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

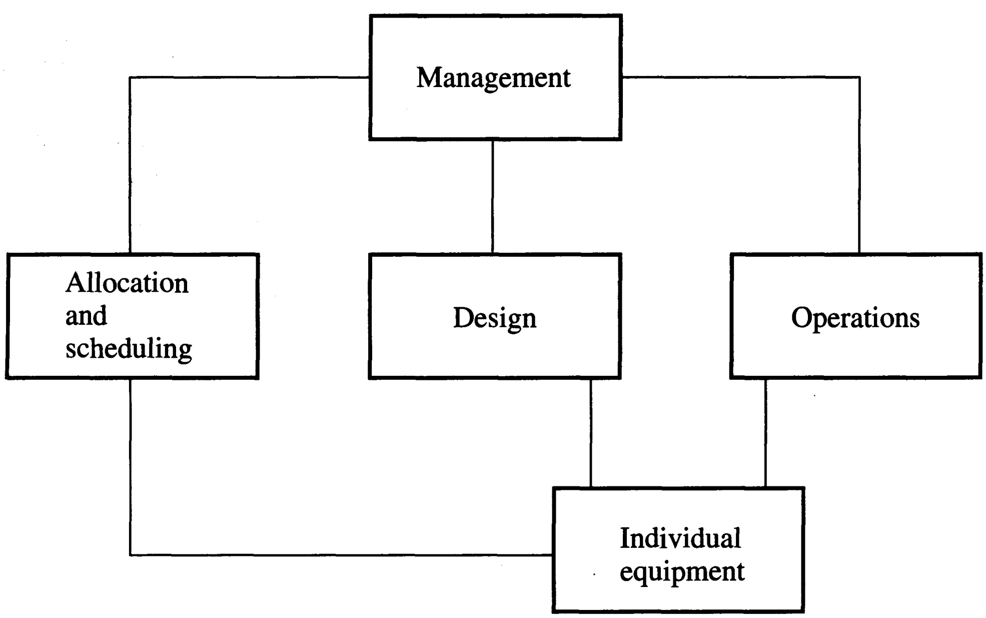


FIGURE 1.1
Hierarchy of levels of optimization.

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

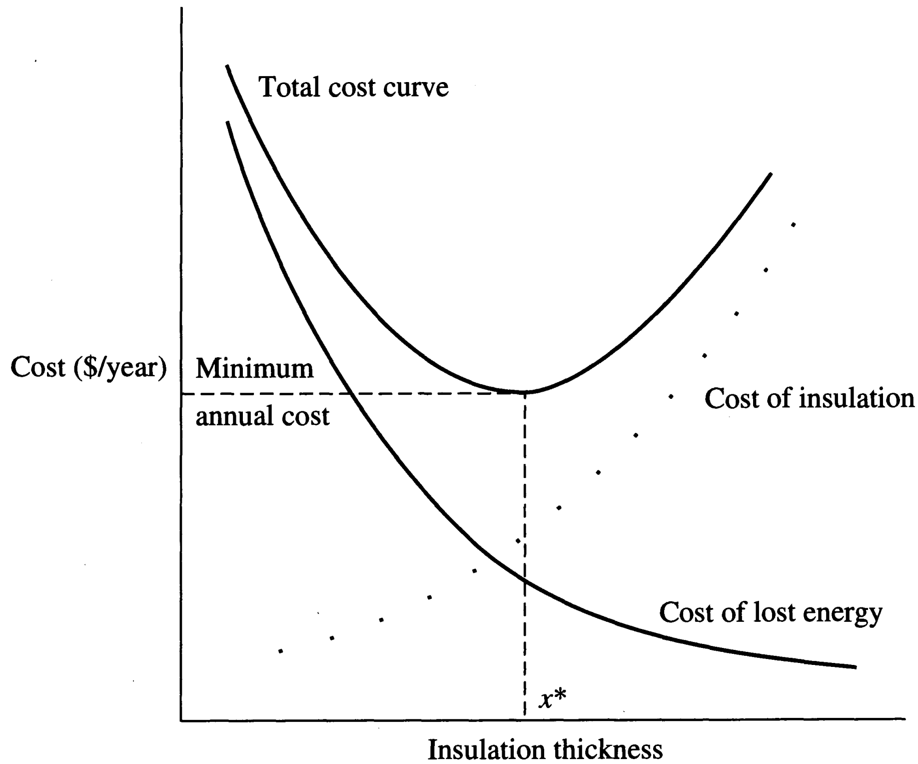


FIGURE E1.1
The effect of insulation thickness on total cost (x^* = optimum thickness). Insulation can be purchased in 0.5-in. increments. (The total cost function is shown as a smooth curve for convenience, although the sum of the two costs would not actually be smooth.)

