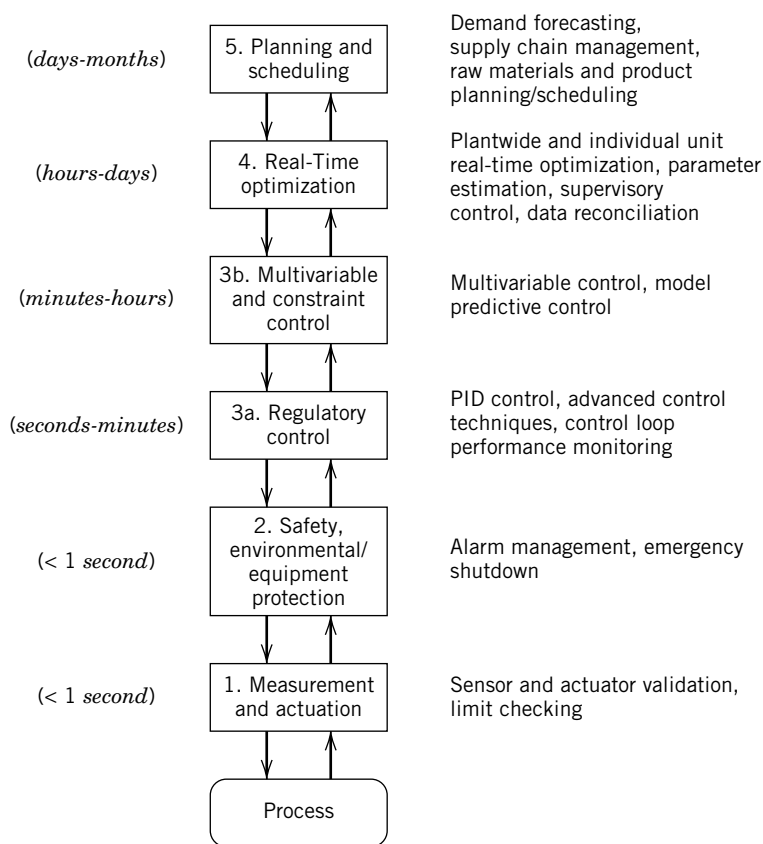
Figure 19.1 The five levels of process control and optimization in manufacturing. Time scales are shown for each level.

lower levels and the lower levels communicating constraints and performance information to the higher levels. The time scale for decision-making at the highest level (planning and scheduling) may be of the order of months, while at lower levels (for example, regulatory control), decisions affecting the process can be made frequently (e.g., in fractions of a second). The main focus of this chapter is on Level 4.

Historically, the focus of optimization in chemical plants has been during the design phase, but since the 1990s this has changed because plant profitability can be enhanced by performing optimization of operating conditions on a repetitive basis. In a large plant, the improved profits attained with RTO can be substantial (Bailey et al., 1993; White, 2010). Optimal operating points can sometimes change markedly from day to day, or even during the course of one day. For example, the price of delivered electrical power can vary by a factor of five from highest to lowest price (due to time-of-day pricing by electrical utilities). Other

changes that require periodic optimization of operating conditions include variations in the quality and cost of feedstocks, processing and storage limits, and product demands. With recent advances in digital hardware and optimization software, RTO can be easily incorporated into computer control systems. The scale at which industrial RTO can be implemented is impressive. Problems with over 100,000 variables and equality/inequality constraints are routinely solved (Georgiou et al., 1997).

19.1 BASIC REQUIREMENTS IN REAL-TIME OPTIMIZATION

The steady-state model used in RTO typically is obtained either from fundamental knowledge of the plant or from experimental data. It utilizes the plant operating conditions for each unit such as temperature, pressure, and feed flow rates to predict properties such as product yields (or distributions), production rates, and measurable product characteristics (e.g., purity,

viscosity, and molecular weight). The economic model involves the costs of raw materials, values of products, and costs of production as functions of operating conditions, projected sales figures, and so on. An objective function is specified in terms of these quantities; in particular, *operating profit* over some specific period of time can be expressed as

$$P = \sum_{s} F_s V_s - \sum_{r} F_r C_r - OC \qquad (19\text{-}1)$$

where

P = operating profit/time

$\sum_{s} F_s V_s$ = sum of product flow rates times respective product values

$\sum_{r} F_r C_r$ = sum of feed flow rate times respective unit cost

OC = operating costs/time

Both the operating and economic models typically will include constraints on

1. *Operating conditions:* Process variables must be within certain limits due to valve ranges (0% to 100% open) and environmental restrictions (e.g., furnace firing constraints).
2. *Feed and production rates:* A feed pump has a maximum capacity; sales are limited by market projections.
3. *Storage and warehousing capacities:* Storage tank capacity cannot be exceeded during periods of low demand.
4. *Product impurities:* A salable product cannot contain more than the maximum amount of a specified contaminant or impurity.

Process operating situations that are relevant to maximizing operating profits include

1. *Sales limited by production.* In this type of market, sales can be increased by increasing production. This can be achieved by optimizing operating conditions and production schedules.
2. *Sales limited by market.* This situation is susceptible to optimization only if improvements in efficiency at current production rates can be obtained. An increase in thermal efficiency, for example, usually leads to a reduction in manufacturing costs (e.g., utilities or feedstocks).
3. *Large throughput.* Units with large production rates (or throughputs) offer great potential for increased profits. Small savings in product costs per unit throughput or incremental improvements in yield, plus large production rates, can result in major increases in profits.

4. *High raw material or energy consumption.* These are major cost factors in a typical plant and thus offer potential savings. For example, the optimal allocation of fuel supplies and steam in a plant can reduce costs by minimizing fuel consumption.
5. *Product quality better than specification.* If the product quality is significantly better than the customer requirements, it can cause excessive production costs and wasted capacity. By operating closer to the customer requirement (e.g., impurity level), cost savings can be obtained, but this strategy also requires lower process variability (see Fig. 1.9).
6. *Losses of valuable or hazardous components through waste streams.* The chemical analysis of plant waste streams, both to air and water, will indicate whether valuable materials are being lost. Adjustment of air/fuel ratios in furnaces to minimize unburned hydrocarbon losses and to reduce nitrogen-oxide emissions is one such example.

Timmons et al. (2000) and Latour (1979) have discussed opportunities for the application of on-line optimization or supervisory control in refinery operations. Three general types of optimization problems commonly encountered in industrial process operations are discussed next.

Operating Conditions

Common examples include optimizing distillation column reflux ratio and reactor temperature. Consider the RTO of a fluidized catalytic cracker (FCC) (Latour, 1979). The FCC reaction temperature largely determines the conversion of a light gas oil feedstock to lighter (i.e., more volatile) components. The product distribution (gasoline, middle distillate, fuel oil, light gases) changes as the degree of conversion is increased. Accurate process models of the product distribution as a function of FCC operating conditions and catalyst type are required for real-time optimization. Feedstock composition, downstream unit capacities (e.g., distillation columns), individual product prices, product demand, feed preheat, gas oil recycle, and utilities requirements must be considered in optimizing an FCC unit. The large throughput of the FCC implies that a small improvement in yield translates to a significant increase in profits. Biegler et al. (1997) have discussed an RTO case study on a hydrocracker and fractionation plant originally formulated by Bailey et al. (1993).

Olefins plants in which ethylene is the main product are another application where RTO has had a

significant impact (Darby and White, 1998; Starks and Arrieta, 2007). A full plant model can have as many as 1,500 submodels, based on the development of fundamental chemical engineering relations for all unit operations involved, that is, furnaces, distillation columns, mixers, compressors, and heat exchangers (Georgiou et al., 1997). In the ExxonMobil olefins plant (Beaumont, TX), the detailed model contained about 200,000 variables and equations, and optimization is used to obtain the values of about 50 targets or set points. Although standard approaches are used for developing separation and heat exchange models, the furnace models are quite elaborate and are typically usually proprietary. In the ExxonMobil application, 12 furnaces are operated in parallel with up to eight possible gas feeds and five liquid feeds (different hydrocarbons) to be cracked, along with three different coil geometries. The key optimization variables are conversion, feed rate, and steam/oil ratio, subject to feedstock availability and equipment constraints. This particular application has led to benefits in the range of millions of dollars per year.

Allocation

Allocation problems involve the optimal distribution of a limited resource among several parallel (alternative) process units. Typical examples include (Latour, 1979; Marlin and Hrymak, 1997):

Steam Generators. Optimum load distribution among several boilers of varying size and efficiency.

Refrigeration Units. Optimum distribution of a fixed refrigeration capacity among several low-temperature condensers associated with distillation columns.

Parallel Distillation Columns. Minimization of "off-spec" products and utilities consumption while maximizing overall capacity.

Planning and Scheduling

Examples of scheduling problems encountered in continuous plants include catalyst regeneration, furnace decoking, and heat exchanger cleaning, which deal with the tradeoff between operating efficiency and lost production due to maintenance. Planning problems normally entail optimization of continuous plant operations over a period of months. This approach is commonly used in refinery optimization. In batch processing, optimal scheduling is crucial to match equipment to product demands and to minimize cycle times. In a batch campaign, several batches of product may be produced using the same recipe. In order to optimize the production process,

the engineer needs to determine the recipe that satisfies product quality requirements; the production rates to fulfill the product demand; the availability of raw material inventories; product storage availability; and the run schedule. Recent examples of optimal batch scheduling include specialty polymer products by McDonald (1998) and pharmaceuticals by Schulz and Rudof (1998). See Chapter 18 for more details on batch processing.

