PART I

PROBLEM FORMULATION

Formulating the problem is perhaps the most crucial step in optimization. Problem formulation requires identifying the essential elements of a conceptual or verbal statement of a given application and organizing them into a prescribed mathematical form, namely,

1. The objective function (economic criterion)
2. The process model (constraints)

The objective function represents such factors as profit, cost, energy, and yield in terms of the key variables of the process being analyzed. The process model and constraints describe the interrelationships of the key variables. It is important to learn a systematic approach for assembling the physical and empirical relations and data involved in an optimization problem, and Chapters 1, 2, and 3 cover the recommended procedures. Chapter 1 presents six steps for optimization that can serve as a general guide for problem solving in design and operations analysis. Numerous examples of problem formulation in chemical engineering are presented to illustrate the steps.

Chapter 2 summarizes the characteristics of process models and explains how to build one. Special attention is focused on developing mathematical models, particularly empirical ones, by fitting empirical data using least squares, which itself is an optimization procedure.

Chapter 3 treats the most common type of objective function, the cost or revenue function. Historically, the majority of optimization applications have involved trade-offs between capital costs and operating costs. The nature of the trade-off depends on a number of assumptions such as the desired rate of return on investment, service life, depreciation method, and so on. While an objective function based on net present value is preferred for the purposes of optimization, discounted cash flow based on spreadsheet analysis can be employed as well.

It is important to recognize that many possible mathematical problem formulations can result from an engineering analysis, depending on the assumptions made and the desired accuracy of the model. To solve an optimization problem, the mathematical formulation of the model must mesh satisfactorily with the computational algorithm to be used. A certain amount of artistry, judgment, and experience is therefore required during the problem formulation phase of optimization.

1

THE NATURE AND ORGANIZATION OF OPTIMIZATION PROBLEMS

OPTIMIZATION IS THE use of specific methods to determine the most cost-effective and efficient solution to a problem or design for a process. This technique is one of the major quantitative tools in industrial decision making. A wide variety of problems in the design, construction, operation, and analysis of chemical plants (as well as many other industrial processes) can be resolved by optimization. In this chapter we examine the basic characteristics of optimization problems and their solution techniques and describe some typical benefits and applications in the chemical and petroleum industries.

1.1 WHAT OPTIMIZATION IS ALL ABOUT

A well-known approach to the principle of optimization was first scribbled centuries ago on the walls of an ancient Roman bathhouse in connection with a choice between two aspirants for emperor of Rome. It read—"De doubus malis, minus est semper aligendum"—of two evils, always choose the lesser.

Optimization pervades the fields of science, engineering, and business. In physics, many different optimal principles have been enunciated, describing natural phenomena in the fields of optics and classical mechanics. The field of statistics treats various principles termed "maximum likelihood," "minimum loss," and "least squares," and business makes use of "maximum profit," "minimum cost," "maximum use of resources," "minimum effort," in its efforts to increase profits. A typical engineering problem can be posed as follows: A process can be represented by some equations or perhaps solely by experimental data. You have a single performance criterion in mind such as minimum cost. The goal of optimization is to find the values of the variables in the process that yield the best value of the performance criterion. A trade-off usually exists between capital and operating costs. The described factors—process or model and the performance criterion—constitute the optimization "problem."

Typical problems in chemical engineering process design or plant operation have many (possibly an infinite number) solutions. Optimization is concerned with selecting the best among the entire set by efficient quantitative methods. Computers and associated software make the necessary computations feasible and cost-effective. To obtain useful information using computers, however, requires (1) critical analysis of the process or design, (2) insight about what the appropriate performance objectives are (i.e., what is to be accomplished), and (3) use of past experience, sometimes called engineering judgment.

1.2 WHY OPTIMIZE?

Why are engineers interested in optimization? What benefits result from using this method rather than making decisions intuitively? Engineers work to improve the initial design of equipment and strive to enhance the operation of that equipment once it is installed so as to realize the largest production, the greatest profit, the minimum cost, the least energy usage, and so on. Monetary value provides a convenient measure of different but otherwise incompatible objectives, but not all problems have to be considered in a monetary (cost versus revenue) framework.

In plant operations, benefits arise from improved plant performance, such as improved yields of valuable products (or reduced yields of contaminants), reduced energy consumption, higher processing rates, and longer times between shutdowns. Optimization can also lead to reduced maintenance costs, less equipment wear, and better staff utilization. In addition, intangible benefits arise from the interactions among plant operators, engineers, and management. It is extremely helpful to systematically identify the objective, constraints, and degrees of freedom in a process or a plant, leading to such benefits as improved quality of design, faster and more reliable troubleshooting, and faster decision making.

Predicting benefits must be done with care. Design and operating variables in most plants are always coupled in some way. If the fuel bill for a distillation column is $3000 per day, a 5-percent savings may justify an energy conservation project. In a unit operation such as distillation, however, it is incorrect to simply sum the heat exchanger duties and claim a percentage reduction in total heat required. A reduction in the reboiler heat duty may influence both the product purity, which can translate to a change in profits, and the condenser cooling requirements. Hence, it may be misleading to ignore the indirect and coupled effects that process variables have on costs.

What about the argument that the formal application of optimization is really not warranted because of the uncertainty that exists in the mathematical representation of the process or the data used in the model of the process? Certainly such an argument has some merit. Engineers have to use judgment in applying optimization techniques to problems that have considerable uncertainty associated with them, both from the standpoint of accuracy and the fact that the plant operating parameters and environs are not always static. In some cases it may be possible to carry out an analysis via deterministic optimization and then add on stochastic features to the analysis to yield quantitative predictions of the degree of uncertainty. Whenever the model of a process is idealized and the input and parameter data only known approximately, the optimization results must be treated judiciously. They can provide upper limits on expectations. Another way to evaluate the influence of uncertain parameters in optimal design is to perform a sensitivity analysis. It is possible that the optimum value of a process variable is unaffected by certain parameters (low sensitivity); therefore, having precise values for these parameters will not be crucial to finding the true optimum. We discuss how a sensitivity analysis is performed later on in this chapter.

1.3 SCOPE AND HIERARCHY OF OPTIMIZATION

Optimization can take place at many levels in a company, ranging from a complex combination of plants and distribution facilities down through individual plants, combinations of units, individual pieces of equipment, subsystems in a piece of equipment, or even smaller entities (Beveridge and Schechter, 1970). Optimization problems can be found at all these levels. Thus, the scope of an optimization problem can be the entire company, a plant, a process, a single unit operation, a single piece of equipment in that operation, or any intermediate system between these. The complexity of analysis may involve only gross features or may examine minute detail, depending upon the use to which the results will be put, the availability of accurate data, and the time available in which to carry out the optimization. In a typical industrial company optimization can be used in three areas (levels): (1) management, (2) process design and equipment specification, and (3) plant operations (see Fig. 1.1).

Management makes decisions concerning project evaluation, product selection, corporate budget, investment in sales versus research and development, and new plant construction (i.e., when and where should new plants be constructed). At this level much of the available information may be qualitative or has a high degree of uncertainty. Many management decisions for optimizing some feature(s) of a large company therefore have the potential to be significantly in error when put into practice, especially if the timing is wrong. In general, the magnitude of the objective function, as measured in dollars, is much larger at the management level than at the other two levels.

Individuals engaged in process design and equipment specification are concerned with the choice of a process and nominal operating conditions. They answer questions such as: Do we design a batch process or a continuous process? How many reactors do we use in producing a petrochemical? What should the configurations of the plant be, and how do we arrange the processes so that the operating efficiency of the plant is at a maximum? What is the optimum size of a unit or combination of units? Such questions can be resolved with the aid of so-called process

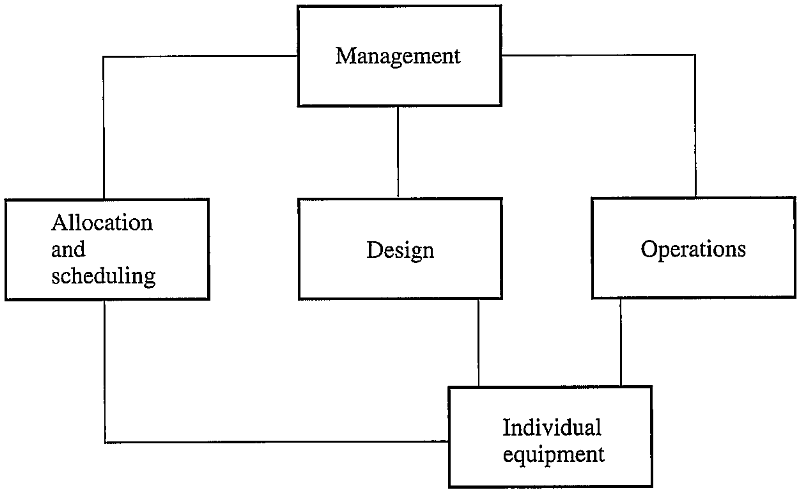

FIGURE 1.1
Hierarchy of levels of optimization.

design simulators or flowsheeting programs. These large computer programs carry out the material and energy balances for individual pieces of equipment and combine them into an overall production unit. Iterative use of such a simulator is often necessary to arrive at a desirable process flowsheet.

Other, more specific decisions are made in process design, including the actual choice of equipment (e.g., more than ten different types of heat exchangers are available) and the selection of construction materials of various process units.

The third constituency employing optimization operates on a totally different time scale than the other two. Process design and equipment specification is usually performed prior to the implementation of the process, and management decisions to implement designs are usually made far in advance of the process design step. On the other hand, optimization of operating conditions is carried out monthly, weekly, daily, hourly, or even, at the extreme, every minute. Plant operations are concerned with operating controls for a given unit at certain temperatures, pressures, or flowrates that are the best in some sense. For example, the selection of the percentage of excess air in a process heater is critical and involves balancing the fuel–air ratio to ensure complete combustion while making the maximum use of the heating potential of the fuel.