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

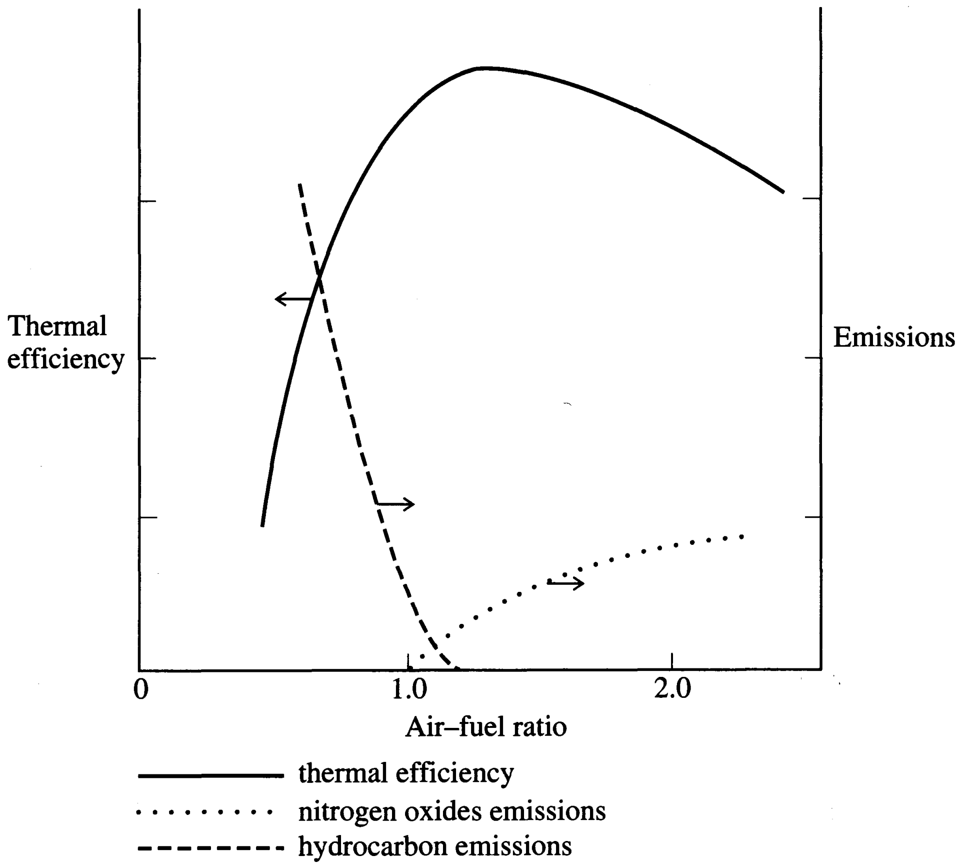


FIGURE E1.2*a*
Efficiency and emissions of a boiler as a function of air–fuel ratio. (1.0 = stoichiometric air–fuel ratio.)

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

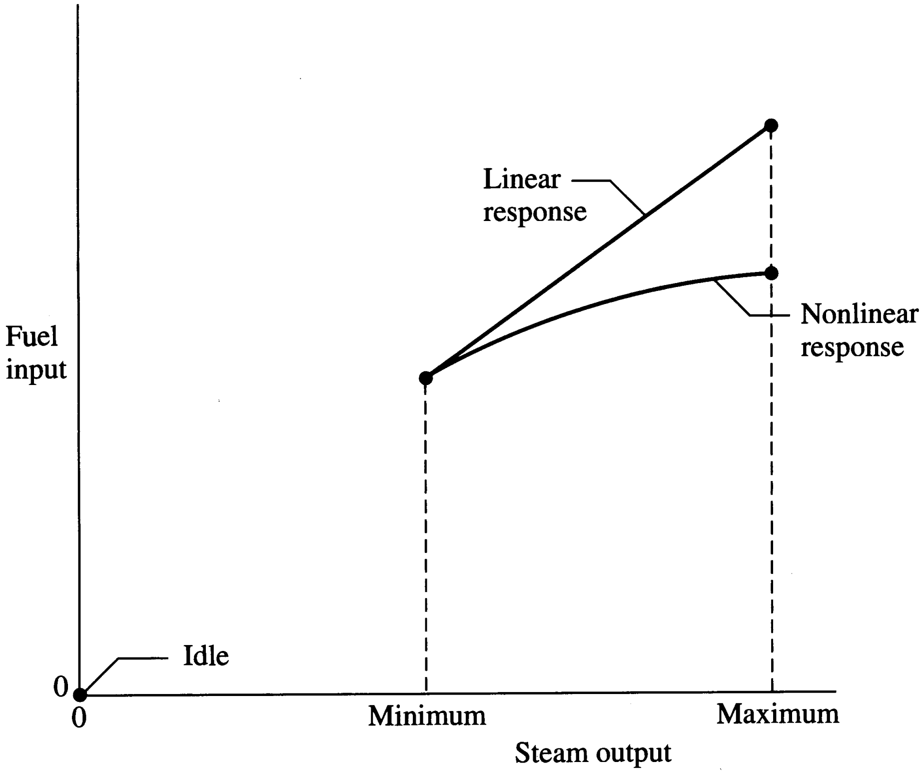


FIGURE E1.2*b*
Discontinuity in operating regimen.