19.1.1 Implementation of RTO in Computer Control

In RTO the computer control system performs all data transfer and optimization calculations and sends set-point information to the controllers. The RTO system should perform all tasks without unduly upsetting plant operations. Several steps are necessary for implementation of RTO, including data gathering and validation (or reconciliation), determination of the plant steady state, updating of model parameters (if necessary) to match current operations, calculation of the new (optimized) set points, and implementation of these set points.

To determine whether a process unit is at steady state, software in the computer control system monitors key plant measurements (e.g., compositions, product rates, flow rates, etc.) and determines whether the plant operating conditions are close enough to steady state to start the RTO sequence. Only when all of the key measurements are within the allowable tolerances is the plant considered to be at steady state and the optimization calculations started; see Cao and Rhinehart (1995) for a statistical technique that determines the existence of steady-state conditions. The optimization software screens the measurements for unreasonable data (gross error detection). Data validity checking automatically adjusts the model updating procedure to reflect the presence of bad data or equipment that has been taken out of service. Data reconciliation based on satisfying material and energy balances can be carried out using separate optimization software (Narasimhan and Jordache, 2000). Data validation and reconciliation is an extremely critical part of any optimization activity. If measurement errors resulting from poor instrument calibration are not considered, the data reconciliation step or subsequent parameter estimation step will not provide meaningful answers (Soderstrom et al., 2000).

The optimization software can update model parameters to match current plant data, using regression techniques. Typical model parameters include exchanger heat transfer coefficients, reactor performance
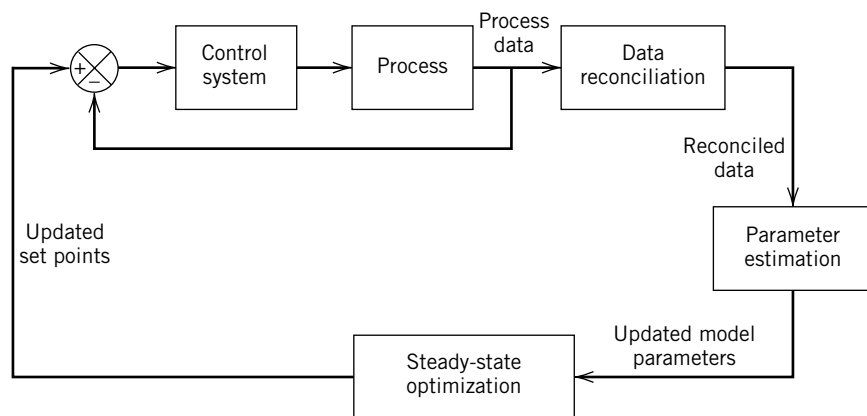
Figure 19.2 A block diagram for RTO and regulatory feedback control.

parameters, and furnace efficiencies. The parameters appear in material and energy balances for each unit in the plant as well as constitutive equations for physical properties. Parameter updating compensates for plant changes and degradation of process equipment, although there is a loss of performance when the model parameters are uncertain or the plant data contain noise (Perkins, 1998). Considerable plant knowledge and experience is required in deciding which parameters to update and which data to use for the updates. After completion of the parameter estimation, the information regarding the current plant constraints, the control status data, and the economic values for feeds, products, utilities, and other operating costs are collected. The department in charge of planning and scheduling updates the economic values on a regular basis. The optimization software then calculates the optimum set points. The steady-state condition of the plant is rechecked after the optimization calculation. If the individual processes are confirmed to still be at the same steady state, then the new set points are transferred to the computer control system for implementation. Subsequently, the process control computer repeats the steady-state detection calculations, restarting the cycle. If the new optimum set points are not statistically different from the previous ones, no changes are made (Marlin and Hrymak, 1997).

The combination of RTO and regulatory control can be viewed as analogous to cascade control. As shown in Fig. 19.2, the outer RTO loop will operate more slowly than the inner loop, and a poor design of this interaction results in poor performance. The dynamic controller (or layer 3) handles the transformation between the steady-state model used in RTO and the actual dynamic operation of the process. If the RTO model and dynamic model have very

different gains, the resulting combination can perform poorly. As in cascade control (cf. Chapter 15), the inner loop should be faster than the outer loop; otherwise poor closed-loop performance may result (Marlin and Hrymak, 1997).

19.2 THE FORMULATION AND SOLUTION OF RTO PROBLEMS

Once a process has been selected for RTO, an appropriate problem statement must be formulated and then solved. As mentioned earlier, the optimization of set points requires

1. The economic model, an objective function to be maximized or minimized, that includes costs and product values
2. The operating model, which includes a steady-state process model and all constraints on the process variables

Edgar et al. (2001) have listed six steps that should be used in solving any practical optimization problem. A summary of the procedure with comments relevant to RTO is given below.

Step 1. *Identify the process variables.* The important input and output variables for the process must be identified. These variables are employed in the objective function and the process model (see Steps 2 and 3).

Step 2. *Select the objective function.* Converting a verbal statement of the RTO goals into a meaningful objective function can be difficult. The verbal statement often contains multiple objectives and implied constraints. To arrive at a single objective function based on operating profit, the quantity and

Table 19.1   Alternative Operating Objectives for a Fluidized Catalytic Cracker (modified from Latour, 1979)

1. Maximize gasoline yield subject to a specified feed rate.
2. Minimize feed rate subject to required gasoline production.
3. Maximize conversion to light products subject to load and compressor/regenerator constraints.
4. Optimize yields subject to fixed feed conditions.
5. Maximize gasoline production with specified cycle oil production.
6. Maximize feed with fixed product distribution.
7. Maximize FCC gasoline plus olefins for alkylate.

quality of each product must be related to the consumption of utilities and the feedstock composition. The specific objective function selected may vary depending on plant configuration as well as the supply/demand situation. Table 19.1 shows different operating objectives that may arise for a fluidized catalytic cracker.

Step 3. *Develop the process model and constraints.* Steady-state process models are formulated, and operating limits for the process variables are identified. The process model can be based on the physics and chemistry of the process (see Chapter 2), or it can be based on empirical relations obtained from experimental process data (see Chapter 6). Inequality constraints arise because many physical variables, such as composition or pressure, can only have positive values, or there may be maximum temperature or maximum pressure restrictions. These inequality constraints are a key part of the optimization problem statement and can have a profound effect on the optimum operating point. In most cases, the optimum lies on a constraint.

Step 4. *Simplify the model and objective function.* Before undertaking any computation, the mathematical statement developed in steps 1–3 may be simplified to be compatible with the most effective solution techniques. A nonlinear objective function and nonlinear constraints can be linearized in order to use a fast, reliable optimization method such as linear programming.

Step 5. *Compute the optimum.* This step involves choosing an optimization technique and calculating the optimum set points. Most of the literature on the subject of optimization is concerned with this step. Over the past 20 years, much progress has been made in developing efficient and robust numerical methods for optimization calculations (Edgar et al., 2001; Griva et al., 2008; Nocedal and Wright, 2006). Virtually all optimization methods are iterative; thus a good

initial estimate of the optimum can reduce the required computer time.

Step 6. *Perform sensitivity studies.* It is useful to know which parameters in an optimization problem are the most important in determining the optimum. By varying model and cost parameters individually and recalculating the optimum, the most sensitive parameters can be identified.

Example 19.1 illustrates the six steps.

EXAMPLE 19.1

A section of a chemical plant makes two specialty products (E, F) from two raw materials (A, B) that are in limited supply. Each product is formed in a separate process as shown in Fig. 19.3. Raw materials A and B do not have to be totally consumed. The reactions involving A and B are as follows:

$$
\begin{array}{lll}
\text{Process 1:} & A + B & \rightarrow E \\
\text{Process 2:} & A + 2B & \rightarrow F
\end{array}
$$
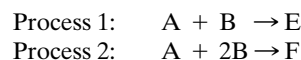
The processing cost includes the costs of utilities and supplies. Labor and other costs are \$200/day for process 1 and \$350/day for process 2. These costs occur even if the production of E or F is zero. Formulate the objective function as the total operating profit per day. List the equality and inequality constraints (Steps 1, 2, and 3).
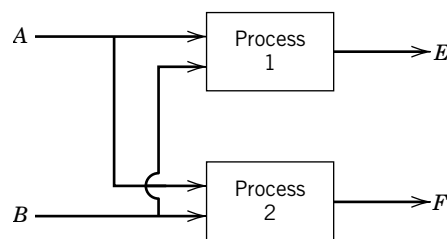

Figure 19.3 A flow diagram of a chemical plant (Example 19.1).