Plant operations deal with the allocation of raw materials on a daily or weekly basis. One classical optimization problem, which is discussed later in this text, is the allocation of raw materials in a refinery. Typical day-to-day optimization in a plant minimizes steam consumption or cooling water consumption.

Plant operations are also concerned with the overall picture of shipping, transportation, and distribution of products to engender minimal costs. For example, the frequency of ordering, the method of scheduling production, and scheduling delivery are critical to maintaining a low-cost operation.

The following attributes of processes affecting costs or profits make them attractive for the application of optimization:

1. *Sales limited by production*: If additional products can be sold beyond current capacity, then economic justification of design modifications is relatively easy. Often, increased production can be attained with only slight changes in operating costs (raw materials, utilities, etc.) and with no change in investment costs. This situation implies a higher profit margin on the incremental sales.
2. *Sales limited by market*: This situation is susceptible to optimization only if improvements in efficiency or productivity can be obtained; hence, the economic incentive for implementation in this case may be less than in the first example because no additional products are made. Reductions in unit manufacturing costs (via optimizing usage of utilities and feedstocks) are generally the main targets.
3. *Large unit throughputs*: High production volume offers great potential for increased profits because small savings in production costs per unit are greatly magnified. Most large chemical and petroleum processes fall into this classification.
4. *High raw material or energy consumption*: Significant savings can be made by reducing consumption of those items with high unit costs.

5. *Product quality exceeds product specifications*: If the product quality is significantly better than that required by the customer, higher than necessary production costs and wasted capacity may occur. By operating close to customer specification (constraints), cost savings can be obtained.
6. *Losses of valuable components through waste streams*: The chemical analysis of various plant exit streams, both to the air and water, should indicate if valuable materials are being lost. Adjustment of air–fuel ratios in furnaces to minimize hydrocarbon emissions and hence fuel consumption is one such example. Pollution regulations also influence permissible air and water emissions.
7. *High labor costs*: In processes in which excessive handling is required, such as in batch operation, bulk quantities can often be handled at lower cost and with a smaller workforce. Revised layouts of facilities can reduce costs. Sometimes no direct reduction in the labor force results, but the intangible benefits of a lessened workload can allow the operator to assume greater responsibility.

Two valuable sources of data for identifying opportunities for optimization include (1) profit and loss statements for the plant or the unit and (2) the periodic operating records for the plant. The profit and loss statement contains much valuable information on sales, prices, manufacturing costs, and profits, and the operating records present information on material and energy balances, unit efficiencies, production levels, and feedstock usage.

Because of the complexity of chemical plants, complete optimization of a given plant can be an extensive undertaking. In the absence of complete optimization we often rely on "incomplete optimization," a special variety of which is termed *suboptimization*. Suboptimization involves optimization for one phase of an operation or a problem while ignoring some factors that have an effect, either obvious or indirect, on other systems or processes in the plant. Suboptimization is often necessary because of economic and practical considerations, limitations on time or personnel, and the difficulty of obtaining answers in a hurry. Suboptimization is useful when neither the problem formulation nor the available techniques permits obtaining a reasonable solution to the full problem. In most practical cases, suboptimization at least provides a rational technique for approaching an optimum.

Recognize, however, that suboptimization of all elements does *not* necessarily ensure attainment of an overall optimum for the *entire* system. Subsystem objectives may not be compatible nor mesh with overall objectives.

1.4 EXAMPLES OF APPLICATIONS OF OPTIMIZATION

Optimization can be applied in numerous ways to chemical processes and plants. Typical projects in which optimization has been used include

1. Determining the best sites for plant location.
2. Routing tankers for the distribution of crude and refined products.
3. Sizing and layout of a pipeline.
4. Designing equipment and an entire plant.

5. Scheduling maintenance and equipment replacement.
6. Operating equipment, such as tubular reactors, columns, and absorbers.
7. Evaluating plant data to construct a model of a process.
8. Minimizing inventory charges.
9. Allocating resources or services among several processes.
10. Planning and scheduling construction.

These examples provide an introduction to the types of variables, objective functions, and constraints that will be encountered in subsequent chapters.

In this section we provide four illustrations of "optimization in practice." that is, optimization of process operations and design. These examples will help illustrate the general features of optimization problems, a topic treated in more detail in Section 1.5.

EXAMPLE 1.1 OPTIMAL INSULATION THICKNESS

Insulation design is a classic example of overall cost saving that is especially pertinent when fuel costs are high. The addition of insulation should save money through reduced heat losses; on the other hand, the insulation material can be expensive. The amount of added insulation needed can be determined by optimization.

Assume that the bare surface of a vessel is at 700°F with an ambient temperature of 70°F. The surface heat loss is 4000 Btu/(h)(ft^2). Add 1 in. of calcium silicate insulation and the loss will drop to 250 Btu/(h)(ft^2). At an installed cost of \$4.00 ft^2 and a cost of energy at \$5.00/10^6 Btu, a savings of \$164 per year (8760 hours of operation) per square foot would be realized. A simplified payback calculation shows a payback period of

$$\frac{\$4.00/(\text{ft}^2)}{\$164/(\text{ft}^2)(\text{year})} = 0.0244 \text{ year, or 9 days}$$

As additional inches of insulation are added, the increments must be justified by the savings obtained. Figure E1.1 shows the outcome of adding more layers of insulation. Since insulation can only be added in 0.5-in. increments, the possible capital costs are shown as a series of dots; these costs are prorated because the insulation lasts for several years before having to be replaced. In Figure E1.1 the energy loss cost is a continuous curve because it can be calculated directly from heat transfer principles. The total cost is also shown as a continuous function. Note that at some point total costs begin increasing as the insulation thickness increases because little or no benefit in heat conservation results. The trade-off between energy cost and capital cost, and the optimum insulation thickness, can be determined by optimization. Further discussion of capital versus operating costs appears in Chapter 3; in particular, see Example 3.3.

EXAMPLE 1.2 OPTIMAL OPERATING CONDITIONS OF A BOILER

Another example of optimization can be encountered in the operation of a boiler. Engineers focus attention on utilities and powerhouse operations within refineries and

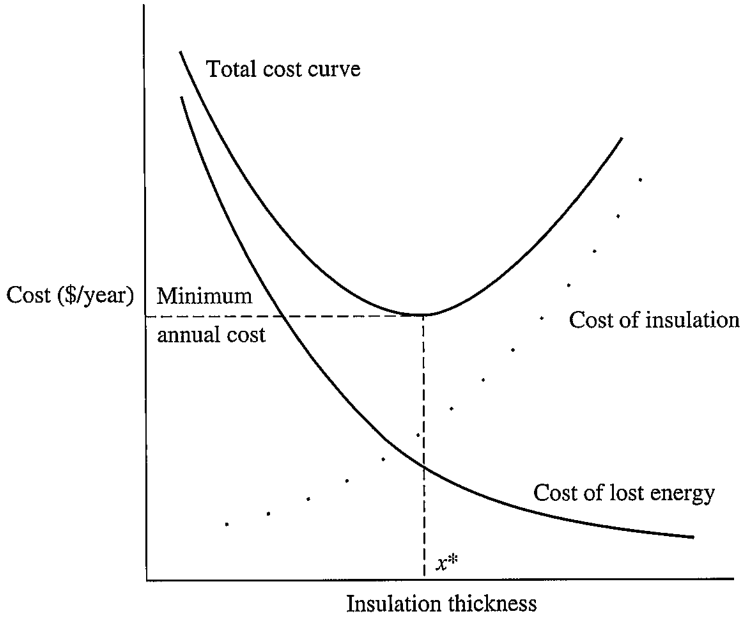

FIGURE E1.1
The effect of insulation thickness on total cost (x^* = optimum thickness). Insulation can be purchased in 0.5-in. increments. (The total cost function is shown as a smooth curve for convenience, although the sum of the two costs would not actually be smooth.)

process plants because of the large amounts of energy consumed by these plants and the potential for significant reduction in the energy required for utilities generation and distribution. Control of environmental emissions adds complexity and constraints in optimizing boiler operations. In a boiler it is desirable to optimize the air–fuel ratio so that the thermal efficiency is maximized; however, environmental regulations encourage operation under fuel-rich conditions and lower combustion temperatures in order to reduce the emissions of nitrogen oxides (NO_x). Unfortunately, such operating conditions also decrease efficiency because some unburned fuel escapes through the stacks, resulting in an increase in undesirable hydrocarbon (HC) emissions. Thus, a conflict in operating criteria arises.

Figure E1.2*a* illustrates the trade-offs between efficiency and emissions, suggesting that more than one performance criterion may exist: We are forced to consider maximizing efficiency versus minimizing emissions, resulting in some compromise of the two objectives.

Another feature of boiler operations is the widely varying demands caused by changes in process operations, plant unit start-ups and shutdowns, and daily and seasonal cycles. Because utility equipment is often operated in parallel, demand swings commonly affect when another boiler, turbine, or other piece of equipment should be brought on line and which one it should be.