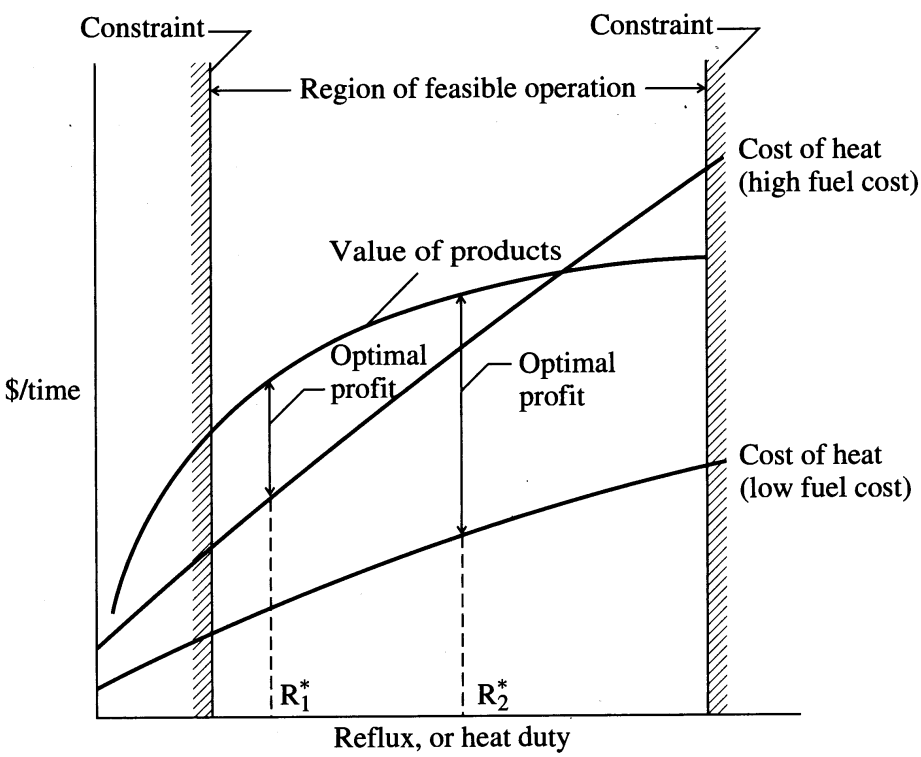


FIGURE E1.3*a*
Illustration of optimal reflux for different fuel costs.

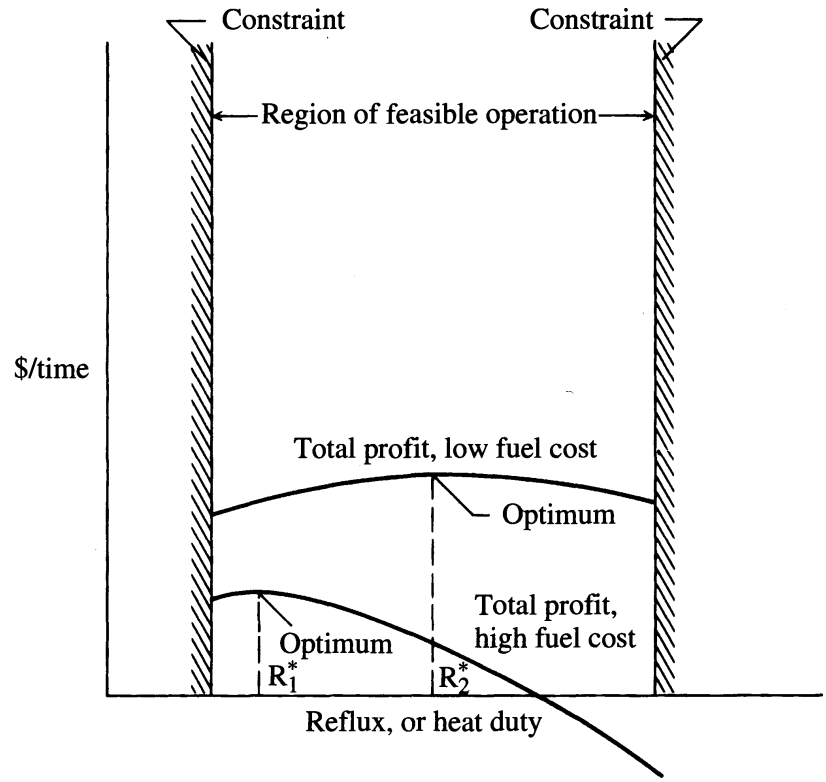


FIGURE E1.3*b*
Total profit for different fuel costs.

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

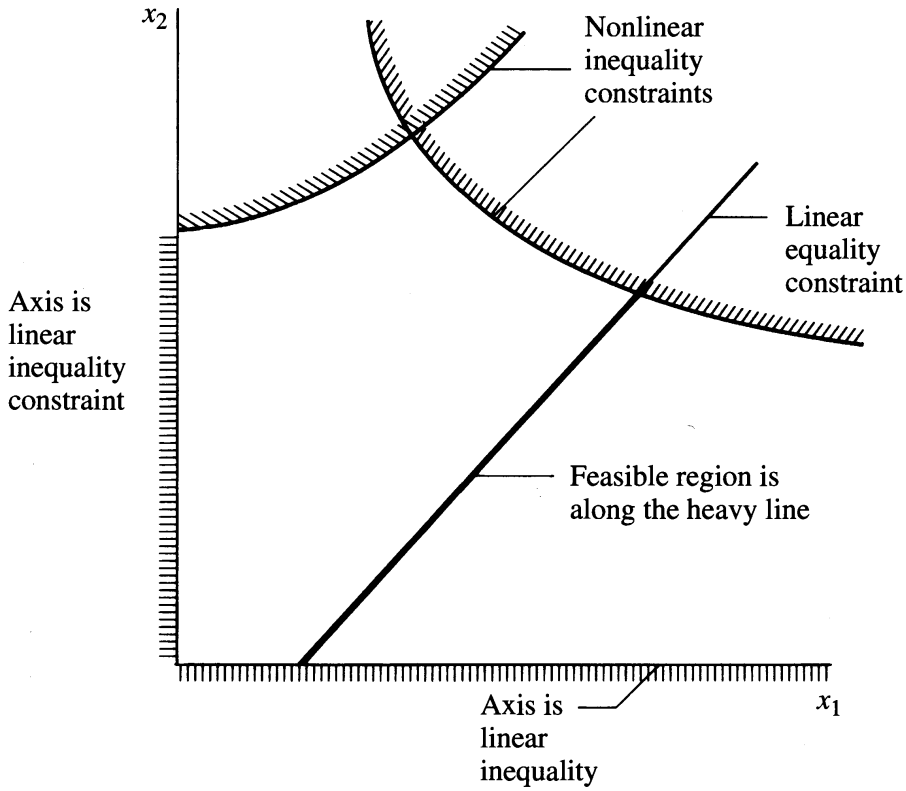


FIGURE 1.2
Feasible region for an optimization problem involving two independent variables. The dashed lines represent the side of the inequality constraints in the plane that form part of the infeasible region. The heavy line shows the feasible region.