Available information

Raw Material	Maximum Available (lb/day)	Cost (¢/lb)
A	40,000	15
B	30,000	20

Process	Product	Reactant Requirements (lb) per lb Product	Processing Cost	Selling Price of Product	Maximum Production Level (lb/day)
1	E	2/3 A, 1/3 B	15 ¢/lb E	40 ¢/lb E	30,000
2	F	1/2 A, 1/2 B	5 ¢/lb F	33 ¢/lb F	30,000

SOLUTION

The optimization problem is formulated using the first three steps delineated above.

Step 1. The relevant process variables are the mass flow rates of reactants and products (see Fig. 19.3):

$$x_1 = \text{lb/day A consumed}$$
$$x_2 = \text{lb/day B consumed}$$
$$x_3 = \text{lb/day E produced}$$
$$x_4 = \text{lb/day F produced}$$

Step 2. In order to use Eq. 19-1 to compute the operating product per day, we need to specify product sales income, feedstock costs, and operating costs:

$$\text{Sales income (\$/day)} = \sum_s F_s V_s = 0.4x_3 + 0.33x_4 \quad (19\text{-}2)$$

$$\text{Feedstock costs (\$/day)} = \sum_r F_r C_r = 0.15x_1 + 0.2x_2 \quad (19\text{-}3)$$

$$\text{Operating costs (\$/day)} = OC = 0.15x_3 + 0.05x_4 \\ + 350 + 200 \quad (19\text{-}4)$$

Substituting into (19-1) yields the daily profit:

$$P = 0.4x_3 + 0.33x_4 - 0.15x_1 - 0.2x_2 \\ - 0.15x_3 - 0.05x_4 - 350 - 200 \\ = 0.25x_3 + 0.28x_4 - 0.15x_1 - 0.2x_2 - 550 \quad (19\text{-}5)$$

Step 3. Not all variables in this problem are unconstrained. First consider the material balance equations, obtained from the reactant requirements, which in this case comprise the process operating model:

$$x_1 = 0.667x_3 + 0.5x_4 \quad (19\text{-}6a)$$

$$x_2 = 0.333x_3 + 0.5x_4 \quad (19\text{-}6b)$$

The limits on the feedstocks and production levels are:

$$0 \le x_1 \le 40,000 \quad (19\text{-}7a)$$

$$0 \le x_2 \le 30,000 \quad (19\text{-}7b)$$

$$0 \le x_3 \le 30,000 \quad (19\text{-}7c)$$

$$0 \le x_4 \le 30,000 \quad (19\text{-}7d)$$

Equations (19-5) through (19-7) constitute the optimization problem to be solved. Because the variables appear linearly in both the objective function and constraints, this formulation is referred to as a *linear programming problem*, which is discussed in Section 19.4.

19.3 UNCONSTRAINED AND CONSTRAINED OPTIMIZATION

Unconstrained optimization refers to the situation where there are no inequality constraints and all equality constraints can be eliminated by variable substitution in the objective function. First we consider single-variable optimization, followed by optimization problems with multiple variables. Because optimization techniques are iterative in nature, we focus mainly on efficient methods that can be applied on-line. Most RTO applications are multivariable problems, which are considerably more challenging than single-variable problems.

19.3.1 Single-Variable Optimization

Some RTO problems involve determining the value of a single independent variable that maximizes (or minimizes) an objective function. Examples of single-variable optimization problems include optimizing the reflux ratio in a distillation column or the air/fuel ratio in a furnace. Optimization methods for single-variable

problems are typically based on the assumption that the objective function $f(x)$ is *unimodal* with respect to x over the region of the search. In other words, a single maximum (or minimum) occurs in this region. To use these methods, it is necessary to specify upper and lower bounds for x^{opt}, the optimum value of x, by evaluating $f(x)$ for trial values of x within these bounds and observing where $f(x)$ is a maximum (or minimum). The values of x nearest this apparent optimum are specified to be the region of the search. This region is also referred to as the *interval of uncertainty* or *bracket*, and is used to initiate the formal optimization procedure.

Efficient single-variable (or *one-dimensional*) optimization methods include Newton and quasi-Newton methods and polynomial approximation (Edgar et al., 2001). The second category includes quadratic interpolation, which utilizes three points in the interval of uncertainty to fit a quadratic polynomial to $f(x)$ over this interval. Let x_a, x_b, and x_c denote three values of x in the interval of uncertainty and f_a, f_b and f_c denote the corresponding values of $f(x)$. Then a quadratic polynomial, $\hat{f}(x) = a_0 + a_1 x + a_2 x^2$, can be fit to these data to provide a local approximation to $f(x)$. The resulting equation for $\hat{f}(x)$ can be differentiated, set equal to zero, and solved for its optimum value, which is denoted by x^*. The expression for x^* is

$$x^* = \frac{1}{2} \frac{(x_b^2 - x_c^2) f_a + (x_c^2 - x_a^2) f_b + (x_a^2 - x_b^2) f_c}{(x_b - x_c) f_a + (x_c - x_a) f_b + (x_a - x_b) f_c}$$

(19-8)

After one iteration, x^* usually is not equal to x^{opt}, because the true function $f(x)$ is not necessarily quadratic. However, x^* is expected to be an improvement over x_a, x_b, and x_c. By saving the best two of the three previous points and finding the actual objective function at x^*, the search can be continued until convergence is indicated.

EXAMPLE 19.2

A free radical reaction involving nitration of decane is carried out in two sequential reactor stages, each of which operates like a continuous stirred-tank reactor (CSTR). Decane and nitrate (as nitric acid) in varying amounts are added to each reactor stage, as shown in Fig. 19.4. The reaction of nitrate with decane is very fast and forms the following products by successive nitration: DNO_3, $D(NO_3)_2$, $D(NO_3)_3$, $D(NO_3)_4$, and so on. The desired product is DNO_3, whereas dinitrate, trinitrate, etc., are undesirable products.

The flow rates of D_1 and D_2 are chosen to satisfy temperature requirements in the reactors, while N_1 and N_2 are optimized to maximize the amount of DNO_3 produced from stage 2, subject to satisfying an overall level of nitration. In this case, we stipulate that $(N_1 + N_2)/(D_1 + D_2) = 0.4$.

There is an excess of D in each stage, and $D_1 = D_2 = 0.5$ mol/s. A steady-state reactor model has been developed to maximize selectivity. Define $r_1 \triangleq N_1/D_1$ and $r_2 \triangleq N_2/(D_1 + D_2)$. The amount of DNO_3 leaving stage 2 (as mol/s in F_2) is given by

$$f_{DNO3} = \frac{r_1 D_1}{(1 + r_1)^2(1 + r_2)} + \frac{r_2 D_2}{(1 + r_1)(1 + r_2)^2}$$

(19-9)

N_i = mol/s nitric acid (to stage i)
D_i = mol/s decane (to stage i)
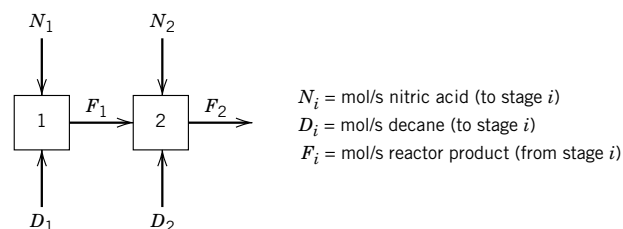F_i = mol/s reactor product (from stage i)

Figure 19.4 A schematic diagram of a two-stage nitration reactor.

This equation can be derived from the steady-state equations for a continuous stirred reactor with the assumption that all reaction rate constants are equal.

Formulate a one-dimensional search problem in r_1 that will permit the optimum values of r_1 and r_2 to be found. Employ quadratic interpolation using an initial interval of $0 \leq r_1 \leq 0.8$. Use enough iterations so that the final value of f_{DNO3} is within ± 0.0001 of the maximum.

SOLUTION

The six steps described earlier are used to formulate the optimization problem.

Step 1. *Identify the process variables.* The process variables to be optimized are N_1 and N_2, the nitric acid molar flow rates for each stage. Because D_1 and D_2 are specified, we can just as well use r_1 and r_2, because the conversion model is stated in terms of r_1 and r_2.

Step 2. *Select the objective function.* The objective is to maximize production of DNO_3 which can be made into useful products, while other nitrates cannot. We assume that the unwanted byproducts have a value of zero. The objective function f is given in (19-9). We do not need to state it explicitly as a profit function, as in Eq. 19-1, because the economic value (selling price) of DNO_3 is merely a multiplicative constant.

Step 3. *Develop models for the process and constraints.* The values of N_1 and N_2 are constrained by the overall nitration level:

$$\frac{N_1 + N_2}{D_1 + D_2} = 0.4$$

(19-10)

which can be expressed in terms of r_1 and r_2 as

$$\frac{r_1 D_1 + r_2 D_1 + r_2 D_2}{D_1 + D_2} = 0.4$$

(19-11)

Inequality constraints on r_1 and r_2 do exist, namely, $r_1 \geq 0$ and $r_2 \geq 0$—because all N_i and D_i are positive. These constraints can be ignored except when the search method incorrectly leads to negative values of r_1 or r_2.