Determining this is complicated by the feature that most powerhouse equipment cannot be operated continuously all the way down to the idle state, as illustrated by Figure E1.2*b* for boilers and turbines. Instead, a range of continuous operation may

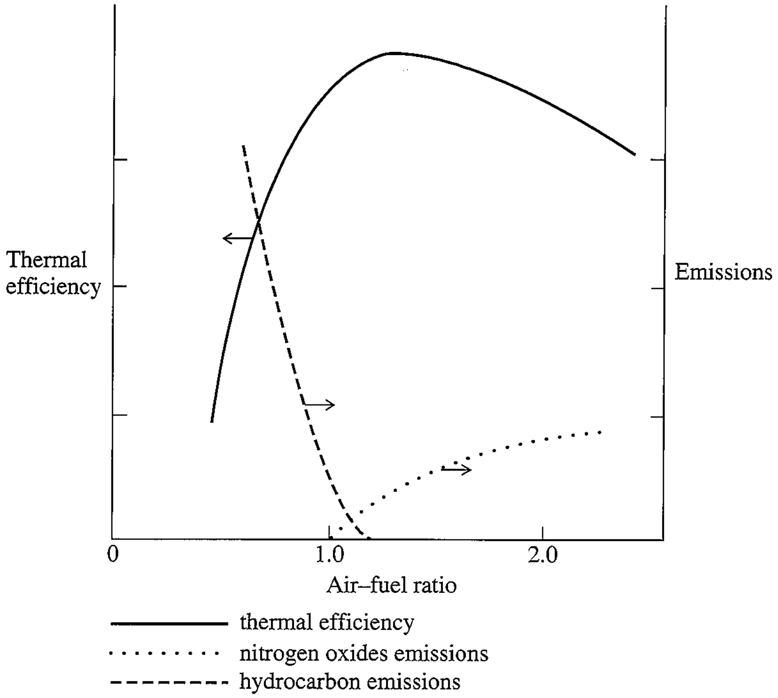

FIGURE E1.2*a*
Efficiency and emissions of a boiler as a function of air–fuel ratio. (1.0 = stoichiometric air–fuel ratio.)

exist for certain conditions, but a discrete jump to a different set of conditions (here idling conditions) may be required if demand changes. In formulating many optimization problems, discrete variables (on–off, high–low, integer 1, 2, 3, 4, etc.) must be accommodated.

EXAMPLE 1.3 OPTIMUM DISTILLATION REFLUX

Prior to 1974, when fuel costs were low, distillation column trains used a strategy involving the substantial consumption of utilities such as steam and cooling water in order to maximize separation (i.e., product purity) for a given tower. However, the operation of any one tower involves certain limitations or constraints on the process, such as the condenser duty, tower tray flooding, or reboiler duty.

The need for energy conservation suggests a different objective, namely minimizing the reflux ratio. In this circumstance, one can ask: How low can the reflux ratio be set? From the viewpoint of optimization, there is an economic minimum value below which the energy savings are less than the cost of product quality degradation. Figures E1.3*a* and E1.3*b* illustrate both alternatives. Operators tend to over-reflux a column because this strategy makes it easier to stay well within the product

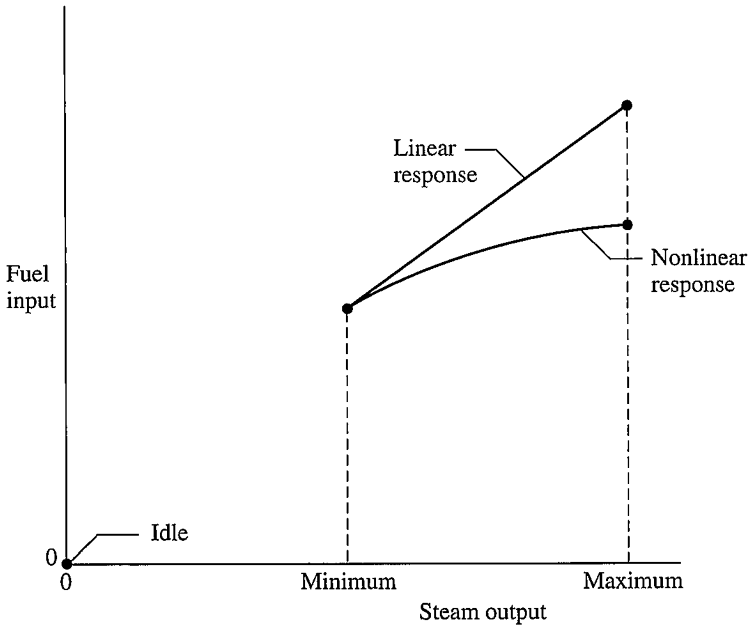

FIGURE E1.2*b*
Discontinuity in operating regimen.

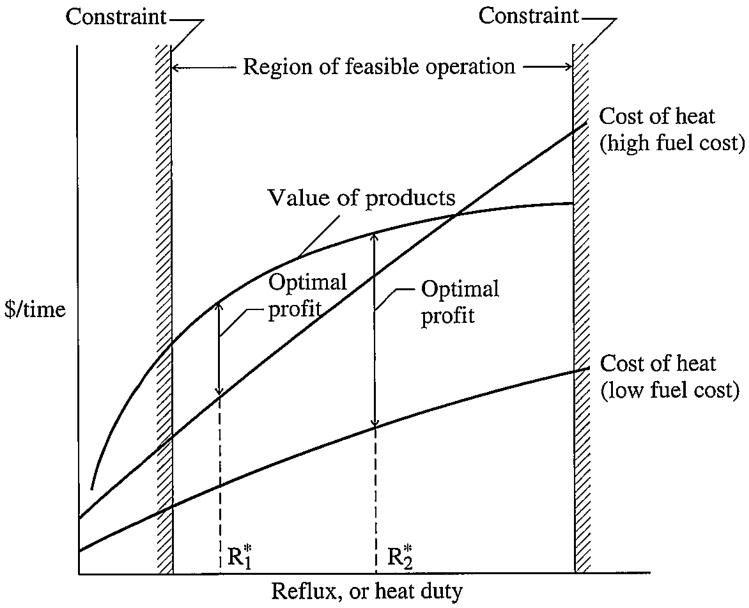

FIGURE E1.3*a*
Illustration of optimal reflux for different fuel costs.

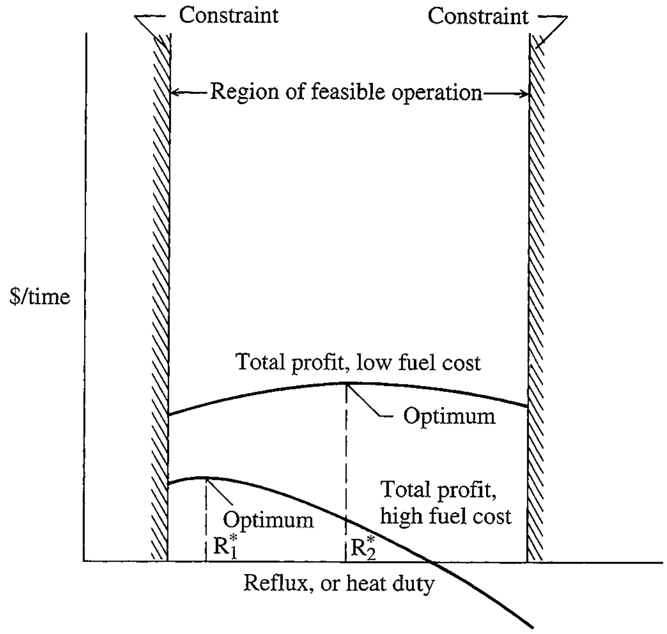

FIGURE E1.3*b*
Total profit for different fuel costs.

specifications. Often columns are operated with a fixed flow control for reflux so that the reflux ratio is higher than needed when feed rates drop off. This issue is discussed in more detail in Chapter 12.

EXAMPLE 1.4 MULTIPLANT PRODUCT DISTRIBUTION

A common problem encountered in large chemical companies involves the distribution of a single product (Y) manufactured at several plant locations. Generally, the product needs to be delivered to several customers located at various distances from each plant. It is, therefore, desirable to determine how much Y must be produced at each of m plants ($Y_1, Y_2, \ldots, Y_m$) and how, for example, Y_m should be allocated to each of n demand points ($Y_{m1}, Y_{m2}, \ldots, Y_{mn}$). The cost-minimizing solution to this problem not only involves the transportation costs between each supply and demand point but also the production cost versus capacity curves for each plant. The individual plants probably vary with respect to their nominal production rate, and some plants may be more efficient than others, having been constructed at a later date. Both of these factors contribute to a unique functionality between production cost and production rate. Because of the particular distribution of transportation costs, it may be desirable to manufacture more product from an old, inefficient plant (at higher cost) than from a new, efficient one because new customers may be located very close to the old plant. On the other hand, if the old plant is operated far above its design rate, costs could become exorbitant, forcing a reallocation by other plants in spite of high transportation costs. In addition, no doubt constraints exist on production levels from each plant that also affect the product distribution plan.

1.5 THE ESSENTIAL FEATURES OF OPTIMIZATION PROBLEMS

Because the solution of optimization problems involves various features of mathematics, the formulation of an optimization problem must use mathematical expressions. Such expressions do not necessarily need to be very complex. Not all problems can be stated or analyzed quantitatively, but we will restrict our coverage to quantitative methods. From a practical viewpoint, it is important to mesh properly the problem statement with the anticipated solution technique.

A wide variety of optimization problems have amazingly similar structures. Indeed, it is this similarity that has enabled the recent progress in optimization techniques. Chemical engineers, petroleum engineers, physicists, chemists, and traffic engineers, among others, have a common interest in precisely the same mathematical problem structures, each with a different application in the real world. We can make use of this structural similarity to develop a framework or methodology within which any problem can be studied. This section describes how any process problem, complex or simple, for which one desires the optimal solution should be organized. To do so, you must (a) consider the model representing the process and (b) choose a suitable objective criterion to guide the decision making.

Every optimization problem contains three essential categories:

1. At least one objective function to be optimized (profit function, cost function, etc.).
2. Equality constraints (equations).
3. Inequality constraints (inequalities).