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:

$$\text{Minimize:} \quad f(\mathbf{x}) \qquad \text{objective function} \tag{a}$$

$$\text{Subject to:} \quad \mathbf{h}(\mathbf{x}) = \mathbf{0} \qquad \text{equality constraints} \tag{b}$$

$$\mathbf{g}(\mathbf{x}) \geq \mathbf{0} \qquad \text{inequality constraints} \tag{c}$$

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

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

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.

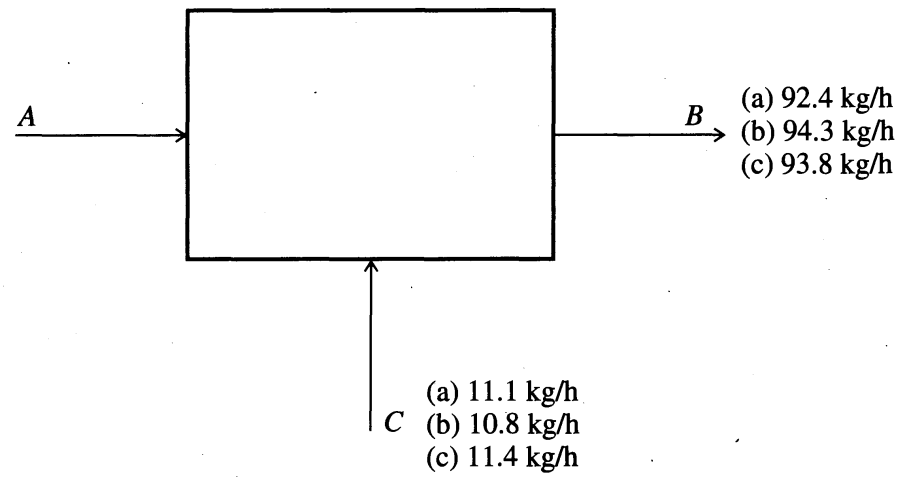


FIGURE E1.6

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:

$$\text{Cost per run} = K_2 + K_3D \qquad (a)$$

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

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

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

$$C = K_1D + n(K_2 + K_3D) \qquad (c)$$

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

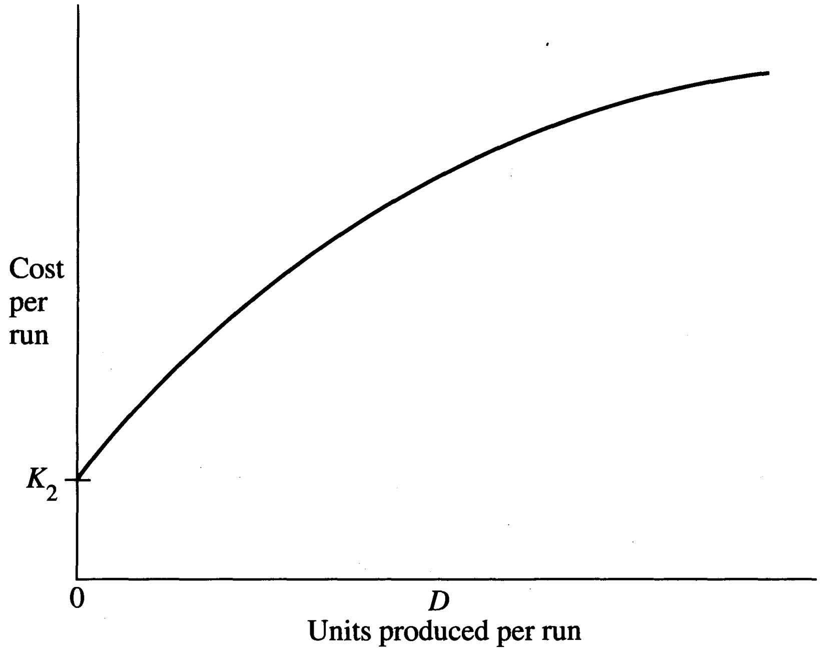


FIGURE E1.7
Nonlinear cost function for manufacturing.

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

$$\frac{dC}{dD} = K_1 - \frac{K_2Q}{D^2} = 0 \tag{e}$$

you can obtain the optimal solution for D

$$D^{\text{opt}} = \sqrt{\frac{K_2Q}{K_1}} \tag{f}$$

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.

$$\frac{d^2C}{dD^2} = \frac{2K_2Q}{D^3} > 0 \tag{g}$$

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

$$C = K_1D + \frac{K_2Q}{D} + \frac{K_4Q}{D^{1/2}} \tag{h}$$

After differentiation and equating the derivative to zero, you get

$$\frac{dC}{dD} = K_1 - \frac{K_2Q}{D^2} - \frac{K_4Q}{2D^{3/2}} = 0 \tag{i}$$

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

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

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 $20 \leq D \leq 60$ 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

$$C^{\text{opt}} = 2\sqrt{K_1K_2Q} + K_3Q \tag{k}$$

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

$$\frac{\partial C^{\text{opt}}}{\partial K_1} = \sqrt{\frac{K_2Q}{K_1}} \tag{l1}$$

$$\frac{\partial C^{\text{opt}}}{\partial K_2} = \sqrt{\frac{K_1Q}{K_2}} \tag{l2}$$

$$\frac{\partial C^{\text{opt}}}{\partial K_3} = Q \tag{l3}$$

$$\frac{\partial C^{\text{opt}}}{\partial Q} = \sqrt{\frac{K_1K_2}{Q}} + K_3 \tag{l4}$$

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.

REFERENCES

Baumol, W. J. *Economic Theory and Operations Analysis*, 3rd ed. Prentice Hall, Englewood Cliffs, New Jersey (1972).

Beveridge, G. S.; and R. S. Schechter. *Optimization: Theory and Practice*, McGraw-Hill, New York (1970).