Step 4. *Simplify the model.* Because $D_1 = D_2 = 0.5$, then, from (19-9),

$$r_2 = 0.4 - 0.5r_1 \qquad (19\text{-}12)$$

We select r_1 to be the independent variable for the one-dimensional search in Eq. 19-9, and then r_2 is a dependent variable. Because r_1 and r_2 are nonnegative, Eq. 19-12 implies that $r_1 \leq 0.8$ and $r_2 \leq 0.4$. After variable substitution, there is only one independent variable (r_1) in the objective function.

Step 5. *Compute the optimum.* Because r_1 lies between 0 and 0.8 (the interval of uncertainty), select the three interior points for the search to be $r_1 = 0.2$, 0.4, and 0.6. The corresponding values of r_2 are 0.3, 0.2, and 0.1. Table 19.2 shows the numerical results for three iterations, along with

objective function values. After the first iteration, the worst point ($r_1 = 0.2$) is discarded and the new point ($r = 0.4536$) is added. After the second iteration, the point with the lowest value of $f(r_1 = 0.6)$ is discarded. The tolerance on the objective function change is satisfied after only three iterations, with the value of r_1 that maximizes f_{DNO3} computed to be $r_1^{opt} = 0.4439$. The converted mononitrate is 0.1348 mol/s from stage 2; the remainder of the nitrate is consumed to make higher molecular weight byproducts.

Step 6. *Perform sensitivity studies.* Based on the results in Table 19.2, the yield is not significantly different from the optimum as long as $0.4 \leq r_1 \leq 0.6$. Practically speaking, this situation is beneficial, because it allows a reasonable range of decane flows to achieve temperature control. If either D_1 or D_2 changes by more than 10%, we should recalculate the optimum. There also might be a need to reoptimize r_1 and r_2 if ambient conditions change (e.g., summer vs. winter operation). Even a 1% change in yield can be economically significant if production rates and the selling price of the product are sufficiently high.

Table 19.2 Search Iterations for Example 19.2 (Quadratic Interpolation)

Iteration	x_a	f_a	x_b	f_b	x_c	f_c	x^*
1	0.2	0.1273	0.4	0.1346	0.6	0.1324	0.4536
2	0.4	0.1346	0.6	0.1324	0.4536	0.1348	0.4439
3	0.4	0.1346	0.4536	0.1348	0.4439	0.1348	(not needed)
	$r_1^{opt} = 0.4439$						

If the function to be optimized is not unimodal, then some care should be taken in applying the quadratic interpolation method. Selecting multiple starting points for the initial scanning before quadratic interpolation is initiated ensures that an appropriate search region has been selected. For a single variable search, scanning the region of search is a fairly simple and fast procedure, but evaluating the presence of multiple optima can become problematic for multivariable optimization problems.

19.3.2   Multivariable Optimization

In multivariable optimization problems, there is no guarantee that a given optimization technique will find the optimum point in a reasonable amount of computer time. The optimization of a general nonlinear multivariable objective function, $f(\boldsymbol{x}) = f(x_1, x_2, \ldots, x_{N_V})$, requires that efficient and robust numerical techniques be employed. Efficiency is important, because the solution requires an iterative approach. Trial-and-error solutions are usually out of the question for problems with more than two or three variables. For

example, consider a four-variable grid search, where an equally spaced grid for each variable is prescribed. For 10 values of each of the 4 variables, there are 10^4 total function evaluations required to find the best answer out of the 10^4 grid intersections. Even then, this computational effort may not yield a result sufficiently close to the true optimum. Grid search is a very inefficient method for multivariable optimization.

The difficulty of optimizing multivariable functions often is resolved by treating the problem as a series of single-variable (or one-dimensional) searches. From a given starting point, a search direction is specified, and then the optimum point along that direction is determined by a one-dimensional search. Then a new search direction is determined, followed by another one-dimensional search in that direction. In choosing an algorithm to determine the search direction, we can draw upon extensive numerical experience with various optimization methods (Griva et al, 2008; Nocedal and Wright, 2006; Edgar et al., 2001).

Multivariable RTO of nonlinear objective functions using function derivatives is recommended with more than two variables. In particular, the conjugate gradient
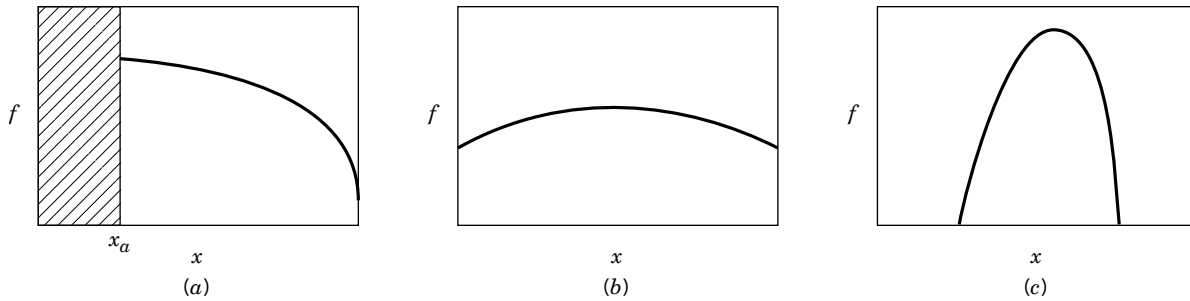
Figure 19.5 Three types of optimal operating conditions.

and quasi-Newton methods (Griva et al, 2008; Edgar et al., 2001) are extremely effective in solving such problems. Applications of multivariable RTO have experienced rapid growth as a result of advances in computer hardware and software. We consider such methods in more detail in Section 19.5.

An important application of unconstrained optimization algorithms is to update parameters in steady-state models from the available data. Usually, only a few model parameters are estimated on-line, and then RTO is based on the updated model. Guidelines for parameter estimation have been provided by Marlin and Hrymak (1997) and Forbes et al. (1994).

Most practical multivariable problems include constraints, which must be treated using enhancements of unconstrained optimization algorithms. The next two sections describe two classes of constrained optimization techniques that are used extensively in the process industries. When constraints are an important part of an optimization problem, constrained techniques must be employed, because an unconstrained method might produce an optimum that violates the constraints, leading to unrealistic values of the process variables. The general form of an optimization problem includes a nonlinear objective function (profit) and nonlinear constraints and is called a *nonlinear programming* problem.

$$\text{maximize} \quad f(x_1, x_2, \ldots, x_{N_V}) \tag{19-13}$$

$$\text{subject to:} \quad h_i(x_1, x_2, \ldots, x_{N_V}) = 0 \ (i = 1, \ldots, N_E) \tag{19-14}$$

$$g_i(x_1, x_2, \ldots, x_{N_V}) \leq 0 \ (i = 1, \ldots, N_I) \tag{19-15}$$

In this case, there are N_V process variables, N_E equality constraints and N_I inequality constraints.

Skogestad (2000) and Perkins (1998) have discussed the interplay of constraints, and the selection of the optimal operating conditions. Skogestad identified three different cases for RTO that are illustrated in Fig. 19.5. In each case, a single variable x is used to maximize a profit function, $f(x)$.

(a) *Constrained optimum:* The optimum value of the profit is obtained when $x = x_a$. Implementation of an active constraint is straightforward; for example, it is easy to keep a valve closed.

(b) *Unconstrained flat optimum:* In this case, the profit is insensitive to the value of x, and small process changes or disturbances do not affect profitability very much.

(c) *Unconstrained sharp optimum:* A more difficult problem for implementation occurs when the profit is sensitive to the value of x. If possible, we may want to select a different input variable for which the corresponding optimum is flatter, so that the operating range can be wider without reducing the profit very much.

In some cases, an actual process variable (such as yield) can be the objective function, and no process model is required. Instead, the process variables are varied systematically to find the best value of the objective function from the specific data set, sometimes involving design of experiments as discussed by Myers and Montgomery (2002). In this way, improvements in the objective function can be obtained gradually. Usually, only a few variables can be optimized in this way, and it is limited to batch operations. Methods used in industrial batch process applications include EVOP (evolutionary operation) and response surface analysis (Edwards and Jutan, 1997; Box and Draper, 1998; Myers and Montgomery, 2002).

19.4   LINEAR PROGRAMMING

An important class of constrained optimization problems has a linear objective function and linear constraints. The solution of these problems is highly structured and can be obtained rapidly via *linear programming* (LP). This powerful approach is widely used in RTO applications.

For processing plants, different types of *linear* inequality and equality constraints often arise that make the LP method of great interest. The constraints can change on a daily or even an hourly basis.

1. *Production constraints.* Equipment throughput restrictions, storage limits, or market constraints (no additional product can be sold) are frequently encountered in manufacturing. These constraints have the form of $x_i \leq c_i$ or $g_i = x_i - c_i \leq 0$ (cf. Eq. 19-15).
2. *Raw material limitations.* Feedstock supplies are frequently limited owing to supplier capability or production levels of other plants within the same company.
3. *Safety restrictions.* Common examples are limitations on operating temperature and pressure.
4. *Product specifications.* Constraints placed on the physical properties or composition of the final product fall into this category. For blends of various liquid products in a refinery, it is commonly assumed that a blend property can be calculated by averaging pure component properties. Thus, a blend of N_c components with physical property values ψ_k and volume fractions y_k (based on volumetric flow rates) has a calculated blend property of

$$\overline{\psi} = \sum_{k=1}^{N_c} \psi_k y_k \qquad (19\text{-}16)$$

If there is an upper limit α on $\overline{\psi}$, the resulting constraint is

$$\sum_{k=1}^{N_c} \psi_k y_k \leq \alpha \qquad (19\text{-}17)$$

5. *Material and energy balances.* Although items 1–4 generally are considered to be inequality constraints, the steady-state material and energy balances are equality constraints.