Categories 2 and 3 constitute the model of the process or equipment; category 1 is sometimes called the *economic model.*

By a *feasible solution* of the optimization problem we mean a set of variables that satisfy categories 2 and 3 to the desired degree of precision. Figure 1.2 illustrates the feasible region or the region of feasible solutions defined by categories 2 and 3. In this case the feasible region consists of a line bounded by two inequality constraints. An *optimal solution* is a set of values of the variables that satisfy the components of categories 2 and 3; this solution also provides an optimal value for the function in category 1. In most cases the optimal solution is a unique one; in some it is not. If you formulate the optimization problem so that there are no residual degrees of freedom among the variables in categories 2 and 3, optimization is

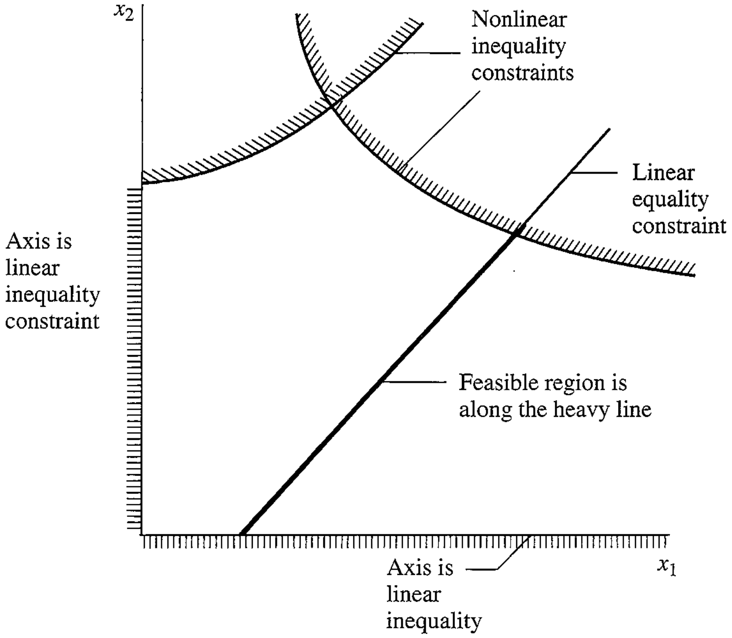

FIGURE 1.2
Feasible region for an optimization problem involving two independent variables. The dashed lines represent the side of the inequality constraints in the plane that form part of the infeasible region. The heavy line shows the feasible region.

not needed to obtain a solution for a problem. More specifically, if m_e equals the number of independent consistent equality constraints and m_i equals the number of independent inequality constraints that are satisfied as equalities (equal to zero), and if the number of variables whose values are unknown is equal to $m_e + m_i$, then at least one solution exists for the relations in components 2 and 3 regardless of the optimization criterion. (Multiple solutions may exist when models in categories 2 and 3 are composed of nonlinear relations.) If a unique solution exists, no optimization is needed to obtain a solution—one just solves a set of equations and need not worry about optimization methods because the unique feasible solution is by definition the optimal one.

On the other hand, if more process variables whose values are unknown exist in category 2 than there are independent equations, the process model is called *underdetermined*; that is, the model has an infinite number of feasible solutions so that the objective function in category 1 is the additional criterion used to reduce the number of solutions to just one (or a few) by specifying what is the "best" solution. Finally, if the equations in category 2 contain more independent equations than variables whose values are unknown, the process model is *overdetermined* and no solution satisfies all the constraints exactly. To resolve the difficulty, we sometimes choose to relax some or all of the constraints. A typical example of an overdetermined model might be the reconciliation of process measurements for a material balance. One approach to yield the desired material balance would be to resolve the set of inconsistent equations by minimizing the sum of the errors of the set of equations (usually by a procedure termed *least squares*).

In this text the following notation will be used for each category of the optimization problem:

Minimize:	$f(\mathbf{x})$	objective function	(a)
Subject to:	$\mathbf{h}(\mathbf{x}) = \mathbf{0}$	equality constraints	(b)
	$\mathbf{g}(\mathbf{x}) \geq \mathbf{0}$	inequality constraints	(c)

where $\mathbf{x}$ is a vector of n variables $(x_1, x_2, \ldots, x_n)$, $\mathbf{h}(\mathbf{x})$ is a vector of equations of dimension m_1, and $\mathbf{g}(\mathbf{x})$ is a vector of inequalities of dimension m_2. The total number of constraints is $m = (m_1 + m_2)$.

EXAMPLE 1.5 OPTIMAL SCHEDULING: FORMULATION OF THE OPTIMATION PROBLEM

In this example we illustrate the formulation of the components of an optimization problem.

We want to schedule the production in two plants, A and B, each of which can manufacture two products: 1 and 2. How should the scheduling take place to maximize profits while meeting the market requirements based on the following data:

	Material processed (lb/day)		Profit ($/lb)	
Plant	**1**	**2**	**1**	**2**
A	M_{A1}	M_{A2}	S_{A1}	S_{A2}
B	M_{B1}	M_{B2}	S_{B1}	S_{B2}

How many days per year (365 days) should each plant operate processing each kind of material? *Hints*: Does the table contain the variables to be optimized? How do you use the information mathematically to formulate the optimization problem? What other factors must you consider?

Solution. How should we start to convert the words of the problem into mathematical statements? First, let us define the variables. There will be four of them (t_{A1},t_{A2}, t_{B1}, and t_{B2}, designated as a set by the vector $\mathbf{t}$) representing, respectively, the number of days per year each plant operates on each material as indicated by the subscripts.

What is the objective function? We select the annual profit so that

$$f(\mathbf{t}) = t_{A1}M_{A1}S_{A1} + t_{A2}M_{A2}S_{A2} + t_{B1}M_{B1}S_{B1} + t_{B2}M_{B2}S_{B2} \qquad (a)$$

Next, do any equality constraints evolve from the problem statement or from implicit assumptions? If each plant runs 365 days per year, two equality constraints arise:

$$t_{A1} + t_{A2} = 365 \tag{b}$$

$$t_{B1} + t_{B2} = 365 \tag{c}$$

Finally, do any inequality constraints evolve from the problem statement or implicit assumptions? On first glance it may appear that there are none, but further thought indicates t must be nonnegative since negative values of t have no physical meaning:

$$t_{Ai} \geq 0 \quad i = 1,2 \tag{d}$$

$$t_{Bi} \geq 0 \quad i = 1,2 \tag{e}$$

Do negative values of the coefficients S have physical meaning?

Other inequality constraints might be added after further analysis, such as a limitation on the total amount of material 2 that can be sold (L_1):

$$t_{A2}M_{A2} + t_{B2}M_{B2} \leq L_1 \tag{f}$$

or a limitation on production rate for each product at each plant, namely

$$\begin{aligned} M_{A1} &\leq L_2 \\ M_{A2} &\leq L_3 \\ M_{B1} &\leq L_4 \\ M_{B2} &\leq L_5 \end{aligned} \tag{g}$$

To find the optimal **t**, we need to optimize (a) subject to constraints (b) to (g).

EXAMPLE 1.6 MATERIAL BALANCE RECONCILIATION

Suppose the flow rates entering and leaving a process are measured periodically. Determine the best value for stream A in kg/h for the process shown from the three hourly measurements indicated of B and C in Figure E1.6, assuming steady-state operation at a fixed operating point. The process model is

$$M_A + M_C = M_B \tag{a}$$

where M is the mass per unit time of throughput.

Solution. We need to set up the objective function first. Let us minimize the sum of the squares of the deviations between input and output as the criterion so that the objective function becomes

$$\begin{aligned} f(M_A) = {} & (M_A + 11.1 - 92.4)^2 + (M_A + 10.8 - 94.3)^2 \\ & + (M_A + 11.4 - 93.8)^2 \end{aligned} \tag{b}$$

A sum of squares is used since this guarantees that $f > 0$ for all values of M_A; a minimum at $f = 0$ implies no error.

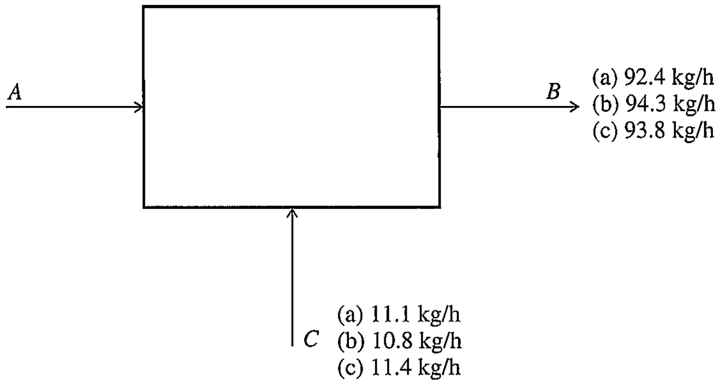

FIGURE E1.6

No equality constraints remain in the problem. Are there any inequality constraints? (*Hint*: What about M_A?) The optimum value of M_A can be found by differentiating f with respect to M_A; this leads to an optimum value for M_A of 82.4 and is the same result as that obtained by computing from the averaged measured values, $M_A = \bar{M}_B - \bar{M}_C$. Other methods of reconciling material (and energy) balances are discussed by Romagnoli and Sanchez (1999).

1.6 GENERAL PROCEDURE FOR SOLVING OPTIMIZATION PROBLEMS

No single method or algorithm of optimization can be applied efficiently to all problems. The method chosen for any particular case depends primarily on (1) the character of the objective function and whether it is known explicitly, (2) the nature of the constraints, and (3) the number of independent and dependent variables.

Table 1.1 lists the six general steps for the analysis and solution of optimization problems. You do not have to follow the cited order exactly, but you should cover all of the steps eventually. Shortcuts in the procedure are allowable, and the easy steps can be performed first. Each of the steps will be examined in more detail in subsequent chapters.

Remember, the general objective in optimization is to choose a set of values of the variables subject to the various constraints that produce the desired optimum response for the chosen objective function.

Steps 1, 2, and 3 deal with the mathematical definition of the problem, that is, identification of variables, specification of the objective function, and statement of the constraints. We devote considerable attention to problem formulation in the remainder of this chapter, as well as in Chapters 2 and 3. If the process to be optimized is very complex, it may be necessary to reformulate the problem so that it can be solved with reasonable effort.