Romagnoli, J. A.; and M. C. Sanchez, *Data Processing and Reconciliation for Chemical Process Operation.* Academic Press, New York (1999).

SUPPLEMENTARY REFERENCES

Hillier, F.; and G. Lieberman. *Introduction to Operations Research.* McGraw-Hill, New York (1995).

Peters, M. S.; and K. D. Timmerhaus. *Plant Design and Economics for Chemical Engineers.* McGraw-Hill, New York (1991).

Reklaitis, G. V.; A. Ravindran, and K. M. Ragsdell. *Engineering Optimization*. John Wiley, New York (1983).

Rudd, D. F.; and C. C. Watson, *Strategy of Process Engineering*. John Wiley, New York (1968).

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

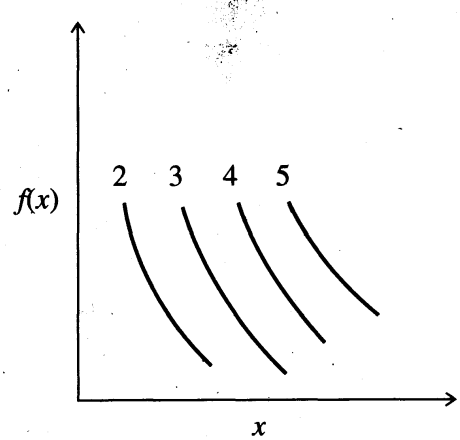


FIGURE P1.7

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.

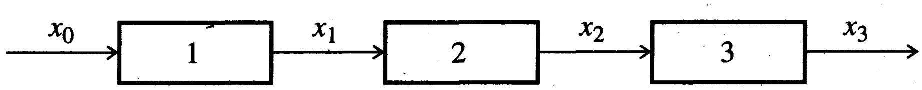


FIGURE P1.9

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.

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

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

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

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

$$x_1, x_2 \geq 0$$

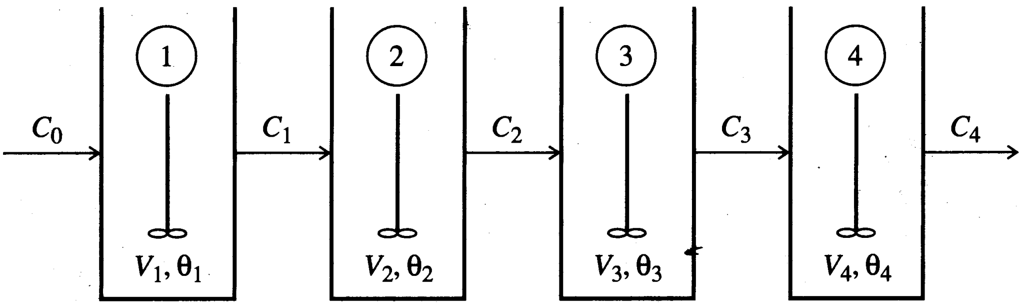


FIGURE P1.11

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 $V_i = 20\ \text{m}^3$. 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

$$\text{Maximize:} \quad \text{B}(1.0)$$

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

(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, $p_2^{\text{opt}} = 2$ 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 ($C_1D^{1.5}$ 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:

Unit	Productivity (h/batch)		
	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.

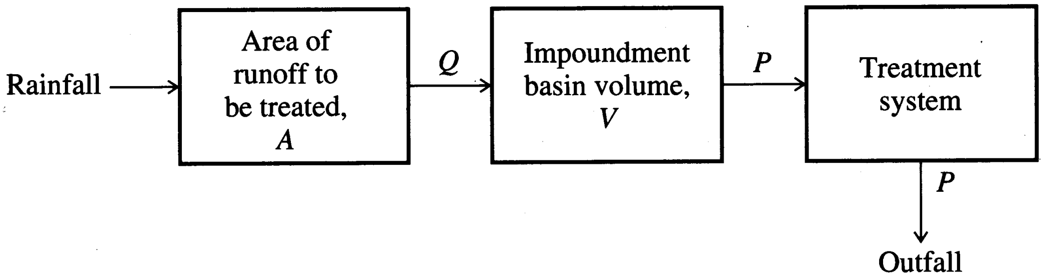


FIGURE P1.21

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?

2

DEVELOPING MODELS FOR OPTIMIZATION

CONSTRAINTS IN OPTIMIZATION arise because a process must describe the physical bounds on the variables, empirical relations, and physical laws that apply to a specific problem, as mentioned in Section 1.4. How to develop models that take into account these constraints is the main focus of this chapter. Mathematical models are employed in all areas of science, engineering, and business to solve problems, design equipment, interpret data, and communicate information. Eykhoff (1974) defined a mathematical model as "a representation of the essential aspects of an existing system (or a system to be constructed) which presents knowledge of that system in a usable form." For the purpose of optimization, we shall be concerned with developing quantitative expressions that will enable us to use mathematics and computer calculations to extract useful information. To optimize a process models may need to be developed for the objective function f, equality constraints $\mathbf{g}$, and inequality constraints $\mathbf{h}$.

Because a model is an abstraction, modeling allows us to avoid repetitive experimentation and measurements. Bear in mind, however, that a model only imitates reality and cannot incorporate all features of the real process being modeled. In the development of a model, you must decide what factors are relevant and how complex the model should be. For example, consider the following questions.

1. Should the process be modeled on a fundamental or empirical level, and what level of effort (time, expenses, manpower) is required for either approach?
2. Can the process be described adequately using physical principles?
3. What is the desired accuracy of the model, and how does its accuracy influence its ultimate use?
4. What measurements are available, and what data are available for model verification?
5. Is the process actually composed of smaller, simpler subsystems that can be more easily analyzed?

The answers to these questions depend on how the model is used. As the model of the process becomes more complex, optimization usually becomes more difficult.