19.4.1 Linear Programming Concepts

For simplicity, consider a multivariable process with two inputs (u_1, u_2) and two outputs (y_1, y_2). The set of inequality constraints for $\boldsymbol{u}$ and $\boldsymbol{y}$ define an *operating window* for the process. A simple example of an operating window for a process with two inputs (to be optimized) is shown in Fig. 19.6. The upper and lower limits for u_1 and u_2 define a rectangular region. There are also upper limits for y_1 and y_2 and a lower limit for y_2. For a linear process model,

$$\boldsymbol{y} = \boldsymbol{K}\boldsymbol{u} \qquad (19\text{-}18)$$

the inequality constraints on $\boldsymbol{y}$ can be converted to constraints in $\boldsymbol{u}$, which reduces the size of the operating
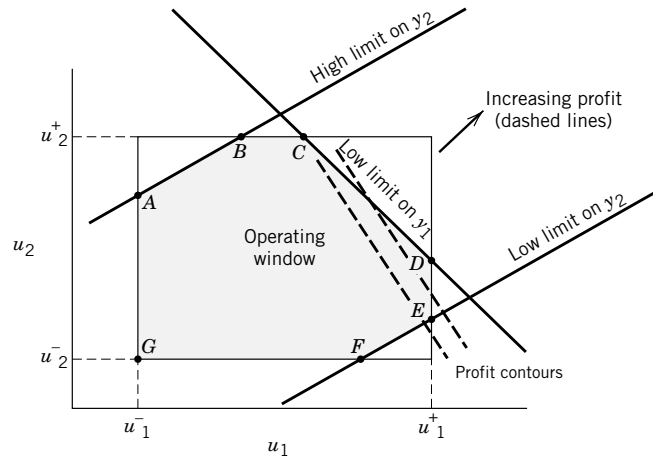

Figure 19.6 Operating window for a 2×2 optimization problem. The dashed lines are objective function contours, increasing from left to right. The maximum profit occurs where the profit line intersects the constraints at vertex D.

window to the shaded region in Fig. 19.6. If a linear cost function is selected, the optimum operating condition occurs on the boundary of the operating window at a point where constraints intersect (Griva et al, 2008; Edgar et al., 2001). These points of intersections are called vertices. Thus, in Fig. 19.6 the optimum operating point, $\boldsymbol{u}^{\mathrm{opt}}$ occurs at one of the seven vertices, points A–G. For the indicated linear profit function (dashed lines), the maximum occurs at vertex D. This graphical concept can be extended to problems with more than two inputs because the operating window is a closed convex region, providing that the process model, cost function, and inequality constraints are all linear. Using Eq. 19-18, we can calculate the optimal set points $\boldsymbol{y}_{\mathrm{sp}}$ from the value of $\boldsymbol{u}^{\mathrm{opt}}$.

The number of independent variables in a constrained optimization problem can be found by a procedure analogous to the degrees of freedom analysis in Chapter 2. For simplicity, suppose that there are no constraints. If there are N_V process variables (which includes process inputs and outputs) and the process model consists of N_E independent equations, then the number of independent variables is $N_F = N_V - N_E$. This means N_F set points can be specified independently to maximize (or minimize) the objective function. The corresponding values of the remaining ($N_V - N_F$) variables can be calculated from the process model. However, the presence of inequality constraints that can become active changes the situation, because the N_F set points cannot be selected arbitrarily. They must satisfy all of the equality and inequality constraints.

The standard linear programming (LP) problem can be stated as follows:

$$\text{minimize } f = \sum_{r=1}^{N_V} c_i x_i \qquad (19\text{-}19)$$

subject to

$$x_i \geq 0 \qquad i = 1, 2, \ldots N_V$$

$$\sum_{j=1}^{N_V} a_{ij}x_j \geq b_i \quad i = 1, 2, \ldots N_I \qquad (19\text{-}20)$$

$$\sum_{j=1}^{N_V} \tilde{a}_{ij}x_j = d_i \quad i = 1, 2, \ldots N_E \qquad (19\text{-}21)$$

The LP solution can be obtained by a method called the Simplex algorithm (Edgar et al., 2001; Griva et al., 2008). The Simplex algorithm can handle virtually any number of inequality constraints and any number of variables in the objective function (subject to computer time limitations, of course). Maximization problems can be converted to the form of (19-19) by multiplying the objective function by -1. Inequality constraints are handled by the introduction of artificial variables called *slack variables*, which convert the inequality constraints (19-20) to equality constraints by subtracting a non-negative slack variable from the left-hand side of each inequality. The slack variable then provides a measure of the distance from the constraint for a given set of variables, and these artificial variables are introduced for computational purposes. When a slack variable is zero, the constraint is active. Because there are a limited number of intersections of constraint boundaries where the optimum must occur, the amount of computer time required to search for the optimum is reduced considerably compared to more general nonlinear optimization problems. Hence, many nonlinear optimization problems (even those with nonlinear constraints) are often linearized so that the LP algorithm can be employed. This procedure allows optimization problems with over 100,000 variables to be solved.

In the 1980s, a major change in optimization software occurred when linear programming solvers and then nonlinear programming solvers were interfaced to spreadsheet software for desktop computers. The spreadsheet has become a popular user interface for entering and manipulating numeric data. Spreadsheet software increasingly incorporates analytic tools that are accessible from the spreadsheet interface and permit access to external databases. For example, Microsoft Excel incorporates an optimization-based routine called Solver that operates on the values and formulas of a spreadsheet model. Current versions (4.0 and later) include LP and NLP solvers and mixed integer programming (MIP) capability for both linear and nonlinear problems. The user specifies a set of cell addresses to be independently adjusted (the decision variables), a set of formula cells whose values are to be constrained (the constraints), and a formula cell designated as the optimization objective, as shown in the following example.

EXAMPLE 19.3

Consider a simple version of a refinery blending and production problem. This example is more illustrative of a scheduling application (Level 5 in Fig. 19.1) that has been used extensively since the 1960s in the chemical process industries. Figure 19.7 is a schematic diagram of feedstocks and products for the refinery (costs and selling prices are given in parentheses). Table 19.3 lists the information pertaining to the expected yields of the two types of crude oils when processed by the refinery. Note that the product distribution from the refinery is quite different for the two crude oils. Table 19.3 also lists the limitations on the established markets for the various products in terms of the allowed maximum daily production. In addition, processing costs are given.

To set up the linear programming problem, formulate an objective function and constraints for the refinery operation. From Fig. 19.7, six variables are involved, namely, the flow rates of the two raw materials and the four products. Solve the LP using the Excel Solver.

SOLUTION

Let the variables be

$$x_1 = \text{bbl/day of crude \#1}$$
$$x_2 = \text{bbl/day of crude \#2}$$
$$x_3 = \text{bbl/day of gasoline}$$
$$x_4 = \text{bbl/day of kerosene}$$
$$x_5 = \text{bbl/day of fuel oil}$$
$$x_6 = \text{bbl/day of residual}$$

The linear objective function f (to be maximized) is the profit, the difference between income and costs:

$$f = \text{income} - \text{raw material cost} - \text{processing cost}$$

where the following items are expressed as dollars per day:

$$\left\{ \begin{array}{l} \text{Income} = 36x_3 + 24x_4 + 21x_5 + 10x_6 \\ \text{Raw material cost} = 24x_1 + 15x_2 \\ \text{Processing cost} = 0.5x_1 + x_2 \end{array} \right\} \quad (19\text{-}22)$$

$$f = 36x_3 + 24x_4 + 21x_5 + 10x_6 - 24.5x_1 - 16x_2 \qquad (19\text{-}23)$$

The yield data provide four linear equality constraints (material balances) relating x_1 through x_6:

Gasoline:	$x_3 = 0.80x_1 + 0.44x_2$	(19-24)
Kerosene:	$x_4 = 0.05x_1 + 0.10x_2$	(19-25)
Fuel oil:	$x_5 = 0.10x_1 + 0.36x_2$	(19-26)
Residual:	$x_6 = 0.05x_1 + 0.10x_2$	(19-27)

Other constraints that exist or are implied in this problem are given in Table 19.3, which lists certain restrictions on the $\{x_i\}$ in terms of production limits. These can be formulated as inequality constraints:

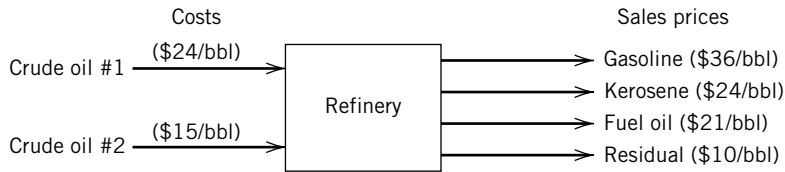|			
Gasoline:	$x_3 \leq 24{,}000$	(19-28)
Kerosene:	$x_4 \leq 2{,}000$	(19-29)
Fuel oil:	$x_5 \leq 6{,}000$	(19-30)

Figure 19.7 Refinery input and output schematic.