Step 4 suggests that the mathematical statement of the problem be simplified as much as possible without losing the essence of the problem. First, you might

TABLE 1.1
The six steps used to solve optimization problems

1. Analyze the process itself so that the process variables and specific characteristics of interest are defined; that is, make a list of all of the variables.
2. Determine the criterion for optimization, and specify the objective function in terms of the variables defined in step 1 together with coefficients. This step provides the performance model (sometimes called the economic model when appropriate).
3. Using mathematical expressions, develop a valid process or equipment model that relates the input–output variables of the process and associated coefficients. Include both equality and inequality constraints. Use well-known physical principles (mass balances, energy balances), empirical relations, implicit concepts, and external restrictions. Identify the independent and dependent variables to get the number of degrees of freedom.
4. If the problem formulation is too large in scope:
   (a) break it up into manageable parts or
   (b) simplify the objective function and model
5. Apply a suitable optimization technique to the mathematical statement of the problem.
6. Check the answers, and examine the sensitivity of the result to changes in the coefficients in the problem and the assumptions.

decide to ignore those variables that have an insignificant effect on the objective function. This step can be done either ad hoc, based on engineering judgment, or by performing a mathematical analysis and determining the weights that should be assigned to each variable via simulation. Second, a variable that appears in a simple form within an equation can be eliminated; that is, it can be solved for explicitly and then eliminated from other equations, the inequalities, and the objective function. Such variables are then deemed to be dependent variables.

As an example, in heat exchanger design, you might initially include the following variables in the problem: heat transfer surface, flow rates, number of shell passes, number of tube passes, number and spacing of the baffles, length of the exchanger, diameter of the tubes and shell, the approach temperature, and the pressure drop. Which of the variables are independent and which are not? This question can become quite complicated in a problem with many variables. You will find that each problem has to be analyzed and treated as an individual case; generalizations are difficult. Often the decision is quite arbitrary although instinct indicates that the controllable variables be initially selected as the independent ones.

If an engineer is familiar with a particular heat exchanger system, he or she might decide that certain variables can be ignored based on the notion of the controlling or dominant heat transfer coefficient. In such a case only one of the flowing streams is important in terms of calculating the heat transfer in the system, and the engineer might decide, at least initially, to eliminate from consideration those variables related to the other stream.

A third strategy can be carried out when the problem has many constraints and many variables. We assume that some variables are fixed and let the remainder of the variables represent degrees of freedom (independent variables) in the optimization procedure. For example, the optimum pressure of a distillation column might occur at the minimum pressure (as limited by condenser cooling).

Finally, analysis of the objective function may permit some simplification of the problem. For example, if one product (A) from a plant is worth \$30 per pound and all other products from the plant are worth \$5 or less per pound, then we might initially decide to maximize the production of A only.

Step 5 in Table 1.1 involves the computation of the optimum point. Quite a few techniques exist to obtain the optimal solution for a problem. We describe several methods in detail later on. In general, the solution of most optimization problems involves the use of a computer to obtain numerical answers. It is fair to state that over the past 20 years, substantial progress has been made in developing efficient and robust digital methods for optimization calculations. Much is known about which methods are most successful, although comparisons of candidate methods often are ad hoc, based on test cases of simple problems. Virtually all numerical optimization methods involve iteration, and the effectiveness of a given technique often depends on a good first guess as to the values of the variables at the optimal solution.

The last entry in Table 1.1 involves checking the candidate solution to determine that it is indeed optimal. In some problems you can check that the sufficient conditions for an optimum are satisfied. More often, an optimal solution may exist, yet you cannot demonstrate that the sufficient conditions are satisfied. All you can do is show by repetitive numerical calculations that the value of the objective function is superior to all known alternatives. A second consideration is the sensitivity of the optimum to changes in parameters in the problem statement. A sensitivity analysis for the objective function value is important and is illustrated as part of the next example.

EXAMPLE 1.7 THE SIX STEPS OF OPTIMIZATION FOR A MANUFACTURING PROBLEM

This example examines a simple problem in detail so that you can understand how to execute the steps for optimization listed in Table 1.1. You also will see in this example that optimization can give insight into the nature of optimal operations and how optimal results might compare with the simple or arbitrary rules of thumb so often used in practice.

Suppose you are a chemical distributor who wishes to optimize the inventory of a specialty chemical. You expect to sell Q barrels of this chemical over a given year at a fixed price with demand spread evenly over the year. If Q = 100,000 barrels (units) per year, you must decide on a production schedule. Unsold production is kept in inventory. To determine the optimal production schedule you must quantify those aspects of the problem that are important from a cost viewpoint [Baumol (1972)].

Step 1. One option is to produce 100,000 units in one run at the beginning of the year and allow the inventory to be reduced to zero at the end of the year (at which time another 100,000 units are manufactured). Another option is to make ten runs of 10,000 apiece. It is clear that much more money is tied up in inventory with the former option than in the latter. Funds tied up in inventory are funds that could be invested in other areas or placed in a savings account. You might therefore conclude that it would be cheaper to make the product ten times a year.

However, if you extend this notion to an extreme and make 100,000 production runs of one unit each (actually one unit every 315 seconds), the decision obviously is impractical, since the cost of producing 100,000 units, one unit at a time, will be exorbitant. It therefore appears that the desired operating procedure lies somewhere in between the two extremes. To arrive at some quantitative answer to this problem, first define the three operating variables that appear to be important: number of units of each run (D), the number of runs per year (n), and the total number of units produced per year (Q). Then you must obtain details about the costs of operations. In so doing, a cost (objective) function and a mathematical model will be developed, as discussed later on. After obtaining a cost model, any constraints on the variables are identified, which allows selection of independent and dependent variables.

Step 2. Let the business costs be split up into two categories: (1) the carrying cost or the cost of inventory and (2) the cost of production. Let D be the number of units produced in one run, and let Q (annual production level) be assigned a known value. If the problem were posed so that a minimum level of inventory is specified, it would not change the structure of the problem.

The cost of the inventory not only includes the cost of the money tied up in the inventory, but also a storage cost, which is a function of the inventory size. Warehouse space must exist to store all the units produced in one run. In the objective function, let the cost of carrying the inventory be K_1D, where the parameter K_1 essentially lumps together the cost of working capital for the inventory itself and the storage costs.

Assume that the annual production cost in the objective function is proportional to the number of production runs required. The cost per run is assumed to be a linear function of D, given by the following equation:

$$\text{Cost per run} = K_2 + K_3D \tag{a}$$

The cost parameter K_2 is a setup cost and denotes a fixed cost of production—equipment must be made ready, cleaned, and so on. The parameter K_3 is an operating cost parameter. The operating cost is assumed to be proportional to the number of units manufactured. Equation (a) may be an unrealistic assumption because the incremental cost of manufacturing could decrease somewhat for large runs; consequently, instead of a linear function, you might choose a nonlinear cost function of the form

$$\text{Cost per run} = K_2 + K_4D^{1/2} \tag{b}$$

as is shown in Figure E1.7. The effect of this alternative assumption will be discussed later. The annual production cost can be found by multiplying either Equation (a) or (b) by the number n of production runs per year.

The total annual manufacturing cost C for the product is the sum of the carrying costs and the production costs, namely

$$C = K_1D + n(K_2 + K_3D) \tag{c}$$

Step 3. The objective function in (c) is a function of two variables: D and n. However, D and n are directly related, namely $n = Q/D$. Therefore, only one independent

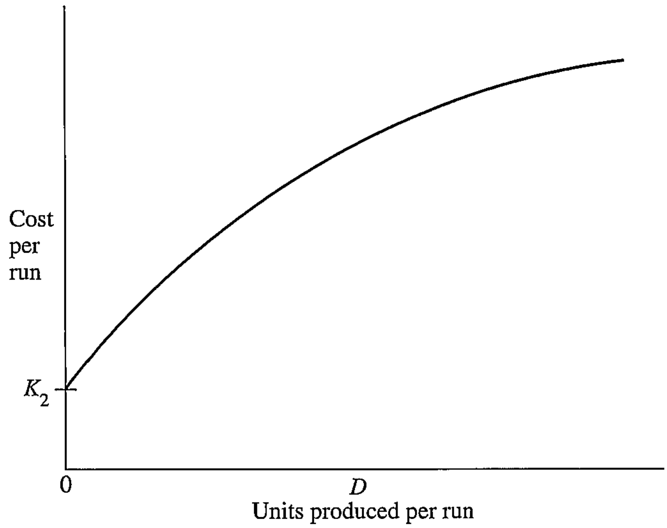

FIGURE E1.7
Nonlinear cost function for manufacturing.

variable exists for this problem, which we select to be D. The dependent variable is therefore n. Eliminating n from the objective function in (c) gives

$$C = K_1D + \frac{K_2Q}{D} + K_3Q \qquad (d)$$

What other constraints exist in this problem? None are stated explicitly, but several implicit constraints exist. One of the assumptions made in arriving at Equation (c) is that over the course of one year, production runs of integer quantities may be involved. Can D be treated as a continuous variable? Such a question is crucial prior to using differential calculus to solve the problem. The occurrence of integer variables in principle prevents the direct calculation of derivatives of functions of integer variables. In the simple example here, with D being the only variable and a large one, you can treat D as continuous. After obtaining the optimal D, the practical value for D is obtained by rounding up or down. There is no guarantee that $n = Q/D$ is an integer; however, as long as you operate from year to year there should be no restriction on n.

What other constraints exist? You know that D must be positive. Do any equality constraints relate D to the other known parameters of the model? If so, then the sole degree of freedom in the process model could be eliminated and optimization would not be needed!

Step 4. Not needed.

Step 5. Look at the total cost function, Equation (c). Observe that the cost function includes a constant term, K_3Q. If the total cost function is differentiated, the term K_3Q vanishes and thus K_3 does not enter into the determination of the optimal value for D. K_3, however, contributes to the total cost.

Two approaches can be employed to solve for the optimal value of D: analytical or numerical. A simple problem has been formulated so that an analytical solution can be obtained. Recall from calculus that if you differentiate the cost function with respect to D and equate the total derivative to zero

$$\frac{dC}{dD} = K_1 - \frac{K_2 Q}{D^2} = 0 \qquad (e)$$

you can obtain the optimal solution for D

$$D^{\text{opt}} = \sqrt{\frac{K_2 Q}{K_1}} \qquad (f)$$

Equation (f) was obtained without knowing specific numerical values for the parameters. If K_1, K_2, or Q change for one reason or another, then the calculation of the new value of D^{opt} is straightforward. Thus, the virtue of an analytical solution (versus a numerical one) is apparent.