In this chapter we will discuss several factors that need to be considered when constructing a process model. In addition, we will examine the use of optimization in estimating the values of unknown coefficients in models to yield a compact and reasonable representation of process data. Additional information can be found in textbooks specializing in mathematical modeling. To illustrate the need to develop models for optimization, consider the following example.

EXAMPLE 2.1 MODELING AND OPTIMIZING BLAST FURNACE OPERATION

Optimizing the operation of the blast furnace is important in every large-scale steel mill. A relatively large number of important variables (several of which cannot be measured) interact in this process in a highly complex manner, numerous constraints must be taken into account, and the age and efficiency of the plant significantly affect the optimum operating point (Deitz, 1997). Consequently, a detailed examination of this problem demonstrates the considerations involved in mathematical modeling of a typical process.

The operation of a blast furnace is semicontinuous. The raw materials are iron ore containing roughly 20 to 60 percent iron as oxides and a variety of other metallic and nonmetallic oxides. These materials are combined with coke, which reacts to form blast furnace gas. Limestone is a flux that helps separate the impurities from the hot metal by influencing the pH. Apart from the blast furnace gas, which may serve as a heating medium in other processes, the output of the furnace consists of molten iron, which includes some impurities (notably carbon and phosphorus) that must be removed in the steelmaking process, and slag, which contains most of the impurities and is of little value. Operation of the blast furnace calls for determination of the amount of each ore, a production rate, and a mode of operation that will maximize the difference between the product value and the cost of producing the required quantity and quality of molten iron. Figure E2.1 shows the flow of materials in the blast furnace, which itself is part of a much larger mill. One ton of hot metal requires about 1.7 tons of iron-bearing materials, 0.5 to 0.65 tons of coke and other fuel, 0.25 tons of fluxes, and 1.8 to 2.0 tons of air. In addition, for each ton of hot metal produced, the process creates 0.2 to 0.4 tons of slag, 0.05 tons or less of flue dust, and 2.5 to 3.5 tons of blast furnace gases. The final product, hot metal, is about 93% iron, with other trace ingredients, including sulfur, silicon, phosphorus, and manganese. The process variables and conceptual models are identified in Figure E2.1 under the column "Process Analysis," which has categories for the objective function, equality constraints, and inequality constraints.

Objective function

To formulate the objective function, two categories of costs have to be considered:

1. Costs associated with the material flows (the input and output variables), such as the costs of purchased materials.
2. Costs associated with the operations related to the process variables in the model.

The terms that make up the objective function (to be maximized) are shown in Figure E.2.1. The profit of the blast furnace can be expressed as

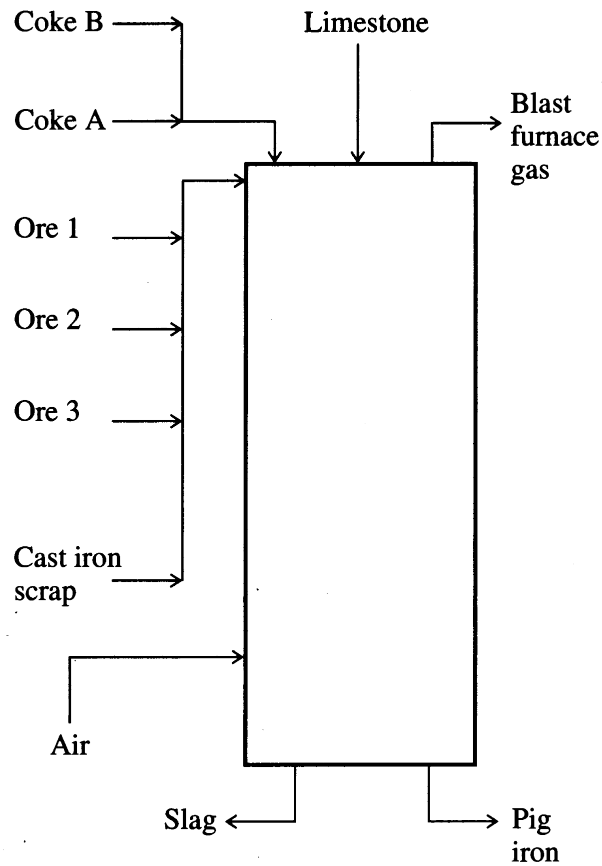
$$f = \sum_{i=7}^{8} c_i x_i - \sum_{i=1}^{6} c_i x_i$$

Equality and inequality constraints

The next step in formulating the problem is to construct a mathematical model of the process by considering the fundamental chemical and physical phenomena and physical limitations that influence the process behavior. For the case of the blast furnace, typical features are

1. *Iron ore*: Ores of different grades are available in restricted quantities. Different ores have varying percentages of iron and different types and amounts of impurities. The proportion of each ore that occurs in the final hot metal is assumed to be fixed by its composition. For example, the amount of fine ore must be limited because too much can disrupt the flow of gas through the furnace and limit production.
2. *Coke*: The amount of coke that may be burned in any furnace is effectively limited by the furnace design, and the hot metal temperature is controlled by the amount

Process



Process Analysis

Objective Function Components

Associated Costs and Revenues:

Ore 1: x_1	material cost c_1
Ore 2: x_2	material cost c_2
Ore 3: x_3	material cost c_3
Cast iron scrap: x_4	material cost c_4
Coke A: x_5	material cost c_5
Coke B: x_6	material c_6
Pig iron: x_7	sales price c_7
Blast furnace gas: x_8	assigned value: c_8

Constraints

Equalities

Material and Energy Balances:

Metal (iron) balance
Slag balance
Carbon balance
Gas balance
Elemental balances (O, H, S, Si, Al, Ca, Mg, P, Ti, K, Cu, Mo, Mn, etc.)
Energy balance

Inequalites

Process Limits:

Coke throughput
Hot metal production rate
Slag volume
Ore availability
Elements in slag
Elements in metal
Basicity
Sales limits

FIGURE E.2.1
Objective function components and types of constraints for a blast furnace.

of coke (or carbon). The coke consumption rate can be based on empirical relationships developed through regression of furnace data.