Table 19.3 Data for the Refinery Feeds and Products

	Volume percent yield		Maximum allowable production (bbl/day)
	Crude #1	Crude #2	
Gasoline	80	44	24,000
Kerosene	5	10	2,000
Fuel oil	10	36	6,000
Processing cost ($/bbl)	0.50	1.00	

One other set of constraints, although not explicitly stated in the formulation of the problem, is composed of the nonnegativity restrictions, namely, $x_i \geq 0$. All process variables must be zero or positive, because it is meaningless to have negative production rates.

The formal statement of the linear programming problem is now complete, consisting of Eqs. 19-23 to 19-30. We can now proceed to solve the LP problem using the Excel Solver option. The problem statement can be introduced into the spreadsheet as illustrated in the Solver Parameter dialog box in Fig. 19.8. There are four equality constraints and three inequality constraints; the first three equality constraints are shown in the dialog box in Fig. 19.8. The objective function is in the target cell A10, and the six variable cells are in cells A4–F4.

In the refinery blending problem, the optimum x obtained by Excel occurs at the intersection of the gasoline and kerosene constraints. For these active constraints, the optimum is therefore

$$x_1 = 26,207$$
$$x_2 = 6,897$$
$$x_3 = 24,000 \text{ (gasoline constraint)}$$
$$x_4 = 2,000 \text{ (kerosene constraint)}$$
$$x_5 = 5,103$$
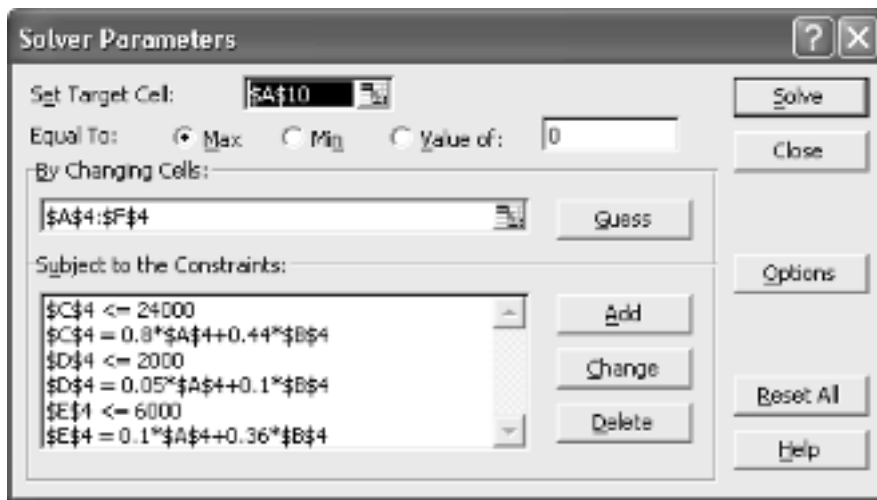$$x_6 = 2,000$$
$$f = \$286,758/\text{day}$$

Figure 19.8 Solver parameter dialog box for Example 19.3 (Refinery LP).

In the process industries, the Simplex algorithm has been applied to a wide range of problems, such as the optimization of a total plant utility system. A general steam utility configuration, typically involving as many as 100 variables and 100 constraints, can be easily optimized using linear programming (Bouilloud, 1969; Edgar et al., 2001; Marlin, 2000). The process variables can be updated on an hourly basis because

steam demands in process units can change. In addition, it may be economical to generate more electricity locally during times of peak demand, due to variable time-of-day electricity pricing by utilities. Larger LP problems are routinely solved in refineries, numbering in the thousands of variables and spanning several months of operations (Pike, 1986).

19.5   QUADRATIC AND NONLINEAR PROGRAMMING

The most general optimization problem occurs when both the objective function and constraints are nonlinear, a case referred to as *nonlinear programming* (NLP), which is stated mathematically in Eqs. 19-13 to 19-15. The leading constrained optimization methods include (Nocedal and Wright, 2006; Griva et al., 2008; Edgar et al., 2001)

1. Quadratic programming
2. Generalized reduced gradient
3. Successive quadratic programming (SQP)
4. Successive linear programming (SLP)

19.5.1   Quadratic Programming

In quadratic programming (QP), the objective function is quadratic and the constraints are linear. Although the solution is iterative, it can be as obtained as quickly as in linear programming.

A quadratic programming problem minimizes a quadratic function of n variables subject to m linear inequality or equality constraints. A convex QP is the simplest form of a nonlinear programming problem with inequality constraints. A number of practical optimization problems are naturally posed as a QP problem, such as constrained least squares and some model predictive control problems.

In compact notation, the quadratic programming problem is

$$\text{Minimize} \quad f(\boldsymbol{x}) = \boldsymbol{c}^T \boldsymbol{x} + \frac{1}{2} \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} \quad (19\text{-}31)$$

$$\text{Subject to} \quad \boldsymbol{A}\boldsymbol{x} = \boldsymbol{b} \quad (19\text{-}32)$$
$$\boldsymbol{x} \geq \boldsymbol{0}$$

where $\boldsymbol{c}$ is a vector $(n \times 1)$, $\boldsymbol{A}$ is an $m \times n$ matrix, and $\boldsymbol{Q}$ is a symmetric $n \times n$ matrix.

The equality constraint of (19-32) may contain some constraints that were originally inequalities but have been converted to equalities by introducing slack variables, as is done for LP problems. Computer codes for quadratic programming allow arbitrary upper and lower bounds on $\boldsymbol{x}$; here we assume $\boldsymbol{x} \geq \boldsymbol{0}$ for simplicity. QP software finds a solution by using LP operations to minimize the sum of constraint violations. Because LP algorithms are employed as part of the QP

calculations, most commercial LP software also contains QP solvers.

19.5.2   Nonlinear Programming Algorithms and Software

One of the older and most accessible NLP algorithms uses iterative linearization and is called the *generalized reduced gradient (GRG)* algorithm. The GRG algorithm employs linear or linearized constraints and uses slack variables to convert all constraints to equality constraints. It then develops a reduced basis by eliminating a subset of the variables, which is removed by inversion of the equalities. The gradient or search direction is then expressed in terms of this reduced basis. The GRG algorithm is used in the Excel Solver. CONOPT is a reduced gradient algorithm that works well for large-scale problems and nonlinear constraints. CONOPT and GRG work best for problems where the number of degrees of freedom is small (the number of constraints is nearly equal to the number of variables).

Successive quadratic programming (SQP) solves a sequence of quadratic programs that approach the solution of the original NLP by linearizing the constraints and using a quadratic approximation to the objective function. Lagrange multipliers are introduced to handle constraints, and the search procedure generally employs some variation of Newton's method, a second-order method that approximates the Hessian matrix using first derivatives (Biegler et al., 1997; Edgar et al., 2001). MINOS and NPSOL, software packages developed in the 1980s, are suitable for programs with large numbers of variables (more variables than equations) and constraints that are linear or nearly linear. *Successive linear programming (SLP)* is used less often for solving RTO problems. It requires linear approximations of both the objective function and constraints but sometimes exhibits poor convergence to optima that are not located at constraint intersections.

Software libraries such as GAMS (General Algebraic Modeling System) or NAG (Numerical Algorithms Group) offer one or more NLP algorithms, but rarely are all algorithms available from a single source. No single NLP algorithm is best for every problem, so several solvers should be tested on a given application. See Nocedal and Wright (2006) for more details on available software.

All of the NLP methods have been utilized to solve nonlinear programming problems in the field of chemical engineering design and operations. Although in the following example we illustrate the use of GRG in the Excel Solver, large-scale NLP problems in RTO are more frequently solved using SQP owing to its superior ability in handling a large number of active constraints.

EXAMPLE 19.4

Consider the problem of minimizing fuel costs in a boiler-house. The boilerhouse contains two turbine generators, each of which can be simultaneously operated with two fuels: fuel oil and medium Btu gas (MBG); see Fig. 19.9. The MBG is produced as a waste off-gas from another part of the plant, and it must be flared if it cannot be used on-site. The goal of the RTO scheme is to find the optimum flow rates of fuel oil and MBG and provide 50 MW of power at all times, so that steady-state operations can be maintained while minimizing costs. It is desirable to use as much of the MBG as possible (which has zero cost) while minimizing consumption of expensive fuel oil. The two turbine generators (G1, G2) have different operating characteristics; the efficiency of G1 is higher than that of G2.

Data collected on the fuel requirements for the two generators yield the following empirical relations:

$$P_1 = 4.5x_1 + 0.1x_1^2 + 4.0x_2 + 0.06x_2^2 \qquad (19\text{-}33)$$
$$P_2 = 4.0x_3 + 0.05x_3^2 + 3.5x_4 + 0.02x_4^2 \qquad (19\text{-}34)$$

where

P_1 = power output (MW) from G1
P_2 = power output (MW) from G2
x_1 = fuel oil to G1 (tons/h)
x_2 = MBG to G1 (fuel units/h)
x_3 = fuel oil to G2 (tons/h)
x_4 = MBG to G2 (fuel units/h)

The total amount of MBG available is 5 fuel units/h. Each generator is also constrained by minimum and maximum power outputs: generator 1 output must lie between 18 and 30 MW, while generator 2 can operate between 14 and 25 MW.