Suppose you are given values of $K_1 = 1.0$, $K_2 = 10{,}000$, $K_3 = 4.0$, and $Q = 100{,}000$. Then D^{opt} from Equation (f) is 31,622.

You can also quickly verify for this problem that D^{opt} from Equation (f) minimizes the objective function by taking the second derivative of C and showing that it is positive. Equation (g) helps demonstrate the sufficient conditions for a minimum.

$$\frac{d^2C}{dD^2} = \frac{2K_2 Q}{D^3} > 0 \qquad (g)$$

Details concerning the necessary and sufficient conditions for minimization are presented in Chapter 4.

Another benefit of obtaining an analytical solution is that you can gain some insight into how production should be scheduled. For example, suppose the optimum number of production runs per year was 4.0 (25,000 units per run), and the projected demand for the product was doubled ($Q = 200{,}000$) for the next year. Using intuition you might decide to double the number of units produced (50,000 units) with 4.0 runs per year. However, as can be seen from the analytical solution, the new value of D^{opt} should be selected according to the square root of Q rather than the first power of Q. This relationship is known as the *economic order quantity* in inventory control and demonstrates some of the pitfalls that may result from making decisions by simple analogies or intuition.

We mentioned earlier that this problem was purposely designed so that an analytical solution could be obtained. Suppose now that the cost per run follows a nonlinear function such as shown earlier in Figure E1.7. Let the cost vary as given by Equation (b), thus allowing for some economy of scale. Then the total cost function becomes

$$C = K_1 D + \frac{K_2 Q}{D} + \frac{K_4 Q}{D^{1/2}} \qquad (h)$$

After differentiation and equating the derivative to zero, you get

$$\frac{dC}{dD} = K_1 - \frac{K_2 Q}{D^2} - \frac{K_4 Q}{2D^{3/2}} = 0 \qquad (i)$$

Note that Equation (i) is a rather complicated polynomial that cannot explicitly be solved for D^{opt}; you have to resort to a numerical solution as discussed in Chapter 5.

A dichotomy arises in attempting to minimize function (h). You can either (1) minimize the cost function (h) directly or (2) find the roots of Equation (i). Which is the best procedure? In general it is easier to minimize C directly by a numerical method rather than take the derivative of C, equate it to zero, and solve the resulting nonlinear equation. This guideline also applies to functions of several variables.

The second derivative of Equation (h) is

$$\frac{d^2C}{dD^2} = \frac{2K_2Q}{D^3} + \frac{3K_4Q}{4D^{5/2}} \qquad (j)$$

A numerical procedure to obtain D^{opt} directly from Equation (d) could also have been carried out by simply choosing values of D and computing the corresponding values of C from Equation (d) ($K_1 = 1.0$; $K_2 = 10{,}000$; $K_3 = 4.0$; $Q = 100{,}000$).

$D \times 10^{-3}$	10	20	30	40	50	60	70	80	90	100
$C \times 10^{-3}$	510	470	463	465	470	477	484	492	501	510

From the listed numerical data you can see that the function has a single minimum in the vicinity of $D = 20{,}000$ to $40{,}000$. Subsequent calculations in this range (on a finer scale) for D will yield a more precise value for D^{opt}.

Observe that the objective function value for $20 \le D \le 60$ does not vary significantly. However, not all functions behave like C in Equation (d)—some exhibit sharp changes in the objective function near the optimum.

Step 6. You should always be aware of the sensitivity of the optimal answer, that is, how much the optimal value of C changes when a variable such as D changes or a coefficient in the objective function changes. Parameter values usually contain errors or uncertainties. Information concerning the sensitivity of the optimum to changes or variations in a parameter is therefore very important in optimal process design. For some problems, a sensitivity analysis can be carried out analytically, but in others the sensitivity coefficients must be determined numerically.

In this example problem, we can analytically calculate the changes in C^{opt} in Equation (d) with respect to changes in the various cost parameters. Substitute D^{opt} from Equation (f) into the total cost function

$$C^{opt} = 2\sqrt{K_1K_2Q} + K_3Q \qquad (k)$$

Next, take the partial derivatives of C^{opt} with respect to K_1, K_2, K_3, and Q

$$\frac{\partial C^{opt}}{\partial K_1} = \sqrt{\frac{K_2Q}{K_1}} \qquad (l1)$$

$$\frac{\partial C^{opt}}{\partial K_2} = \sqrt{\frac{K_1Q}{K_2}} \qquad (l2)$$

$$\frac{\partial C^{opt}}{\partial K_3} = Q \qquad (l3)$$

$$\frac{\partial C^{opt}}{\partial Q} = \sqrt{\frac{K_1K_2}{Q}} + K_3 \qquad (l4)$$

Equations ($l1$) through ($l4$) are absolute sensitivity coefficients.

Similarly, we can develop expressions for the sensitivity of D^{opt}:

$$D^{\text{opt}} = \sqrt{\frac{K_2 Q}{K_1}} \tag{f}$$

$$\frac{\partial D^{\text{opt}}}{\partial K_1} = \frac{-1}{2K_1}\sqrt{\frac{K_2 Q}{K_1}} \tag{m1}$$

$$\frac{\partial D^{\text{opt}}}{\partial K_2} = \frac{1}{2K_2}\sqrt{\frac{K_2 Q}{K_1}} \tag{m2}$$

$$\frac{\partial D^{\text{opt}}}{\partial K_3} = 0 \tag{m3}$$

$$\frac{\partial D^{\text{opt}}}{\partial Q} = \frac{1}{2Q}\sqrt{\frac{K_2 Q}{K_1}} \tag{m4}$$

Suppose we now substitute numerical values for the constants in order to clarify how these sensitivity functions might be used. For

$$Q = 100{,}000 \qquad K_1 = 1.0 \quad K_2 = 10{,}000 \qquad K_3 = 4.0$$

then

$$D^{\text{opt}} = 31{,}622$$

$$C^{\text{opt}} = D^{\text{opt}} + \frac{10^9}{D^{\text{opt}}} + 400{,}000 = \$463{,}240$$

$$\frac{\partial C^{\text{opt}}}{\partial K_1} = 31{,}620 \qquad \frac{\partial D^{\text{opt}}}{\partial K_1} = -15{,}810$$

$$\frac{\partial C^{\text{opt}}}{\partial K_2} = 3.162 \qquad \frac{\partial D^{\text{opt}}}{\partial K_2} = 1.581$$

$$\frac{\partial C^{\text{opt}}}{\partial K_3} = 100{,}000 \qquad \frac{\partial D^{\text{opt}}}{\partial K_3} = 0$$

$$\frac{\partial C^{\text{opt}}}{\partial Q} = 4.316 \qquad \frac{\partial D^{\text{opt}}}{\partial Q} = 0.158$$

What can we conclude from the preceding numerical values? It appears that D^{opt} is extremely sensitive to K_1, but not to Q. However, you must realize that a one-unit change in Q (100,000) is quite different from a one-unit change in K_1 (0.5). Therefore, in order to put the sensitivities on a more meaningful basis, you should compute the relative sensitivities: for example, the relative sensitivity of C^{opt} to K_1 is

$$S_{K_1}^{C} = \frac{\partial C^{\text{opt}}/C^{\text{opt}}}{\partial K_1/K_1} = \frac{\partial \ln C^{\text{opt}}}{\partial \ln K_1} = \sqrt{\frac{K_2 Q}{K_1}} \cdot \frac{K_1}{C^{\text{opt}}} = \frac{31{,}622(1.0)}{463{,}240} = 0.0683 \tag{n}$$

Application of the preceding idea for the other variables yields the other relative sensitivities for C^{opt}. Numerical values are

$$S_{K_3}^{C} = 0.863$$

$$S_{K_2}^{C} = 0.0683 \qquad S_{Q}^{C} = 0.932$$

Changes in the parameters Q and K_3 have the largest relative influence on C^{opt}, significantly more than K_1 or K_2. The relative sensitivities for D^{opt} are

$$S_{K_1}^{D} = -0.5 \qquad S_{K_2}^{D} = S_{Q}^{D} = 0.5 \qquad S_{K_3}^{D} = 0$$

so that all the parameters except for K_3 have the same influence (in terms of absolute value of fractional changes) on the optimum value of D.

For a problem for which we cannot obtain an analytical solution, you need to determine sensitivities numerically. You compute (1) the cost for the base case, that is, for a specified value of a parameter; (2) change each parameter separately (one at a time) by some arbitrarily small value, such as plus 1 percent or 10 percent, and then calculate the new cost. You might repeat the procedure for minus 1 percent or 10 percent. The variation of the parameter, of course, can be made arbitrarily small to approximate a differential; however, when the change approaches an infinitesimal value, the numerical error engendered may confound the calculations.

1.7 OBSTACLES TO OPTIMIZATION

If the objective function and constraints in an optimization problem are "nicely behaved," optimization presents no great difficulty. In particular, if the objective function and constraints are all linear, a powerful method known as linear programming can be used to solve the optimization problem (refer to Chapter 7). For this specific type of problem it is known that a unique solution exists if any solution exists. However, most optimization problems in their natural formulation are not linear.

To make it possible to work with the relative simplicity of a linear problem, we often modify the mathematical description of the physical process so that it fits the available method of solution. Many persons employing computer codes for optimization do not fully appreciate the relation between the original problem and the problem being solved; the computer shows its neatly printed output with an authority that the reader feels unwilling, or unable, to question.

In this text we will discuss optimization problems based on behavior of physical systems that have a complicated objective function or constraints: for these problems some optimization procedures may be inappropriate and sometimes misleading. Often optimization problems exhibit one or more of the following characteristics, causing a failure in the calculation of the desired optimal solution:

1. The objective function or the constraint functions may have finite discontinuities in the continuous parameter values. For example, the price of a compressor or

heat exchanger may not change continuously as a function of variables such as size, pressure, temperature, and so on. Consequently, increasing the level of a parameter in some ranges has no effect on cost, whereas in other ranges a jump in cost occurs.