3. *Slag*: For technical reasons, the level of impurities in the slag must be controlled. There is an upper limit on the percentage of magnesium, upper and lower limits on the percentage of silicon and aluminum, and close limits on the "basicity" ratio $(CaO + MgO)/(SiO_2 + A1_2O_3)$. The basicity ratio controls the viscosity and melting point of the slag, which in turn affect the hearth temperature and grade of iron produced.

The basicity ratio can be expressed in terms of the blast furnace feeds x_i as follows:

$$\frac{\sum_{i=1}^{4} w_{2i}x_i + \sum_{i=1}^{4} w_{3i}x_i}{\sum_{i=1}^{4} w_{4i}x_i + \sum_{i=1}^{4} w_{5i}x_i}$$

where w_{2i} = weight fraction of CaO in feed i
w_{3i} = weight fraction of MgO in feed i
w_{4i} = weight fraction of SiO_2 in feed i
w_{5i} = weight fraction of $A1_2O_3$ in feed i

4. *Phosphorus*: All phosphorus in the raw material finds its way into the molten metal. There is an upper limit on the phosphorus permitted, although precise quantities are sometimes prescribed. In general, it is cheaper to produce higher phosphorus iron, but more expensive to refine it.

From these and other considerations you can prepare:

1. A set of input and output variables.
2. A set of steady-state input–output material and energy balances (equality constraints).
3. A set of explicit empirical relations (equality constraints).
4. A set of restrictions (inequality constraints) on the input and output variables as indicated in Figure E.2.1.

2.1 CLASSIFICATION OF MODELS

Two general categories of models exist:

1. Those based on physical theory.
2. Those based on strictly empirical descriptions (so-called black box models).

Mathematical models based on physical and chemical laws (e.g., mass and energy balances, thermodynamics, chemical reaction kinetics) are frequently employed in optimization applications (refer to the examples in Chapters 11 through 16). These models are conceptually attractive because a general model for any system size can be developed even before the system is constructed. A detailed exposition of fundamental mathematical models in chemical engineering is beyond our scope here, although we present numerous examples of physiochemical models throughout the book, especially in Chapters 11 to 16. Empirical models, on the other hand, are attractive when a physical model cannot be developed due to limited time or resources. Input–output data are necessary in order to fit unknown coefficients in either type of the model.

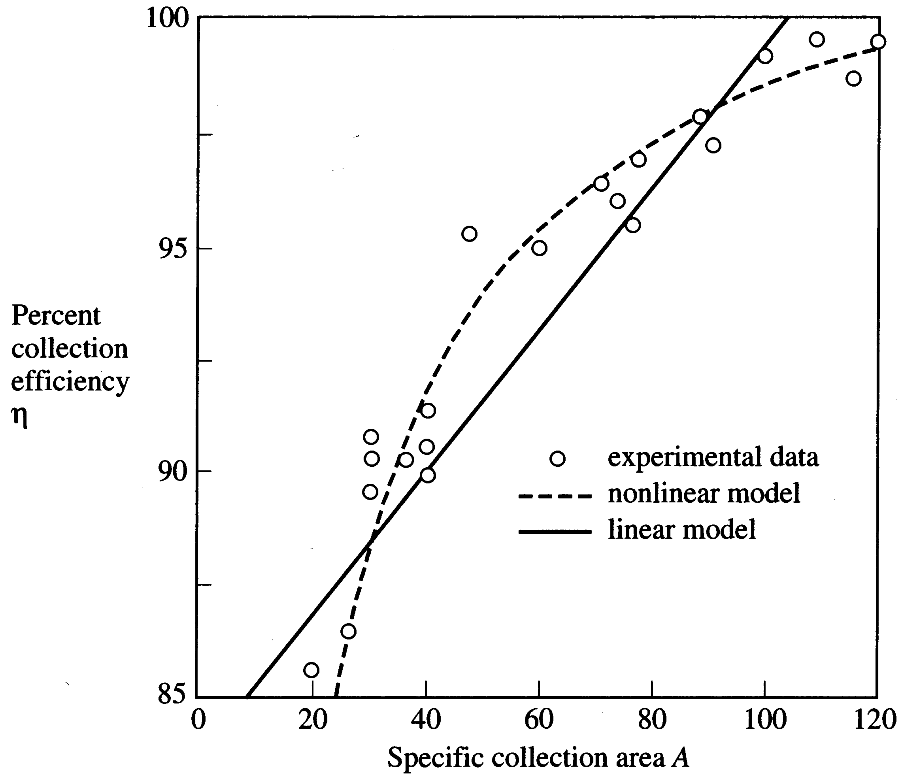


FIGURE E2.2
ESP collection efficiency versus specific collection area for a linear model $\eta = 0.129A + 85.7$ and a nonlinear model $\eta = 100\{1 - [e^{-0.0264A}/(4.082 - 3.15 \times 10^{-6} A)]\}$.

EXAMPLE 2.2 MODELS OF AN ELECTROSTATIC PRECIPITATOR

A coal combustion pilot plant is used to obtain efficiency data on the collection of particulate matter by an electrostatics precipitator (ESP). The ESP performance is varied by changing the surface area of the collecting plates. Figure E2.2 shows the data collected to estimate the coefficients in a model to represent efficiency η as a function of the specific collection area A, measured as plate area/volumetric flow rate.