Formulate the optimization problem by applying the methodology described in Section 19.2. Then solve for the optimum operating conditions $(x_1, x_2, x_3, x_4, P_1, P_2)$ using the Excel Solver.
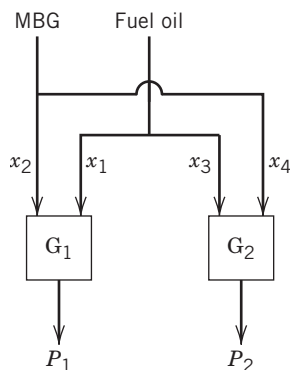

MBG   Fuel oil

x_2 x_1 x_3 x_4

G_1 G_2

P_1 P_2

Figure 19.9 The allocation of two fuels in a boilerhouse with two turbine generators (G_1, G_2).

SOLUTION

Step 1. *Identify the variables.* Use x_1 through x_4 as the four process variables. Variables P_1 and P_2 are dependent because of the equality constraints (see Steps 3 and 4).

Step 2. *Select the objective function.* The way to minimize the cost of operation is to minimize the amount of fuel oil consumed. This implies that we should use as much MBG as possible, because it has zero cost. The objective function can be stated in terms of variables defined above; that is, we wish to minimize

$$f = x_1 + x_3 \qquad (19\text{-}35)$$

Step 3. *Specify process model and constraints.* The constraints given in the problem statement are as follows:

(1) Power relations

$$P_1 = 4.5x_1 + 0.1x_1^2 + 4.0x_2 + 0.06x_2^2 \qquad (19\text{-}33)$$
$$P_2 = 4.0x_3 + 0.05x_3^2 + 3.5x_4 + 0.2x_4^2 \qquad (19\text{-}34)$$

(2)   Power range $18 \le P_1 \le 30$ $(19\text{-}36)$

$14 \le P_2 \le 25$ $(19\text{-}37)$

(3)   Total power $50 = P_1 + P_2$ $(19\text{-}38)$

(4)   MBG supply $5 = x_2 + x_4$ $(19\text{-}39)$

Note that all variables defined above are nonnegative.

Step 4. *Simplify the model and objective function.* Although there are two independent variables in this problem (six variables and four equality constraints), there is no need to carry out variable substitution or further simplification, because the Excel Solver can easily handle the solution of this fairly small NLP problem.

Step 5. *Compute the optimum.* The Solver dialog box is shown in Fig. 19.10. The objective function value is in the target cell of the spreadsheet, written as a function of $x_1 - x_4$ (Eq. 19-35). These four variables are changed in the series of cells A4–D4. The constraints shown above are expressed in cells B12, B9, E12, and E9.

At the optimum $f = 6.54$, $x_1 = 1.82$, and $x_3 = 4.72$, meaning that 1.82 tons/h of fuel oil are delivered to generator G1, while 4.72 tons/h are used in G2. G1 utilizes all of the MBG (x_2), while G2 uses none ($x_4 = 0$), due to its lower efficiency with MBG.

Step 6. *Perform a sensitivity analysis.* Many operating strategies may be satisfactory, though not optimal, for the above problem. The procedure discussed above can also be repeated if parameters in the original constraint equations are changed as plant operating conditions vary. For example, suppose the total power requirement is changed to 55 MW; as an exercise, determine whether any of the active constraints change for the increased power requirement.
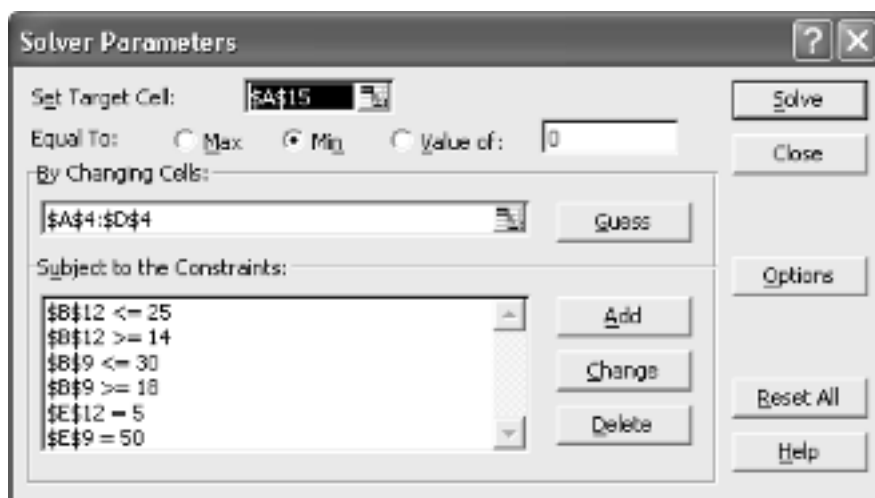
Figure 19.10 Excel Solver parameter dialog box.

SUMMARY

Although the economic benefits from feedback control are not always readily quantifiable, RTO offers a direct method of maximizing the steady-state profitability of a process or group of processes. The optimization of the set points is performed as frequently as necessary, depending on changes in operating conditions or constraints. It is important to formulate the optimization problem carefully; a methodology for formulation and solution of optimization problems is presented in this chapter. A wide range of optimization techniques can be used, depending on (1) the number of variables, (2) the nature of the equality and inequality constraints, and (3) the nature of the objective function. Because we have presented only introductory concepts in optimization here, the reader is advised to consult other comprehensive references on optimization such as Edgar et al. (2001) before choosing a particular method for RTO.

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EXERCISES

19.1 A laboratory filtration study has been carried out at constant rate. The filtration time (t_f in hours) required to build up a specific cake thickness has been correlated as

$$t_f = 5.3 \, x_i e^{-3.6 x_i + 2.7}$$

where x_i = mass fraction solids in the cake. Find the value of x_i that maximizes t_f using quadratic interpolation.

19.2 The thermal efficiency of a natural gas boiler versus air/fuel ratio is plotted in Fig. E19.2. Using physical arguments, explain why a maximum occurs.
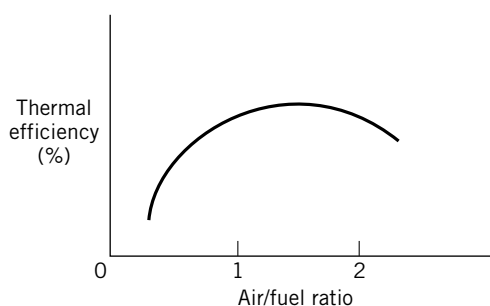

Figure E19.2

19.3 A plasma etcher has a yield of good chips that is influenced by pressure (X_1) and gas flow rate (X_2). Both X_1 and X_2 are scaled variables ($0 \le X_i \le 2$). A model has been developed based on operating data as follows:

$$Y = -0.1X_1^4 + 0.2X_2X_1^2 - 0.09X_2^2 - 0.11X_1^2 + 0.15X_1 + 0.5$$

Use Excel to maximize yield Y, using starting points of (1,1) and (0,0).

19.4 A specialty chemical is produced in a batch reactor. The time required to successfully complete one batch of product depends on the amount charged to (and produced from) the reactor. Using reactor data, a correlation is $t = 2.0P^{0.4}$, where P is the amount of product in pounds per batch and t is given in hours. A certain amount of nonproduction time is associated with each batch for charging, discharging, and minor maintenance, namely, 14 h/batch. The operating cost for the batch system is $50/h. Other costs, including storage, depend on the size of each batch and have been estimated to be C_1 = $800 $P^{0.7}$($/yr). The required annual production is 300,000 lb/yr, and the process can be operated 320 days/yr (24 h/day). Total raw material cost at this production level is $400,000/yr.

(a) Formulate an objective function using P as the only variable. (Show algebraic substitution.)

(b) What are the constraints on P?

(c) Solve for the optimum value of P analytically. Check that it is a minimum. Also check applicable constraints.

19.5 A refinery processes two crude oils that have the yields shown in the following table. Because of equipment and storage limitations, production of gasoline, kerosene, and fuel oil must be limited as shown below. There are no plant limitations on the production of other products such as gas oils. The profit on processing crude No. 1 is $2.00/bbl, and on crude No. 2 it is $1.40/bbl. Find the optimum daily feed rates of the two crudes to this plant via linear programming using the Excel Solver.

Yields (Volume %)		
	Crude No. 1	Crude No. 2	Maximum Allowable Production Rate (bbl/day)
Gasoline	70	31	6,000
Kerosene	6	9	2,400
Fuel oil	24	60	12,000

19.6 Linear programming is to be used to optimize the operation of the solvent splitter column shown in Fig. E19.6. The feed is naphtha, which has a value of $40/bbl in its alternate use as a gasoline blending stock. The light ends sell at $50/bbl, while the bottoms are passed through a second distillation column to yield two solvents. A medium solvent comprising 50 to 70% of the bottoms can be sold for $70/bbl., while the remaining heavy solvent (30 to 50% of the bottoms) can be sold for $40/bbl.