2. The objective function or the constraint functions may be nonlinear functions of the variables. When considering real process equipment, the existence of truly linear behavior and system behavior is somewhat of a rarity. This does not preclude the use of linear approximations, but the results of such approximations must be interpreted with considerable care.
3. The objective function or the constraint functions may be defined in terms of complicated interactions of the variables. A familiar case of interaction is the temperature and pressure dependence in the design of pressure vessels. For example, if the objective function is given as $f = 15.5x_1x_2^{1/2}$, the interaction between x_1 and x_2 precludes the determination of unique values of x_1 and x_2. Many other more complicated and subtle interactions are common in engineering systems. The interaction prevents calculation of unique values of the variables at the optimum.
4. The objective function or the constraint functions may exhibit nearly "flat" behavior for some ranges of variables or exponential behavior for other ranges. This means that the value of the objective function or a constraint is not sensitive or is very sensitive, respectively, to changes in the value of the variables.
5. The objective function may exhibit many local optima, whereas the global optimum is sought. A solution to the optimization problem may be obtained that is less satisfactory than another solution elsewhere in the region. The better solution may be reached only by initiating the search for the optimum from a different starting point.

In subsequent chapters we will examine these obstacles and discuss some ways of mitigating such difficulties in performing optimization, but you should be aware these difficulties cannot always be alleviated.

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PROBLEMS

For each of the following six problems, formulate the objective function, the equality constraints (if any), and the inequality constraints (if any). Specify and list the independent variables, the number of degrees of freedom, and the coefficients in the optimization problem. Solve the problem using calculus as needed, and state the complete optimal solution values.

1.1 A poster is to contain 300 cm^2 of printed matter with margins of 6 cm at the top and bottom and 4 cm at each side. Find the overall dimensions that minimize the total area of the poster.

1.2 A box with a square base and open top is to hold 1000 cm^3. Find the dimensions that require the least material (assume uniform thickness of material) to construct the box.

1.3 Find the area of the largest rectangle with its lower base on the x axis and whose corners are bounded at the top by the curve $y = 10 - x^2$.

1.4 Three points x are selected a distance h apart (x_0, $x_0 + h$, $x_0 + 2h$), with corresponding values f_0, f_1, and f_2. Find the maximum or minimum attained by a quadratic function passing through all three points. *Hint*: Find the coefficients of the quadratic function first.

1.5 Find the point on the curve $f = 2x^2 + 3x + 1$ nearest the origin.

1.6 Find the volume of the largest right circular cylinder that can be inscribed inside a sphere of radius R.

1.7 In a particular process the value of the product $f(x)$ is a function of the concentration x of ammonia expressed as a mole fraction. The following figure shows several values

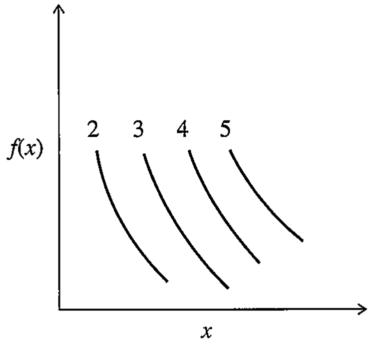

FIGURE P1.7

of $f(x)$. No units or values are designated for either of the axes. Duplicate the figure, and insert on the duplicate the constraint(s) involved in the problem by drawing very heavy lines or curves on the diagram.

1.8 A trucking company has borrowed \$600,000 for new equipment and is contemplating three kinds of trucks. Truck A costs \$10,000, truck B \$20,000, and truck C \$23,000. How many trucks of each kind should be ordered to obtain the greatest capacity in ton-miles per day based on the following data?

Truck A requires one driver per day and produces 2100 ton-miles per day.
Truck B requires two drivers per day and produces 3600 ton-miles per day.
Truck C requires two drivers per day and produces 3780 ton-miles per day.
There is a limit of 30 trucks and 145 drivers.

Formulate a *complete* mathematical statement of the problem, and label each individual part, identifying the objective function and constraints with the correct units (\$, days, etc.). Make a list of the variables by names and symbol plus units. Do *not* solve.

1.9 In a rough preliminary design for a waste treatment plant the cost of the components are as follows (in order of operation)

1. Primary clarifier: $\$19.4\ x_1^{-1.47}$
2. Trickling filter: $\$16.8\ x_2^{-1.66}$
3. Activated sludge unit: $\$91.5\ x_3^{-0.30}$

where the x's are the fraction of the 5-day biochemical oxygen demand (BOD) exiting each respective unit in the process, that is, the exit concentrations of material to be removed.

The required removal in each unit should be adjusted so that the final exit concentration x_3 must be less than 0.05. Formulate (only) the optimization problem listing the objective function and constraints.

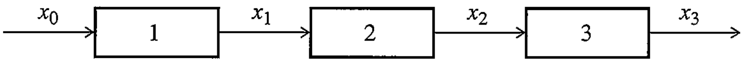

FIGURE P1.9

1.10 Examine the following optimization problem. State the total number of variables, and list them. State the number of independent variables, and list a set.

$$\text{Minimize:}\quad f(x) = 4x_1 - x_2^2 - 12$$

$$\text{Subject to:}\quad 25 - x_1^2 - x_2^2 = 0$$

$$10x_1 - x_1^2 + 10x_2 - x_2^2 - 34 \geq 0$$

$$(x_1 - 3)^2 + (x_2 - 1)^2 \geq 0$$

$$x_1, x_2 \geq 0$$

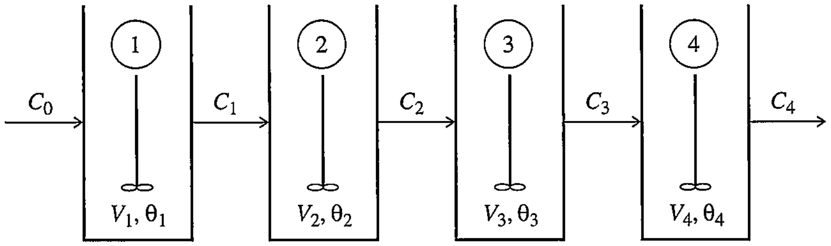

FIGURE P1.11

1.11 A series of four well-mixed reactors operate isothermally in the steady state. Examine the figure. All the tanks do not have the same volume, but the sum of $V_i = 20$ m^3. The component whose concentration is designated by C reacts according to the following mechanism: $r = -kC^n$ in each tank.

Determine the values of the tank volumes (really residence times of the component) in each of the four tanks for steady-state operation with a fixed fluid flow rate of q so as to maximize the yield of product C_4. Note $(V_i/q_i) = \theta_i$, the residence time. Use the following data for the coefficients in the problem

$$n = 2.5 \qquad k = 0.00625\ [\text{m}^3/(\text{kg mol})]^{-1.5}(\text{s})^{-1}$$

$$C_0 = 20 \text{ kg mol/m}^3 \qquad q = 71 \text{ m}^3/\text{h}$$

The units for k are fixed by the constant 0.00625.

List:

1. The objective function
2. The variables
3. The equality constraints
4. The inequality constraints

What are the independent variables? The dependent variables? Do not solve the problem, just set it up so it can be solved.

1.12 A certain gas contains moisture, which you need to remove by compression and cooling so that the gas will finally contain not more than 1% moisture (by volume). If the cost of the compression equipment is

$$\text{Cost in \$} = (\text{pressure in psi})^{1.40}$$

and the cost of the cooling equipment is

$$\text{Cost in \$} = (350 - \text{temperature in kelvin})^{1.9}$$

what is the best temperature to use?

Define the objective function, the independent and the dependent variables, and the constraints first. Then set this problem up, and list all of the steps to solve it. You do not have to solve the final (nonlinear) equations you derive for T. *Hint*: The vapor pressure of water (p^*) is related to the temperature T in °C by Antoine's equation:

$$\log_{10} p^* = 8.10765 - \frac{1750.286}{235.0 + T}$$

1.13 The following problem is formulated as an optimization problem. A batch reactor operating over a 1-h period produces two products according to the parallel reaction mechanism: $A \rightarrow B$, $A \rightarrow C$. Both reactions are irreversible and first order in A and have rate constants given by

$$k_i = k_{io} \exp\{E_i/RT\} \quad i = 1,2$$

where
$$\begin{aligned} k_{10} &= 10^6/\text{s} \\ k_{20} &= 5.10^{11}/\text{s} \\ E_1 &= 10{,}000 \text{ cal/gmol} \\ E_2 &= 20{,}000 \text{ cal/gmol} \end{aligned}$$

The objective is to find the temperature–time profile that maximizes the yield of B for operating temperatures below 282°F. The optimal control problem is therefore

$$\begin{aligned} \text{Maximize:} \quad & \text{B}(1.0) \\ \text{Subject to:} \quad & \frac{dA}{dt} = -(k_1 + k_2)A \\ & \frac{dB}{dt} = k_1 A \\ & A(0) = A_0 \\ & B(0) = 0 \\ & T \leq 282°\text{F} \end{aligned}$$

(a) What are the independent variables in the problem?
(b) What are the dependent variables in the problem?
(c) What are the equality constraints?
(d) What are the inequality constraints?
(e) What procedure would you recommend to solve the problem?