Another part of the plant requires 200 bbl/day of medium solvent; an additional 200 bbl/day can be sold to an external market. The maximum feed that can be processed in column 1 is 2,000 bbl/day. The operational cost (i.e., utilities) associated
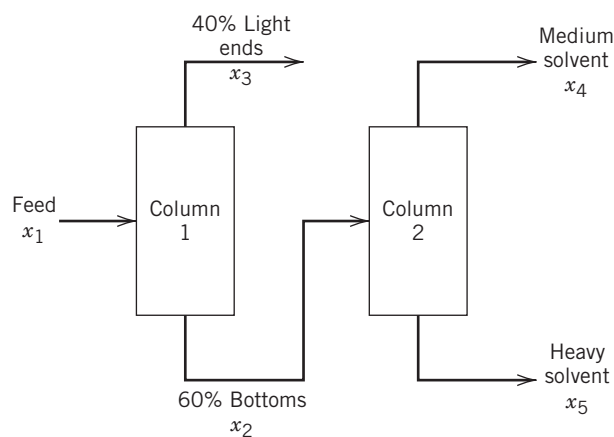
Figure E19.6

with each distillation column is $2.00/bbl feed. The operating range for column 2 is given as the percentage split of medium and heavy solvent. Solve the linear programming problem to determine the maximum revenue and percentages of output streams in column 2.

19.7 Reconciliation of inaccurate process measurements is an important problem in process control that can be solved using optimization techniques. The flow rates of streams B and C have been measured three times during the current shift (shown in Fig. E19.7). Some errors in the measurement devices exist. Assuming steady-state operation (w_A = constant), find the optimal value of w_A (flow rate in kg/h) that minimizes the sum of the squares of the errors for the material balance, $w_A + w_C = w_B$.
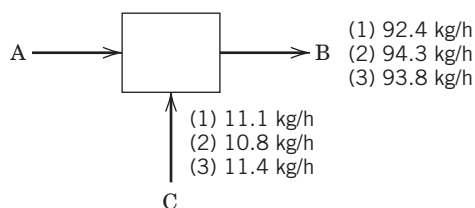

Figure E19.7

19.8 A reactor converts reactant BC to product CB by heating the material in the presence of an additive A (mole fraction = x_A). The additive can be injected into the reactor, while steam can be injected into a heating coil inside the reactor to provide heat. Some conversion can be obtained by heating without addition of A, and vice versa. The product CB can be sold for $50 per lb-mol. For 1 lb-mol of feed, the cost of the additive (in dollars per lb-mol feed) as a function of x_A is given by the formula $2.0 + 10x_A + 20x_A^2$. The cost of the steam (in dollars per lb-mol feed) as a function of S is $1.0 + 0.003S + 2.0 \times 10^{-6}S^2$ (S = lb steam/lb-mol feed). The yield equation is $y_{CB} = 0.1 + 0.3x_A + 0.0001S - 0.0001x_A S$.

$$y_{CB} = \frac{\text{lb-mol product CB}}{\text{lb-mol feed}}$$

(a) Formulate the profit function (basis of 1.0 lb-mol feed) in terms of x_A and S.

$$f = \text{income} - \text{costs}$$

(b) Maximize f subject to the constraints

$$0 \le x_A \le 1 \quad S \ge 0$$

19.9 Optimization methods can be used to fit equations to data. Parameter estimation involves the computation of unknown parameters that minimize the squared error between data and the proposed mathematical model. The step response of an overdamped second-order dynamic process can be described using the equation

$$\frac{y(t)}{K} = \left(1 - \frac{\tau_1 e^{-t/\tau_1} - \tau_2 e^{-t/\tau_2}}{\tau_1 - \tau_2}\right)$$

where τ_1 and τ_2 are process time constants and K is the process gain.

The following normalized data have been obtained from a unit step test (K is equal to $y(\infty)$):

time, t	0	1	2	3	4	5
y_i/K	0.0	0.0583	0.2167	0.360	0.488	0.600
t	6	7	8	9	10	
y_i/K	0.692	0.772	0.833	0.888	0.925	

Use Excel with a starting point (1,0) to find values of τ_1 and τ_2 that minimize the sum of squares of the errors. Compare your answer with that obtained using MATLAB.

19.10 A brewery has the capability of producing a range of beers by blending existing stocks. Two beers (suds and premium) are currently available, with alcohol concentrations of 3.5% for suds and 5.0% for premium. The manufacturing cost for suds is $0.25/gal, and for premium it is $0.40/gal. In making blends, water can be added at no cost. An order for 10,000 gal of beer at 4.0% has been received for this week. There is a limited amount of suds available (9,000 gal), and, because of aging problems, the brewery must use at least 2,000 gal of suds this week. What amounts of suds, premium, and water must be blended to fill the order at minimum cost?

19.11 A specialty chemicals facility manufactures two products A and B in barrels. Products A and B utilize the same raw material; A uses 120 kg/bbl, while B requires 100 kg/bbl. There is an upper limit on the raw material supply of 9,000 kg/day. Another constraint is warehouse storage space (40 m² total; both A and B require 0.5 m²/bbl). In addition, production time is limited to 7 h per day. A and B can be produced at 20 bbl/h and 10 bbl/h, respectively. If the profit per bbl is $10 for A and $14 for B, find the production levels that maximize profit.

19.12 Supervisory control often involves the optimization of set points in order to maximize profit. Can the same results be achieved by optimizing PID controller tuning (K_c, τ_I, τ_D), in order to maximize profits? Are regulatory (feedback) control and supervisory control complementary?

19.13 A dynamic model of a continuous-flow, biological chemostat has the form

$$\dot{X} = 0.063\,C - D\,x$$
$$\dot{C} = 0.9\,S\,[\,X - C\,] - 0.7\,C - D\,C$$
$$\dot{S} = -0.9\,S\,[\,X - C\,] + D\,[\,10 - S\,]$$

where X is the biomass concentration, S is the substrate concentration, and C is a metabolic intermediate concentration. The dilution rate, D, is an independent variable, which is defined to be the flow rate divided by the chemostat volume.

Determine the value of D, which maximizes the steady-state production rate of biomass, f, given by

$$f = DX$$

19.14 A reversible chemical reaction, $A \rightleftarrows B$, occurs in the isothermal continuous stirred-tank reactor shown in Fig. E19.14. The rate expressions for the forward and reverse reactions are

$$r_1 = k_1 C_A$$
$$r_2 = k_2 C_B$$

Using the information given below, use a numerical search procedure to determine the value of F_B (L/h) that maximizes the production rate of C_B (i.e., the amount of C_B that leaves the reactor, mol B/h). The allowable values of F_B are $0 \le F_B \le 200$ L/h.
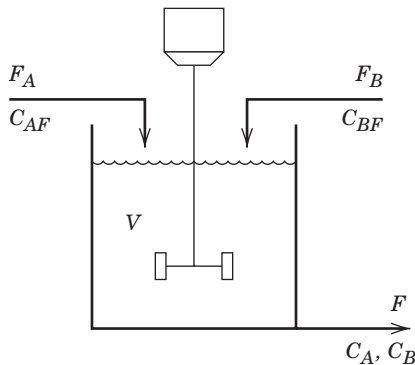

Figure E19.14

Available information

 (i) The reactor is perfectly mixed.
 (ii) The volume of liquid, V, is maintained constant using an overflow line (not shown in the diagram).
(iii) The following parameters are kept constant at the indicated numerical values:

$$V = 200 \text{ L} \qquad F_A = 150 \text{ L/h}$$
$$C_{AF} = 0.3 \text{ mol A/L} \quad C_{BF} = 0.3 \text{ mol B/L}$$
$$k_1 = 2\text{h}^{-1} \qquad k_2 = 1.5 \text{ h}^{-1}$$

19.15 A reversible chemical reaction, $A \rightleftarrows B$, occurs in the isothermal continuous stirred-tank reactor shown in Fig. E19.14. The rate expressions for the forward and reverse reactions are

$$r_1 = k_1 C_A \qquad r_2 = k_2 C_B$$

where the rate constants have the following temperature dependence:

$$k_1 = 3.0 \times 10^6 \exp(-5000/T)$$
$$k_2 = 6.0 \times 10^6 \exp(-5500/T)$$

Each rate constant has units of h^{-1}, and T is in K.

Use the MATLAB Optimization Toolbox or Excel to determine the optimum values of temperature $T(K)$ and flow rate F_B (L/h) that maximize the steady-state production rate of component B. The allowable values are $0 \le F_B \le 200$ and $300 \le T \le 500$.

Available information

 (i) The reactor is perfectly mixed.
 (ii) The volume of liquid, V, is maintained constant using an overflow line (not shown in the diagram).
(iii) The following parameters are kept constant at the indicated numerical values:

$$V = 200 \text{ L} \qquad F_A = 150 \text{ L/h}$$
$$C_{AF} = 0.3 \text{ mol A/L} \quad C_{BF} = 0.3 \text{ mol B/L}$$