1.14 The computation of chemical equilibria can be posed as an optimization problem with linear side conditions. For any infinitesimal process in which the amounts of species present may be changed by either the transfer of species to or from a phase or by chemical reaction, the change in the Gibbs free energy is

$$dG = S\,dT + V\,dp + \sum_i \mu_i\,dn_i \tag{1}$$

Here G, S, T, and p are the Gibbs free energy, the entropy, the temperature, and the (total) pressure, respectively. The partial molal free energy of species number i is μ_i, and n_i is the number of moles of species number i in the system. If it is assumed that the temperature and pressure are held constant during the process, dT and dp both vanish. If we now make changes in the n_i such that $dn_i = dkn_i$, so that the changes in the n_i are in the same proportion k, then, since G is an extensive quantity, we must have $dG = dkG$. This implies that

$$G = \sum_i \mu_i n_i \tag{2}$$

Comparison of Equations (1) and (2) shows that the chemical potentials are intensive quantities, that is, they do not depend on the amount of each species, because if all the n_i are increased in the same proportion at constant T and p, the μ_i must remain unchanged for G to increase in the same rate as the n_i. This invariance property of the μ_i is of the utmost importance in restricting the possible forms that the μ_i may take.

Equation (2) expresses the Gibbs free energy in terms of the mole numbers n_i, which appear both explicitly and implicitly (in the μ_i) on the right-hand side. The Gibbs free energy is a minimum when the system is at equilibrium. The basic problem, then, becomes that of finding that set of n_i that makes G a minimum.

(a) Formulate in symbols the optimization problem using the previous notation with n_i^* being the number of moles of the compounds at equilibrium and M the number of elements present in the system. The initial number of moles of each compound is presumed to be known.
(b) Introduce into the preceding formulation the quantities needed to solve the following problem:

Calculate the fraction of steam that is decomposed in the water–gas shift reaction

$$CO(g) + H_2O(g) \rightleftharpoons CO_2(g) + H_2(g)$$

at $T = 1530°F$ and $p = 10$ atm starting with 1 mol of H_2O and 1 mol of CO. Assume the mixture is an ideal gas. Do not solve the problem.

Hints: You can find (from a thermodynamics book) that the chemical potential can be written as

$$\mu_i = \mu_i^\circ + RT\ln p + RT\ln x_i = \mu_i^\circ + RT\ln p_i \tag{3}$$

where x_i = mole fraction of a compound in the gas phase

$p_i = px_i$

$\mu_{i,T}^0 = (\Delta G_T^0)_i$

$-(\Delta G_T^0) = RT\ln K_x$, with K_x being the equilibrium constant for the reaction.

1.15 For a two-stage adiabatic compressor where the gas is cooled to the inlet gas temperature between stages, the theoretical work is given by

$$W = \frac{kp_1V_1}{k-1}\left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} - 2 + \left(\frac{p_3}{p_2}\right)^{(k-1)/k}\right]$$

where $k = C_p/C_v$

p_1 = inlet pressure

p_2 = intermediate stage pressure

p_3 = outlet pressure
V_1 = inlet volume

We wish to optimize the intermediate pressure p_2 so that the work is a minimum. Show that if $p_1 = 1$ atm and $p_3 = 4$ atm, $p_2^{opt} = 2$ atm.

1.16 You are the manufacturer of PCl_3, which you sell in barrels at a rate of P barrels per day. The cost per barrel produced is

$$C = 50 + 0.1P + 9000/P \text{ in dollars/barrel}$$

For example, for $P = 100$ barrels/day, $C = \$150$/barrel. The selling price per barrel is \$300. Determine

(a) The production level giving the minimum cost per barrel.
(b) The production level which maximizes the profit per day.
(c) The production level at zero profit.
(d) Why are the answers in (a) and (b) different?

1.17 It is desired to cool a gas [$C_p = 0.3$ Btu/(lb)(°F)] from 195 to 90°F, using cooling water at 80°F. Water costs \$0.20/1000 ft^3, and the annual fixed charges for the exchanger are \$0.50/ft^2 of inside surface, with a diameter of 0.0875 ft. The heat transfer coefficient is $U = 8$ Btu/(h)(ft^2)(°F) for a gas rate of 3000 lb/h. Plot the annual cost of cooling water and fixed charges for the exchanger as a function of the outlet water temperature. What is the minimum total cost? How would you formulate the problem to obtain a more meaningful result? *Hint*: Which variable is the manipulated variable?

1.18 The total cost (in dollars per year) for pipeline installation and operation for an incompressible fluid can be expressed as follows:

$$C = C_1 D^{1.5} \cdot L + C_2 m \Delta p/\rho$$

where C_1 = the installed cost of the pipe per foot of length computed on an annual basis ($C_1 D^{1.5}$ is expressed in dollars per year per foot length, C_2 is based on \$0.05/kWh, 365 days/year and 60 percent pump efficiency).
D = diameter (to be optimized)
L = pipeline length = 100 miles
m = mass flow rate = 200,000 lb/h
Δp = $2\rho v^2 L/(Dg_c) \cdot f$ = pressure drop, psi
ρ = density = 60 lb/ft^3
v = velocity = $(4m)/(\rho\pi D^2)$
f = friction factor = $(0.046\mu^{0.2})/(D^{0.2} v^{0.2} \rho^{0.2})$
μ = viscosity = 1 cP

(a) Find general expressions for D^{opt}, v^{opt}, and C^{opt}.
(b) For $C_1 = 0.3$ (D expressed in inches for installed cost), calculate D^{opt} and v^{opt} for the following pairs of values of μ and ρ (watch your units!)

$$\mu = 0.2 \text{ cP}, 1 \text{ cP}, 10 \text{ cP}$$

$$\rho = 50 \text{ lb/ft}^3, 60 \text{ lb/ft}^3, 80 \text{ lb/ft}^3$$

1.19 Calculate the relative sensitivities of D^{opt} and C^{opt} in Problem 1.18 to changes in ρ, μ, m, and C_2 (cost of electricity). Use the base case parameters as given in Problem 1.18, with $C_1 = 0.3$.

Pose each of the following problems as an optimization problem. Include all of the features mentioned in connection with the first four steps of Table 1.1, but do not solve the problem.

1.20 A chemical manufacturing firm has discontinued production of a certain unprofitable product line. This has created considerable excess production capacity on the three existing batch production facilities that operate separately. Management is considering devoting this excess capacity to one or more of three new products; call them products 1, 2, and 3. The available capacity on the existing units which might limit output is summarized in the following table:

Unit	Available time (h/week)
A	20
B	10
C	5

Each of the three new products requires the following processing time for completion:

	Productivity (h/batch)		
Unit	Product 1	Product 2	Product 3
A	0.8	0.2	0.3
B	0.4	0.3	—
C	0.2	—	0.1

The sales department indicates that the sales potential for products 1 and 2 exceeds the maximum production rate and that the sales potential for product 3 is 20 batches per week. The profit per batch would be \$20, \$6, and \$8, respectively, on products 1, 2, and 3.

How much of each product should be produced to maximize profits of the company? Formulate the objective function and constraints, but do not solve.

1.21 You are asked to design an efficient treatment system for runoff from rainfall in an ethylene plant. The accompanying figure gives the general scheme to be used.

The rainfall frequency data for each recurrence interval fits an empirical equation in the form of

$$R = a + b(t)^2$$

where R = cumulative inches of rain during time t
t = time, h
a and b = constants that have to be determined by fitting the observed rainfall data

Four assumptions should be made:

1. The basin is empty at the beginning of the maximum intensity rain.
2. As soon as water starts to accumulate in the basin, the treatment system is started and water is pumped out of the basin.

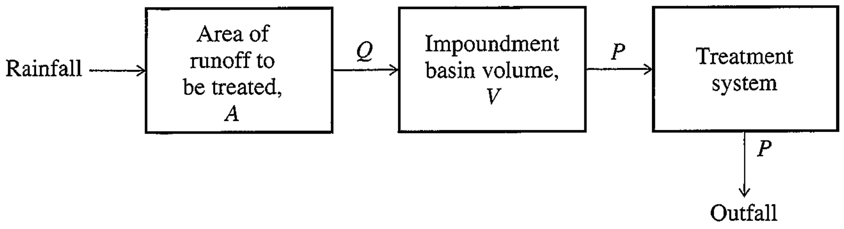

FIGURE P1.21

3. Stormwater is assumed to enter the basin as soon as it falls. (This is normally a good assumption since the rate at which water enters the basin is small relative to the rate at which it leaves the basin during a maximum intensity rain.)
4. All the rainfall becomes runoff.

The basin must not overflow so that any amount of water that would cause the basin to overflow must be pumped out and treated. What is the minimum pumping rate P required?

Other notation: Q = Volumetric flow rate of water entering basin
P = Volumetric treatment rate in processing plant

1.22 Optimization of a distributed parameter system can be posed in various ways. An example is a packed, tubular reactor with radial diffusion. Assume a single reversible reaction takes place. To set up the problem as a nonlinear programming problem, write the appropriate balances (constraints) including initial and boundary conditions using the following notation:

x = Extent of reaction $\quad$ t = Time
T = Dimensions temperature $\quad$ r = Dimensionless radial coordinate

Do the differential equations have to be expressed in the form of analytical solutions?

The objective function is to maximize the total conversion in the effluent from the reactor over the cross-sectional area at any instant of time. Keep in mind that the heat flux through the wall is subject to physical bounds.

1.23 Calculate a new expression for D^{opt} if $f = 0.005$ (rough pipe), independent of the Reynolds number. Compare your results with these from Problem 1.18 for $\mu = 1$ cP and $\rho = 60$ lb/ft^3.

1.24 A shell-and-tube heat exchanger has a total cost of $C = \$7000 + \$250\,D^{2.5}L + \$200\,DL$, where D is the diameter (ft) and L is the length (ft). What is the absolute and the relative sensitivity of the total cost with respect to the diameter?

If an inequality constraint exists for the heat exchanger

$$20\left(\frac{\pi D^2}{4}\right)L \geq 300$$

how must the sensitivity calculation be modified?

1.25 Empirical cost correlations for equipment are often of the following form:

$$\ln C = a_0 + a_1 \ln S + a_2(\ln S)^2$$

where C is the base cost per unit and S is the size per unit. Obtain an analytical expression for the minimum cost in terms of S, and, if possible, find the expression that gives the value of S at the minimum cost. Also write down an analytical expression for the *relative* sensitivity of C with respect to S.

1.26 What are three major difficulties experienced in formulating optimization problems?