Two models of different complexity have been proposed to fit the performance data:

$$\text{Model 1:} \quad \eta = b_1 A + b_2$$

$$\text{Model 2:} \quad \eta = 100\left[1 - \frac{e^{-\gamma_1 A}}{\gamma_2 + \gamma_3 A}\right]$$

Model 1 is linear in the coefficients, and model 2 is nonlinear in the coefficients. The mathematical structure of model 2 has a fundamental basis that takes into account the physical characteristics of the particulate matter, including particle size and electrical properties, but we do not have the space to derive the equation here.

Which model is better?

Solution. The coefficients in the two models were fitted using MATLAB, yielding the following results:

Model 1: $b_1 = 0.129 \quad b_2 = 85.7$

Model 2: $\gamma_1 = 0.0264 \quad \gamma_2 = 4.082 \quad \gamma_3 = -0.00000315$

As can be seen in Figure E2.2, model 2 provides a better fit than model 1 over the range of areas A considered, but model 2 may present some difficulties when used as a constraint inserted into an optimization code.

The electrostatic precipitator in Example 2.2 is typical of industrial processes; the operation of most process equipment is so complicated that application of fundamental physical laws may not produce a suitable model. For example, thermodynamic or chemical kinetics data may be required in such a model but may not be available. On the other hand, although the development of black box models may require less effort and the resulting models may be simpler in form, empirical models are usually only relevant for restricted ranges of operation and scale-up. Thus, a model such as ESP model 1 might need to be completely reformulated for a different size range of particulate matter or for a different type of coal. You might have to use a series of black box models to achieve suitable accuracy for different operating conditions.

In addition to classifying models as theoretically based versus empirical, we can generally group models according to the following types:

Linear versus nonlinear.
Steady state versus unsteady state.
Lumped parameter versus distributed parameter.
Continuous versus discrete variables.

Linear versus nonlinear

Linear models exhibit the important property of superposition; nonlinear ones do not. Equations (and hence models) are linear if the dependent variables or their derivatives appear only to the first power: otherwise they are nonlinear. In practice the ability to use linear models is of great significance because they are an order of magnitude easier to manipulate and solve than nonlinear ones.

To test for the linearity of a model, examine the equation(s) that represents the process. If any one term is nonlinear, the model itself is nonlinear. By implication, the process is nonlinear.

Examine models 1 and 2 for the electrostatic precipitator. Is model 1 linear in A? Model 2? The superposition test in each case is: Does

$$J(ax_1 + bx_2) = aJ(x_1) + bJ(x_2) \tag{2.1a}$$

and

$$J(kx) = kJ(x) \tag{2.1b}$$

where J = any operator contained in the model such as square, differentiation, and so on.
k = a constant
x_1 and x_2 = variables

ESP model 1 is linear in A

$$J(b_1A + b_2) = b_1J(A) + b_2$$

but ESP model 2 is nonlinear because

$$\left(\frac{e^{-\gamma_1(A_1 + A_2)}}{\gamma_2 + \gamma_3(A_1 + A_2)}\right) \neq \left(\frac{e^{-\gamma_1 A_1}}{\gamma_2 + \gamma_3 A_2}\right) + \left(\frac{e^{-\gamma_1 A_2}}{\gamma_2 + \gamma_3 A_2}\right)$$

Steady state versus unsteady state

Other synonyms for steady state are time-invariant, static, or stationary. These terms refer to a process in which the values of the dependent variables remain constant with respect to time. Unsteady state processes are also called nonsteady state, transient, or dynamic and represent the situation when the process-dependent variables change with time. A typical example of an unsteady state process is the operation of a batch distillation column, which would exhibit a time-varying product composition. A transient model reduces to a steady state model when $\partial/\partial t = 0$. Most optimization problems treated in this book are based on steady state models. Optimization problems involving dynamic models usually pertain to "optimal control" or real-time optimization problems (see Chapter 16)

Distributed versus lumped parameters

Briefly, a lumped parameter representation means that spatial variations are ignored and that the various properties and the state of the system can be considered homogeneous throughout the entire volume. A distributed parameter representation, on the other hand, takes into account detailed variations in behavior from point to point throughout the system. In Figure 2.1, compare these definitions for a well-stirred reactor and a tubular reactor with axial flow. In the first case, we assume that mixing is complete so no concentration or temperature gradient occurs in the reactor, hence a lumped parameter mathematical model would be appropriate. In contrast, the tubular reactor has concentration or temperature variations along the axial direction and perhaps in the radial direction, hence a distributed parameter model would be required. All real systems are, of course, distributed because some variations of states occur throughout them. Because the spatial variations often are relatively small, they may be ignored, leading to a lumped approximation. If both spatial and transient characteristics are to be included in a model, a partial differential equation or a series of stages is required to describe the process behavior.

It is not easy to determine whether lumping in a process model is a valid technique for representing the process. A good rule of thumb is that if the response is essentially the same at all points in the process, then the model can be lumped as a single unit. If the response shows significant instantaneous differences in any direction along the vessel, then the problem should be treated using an appropriate differential equation or series of compartments. In an optimization problem it is desirable to simplify a distributed model by using an equivalent lumped parameter system, although you must be careful to avoid masking the salient features of the distributed element (hence building an inadequate model). In this text, we will mainly consider optimization techniques applied to lumped systems.

Continuous versus discrete variables

Continuous variables can assume any value within an interval; discrete variables can take only distinct values. An example of a discrete variable is one that assumes integer values only. Often in chemical engineering discrete variables and continuous variables occur simultaneously in a problem. If you wish to optimize a compressor system, for example, you must select the number of compressor stages (an integer) in addition to the suction and production pressure of each stage (positive continuous variables). Optimization problems without discrete variables are far easier to solve than those with even one discrete variable. Refer to Chapter 9 for more information about the effect of discrete variables in optimization.

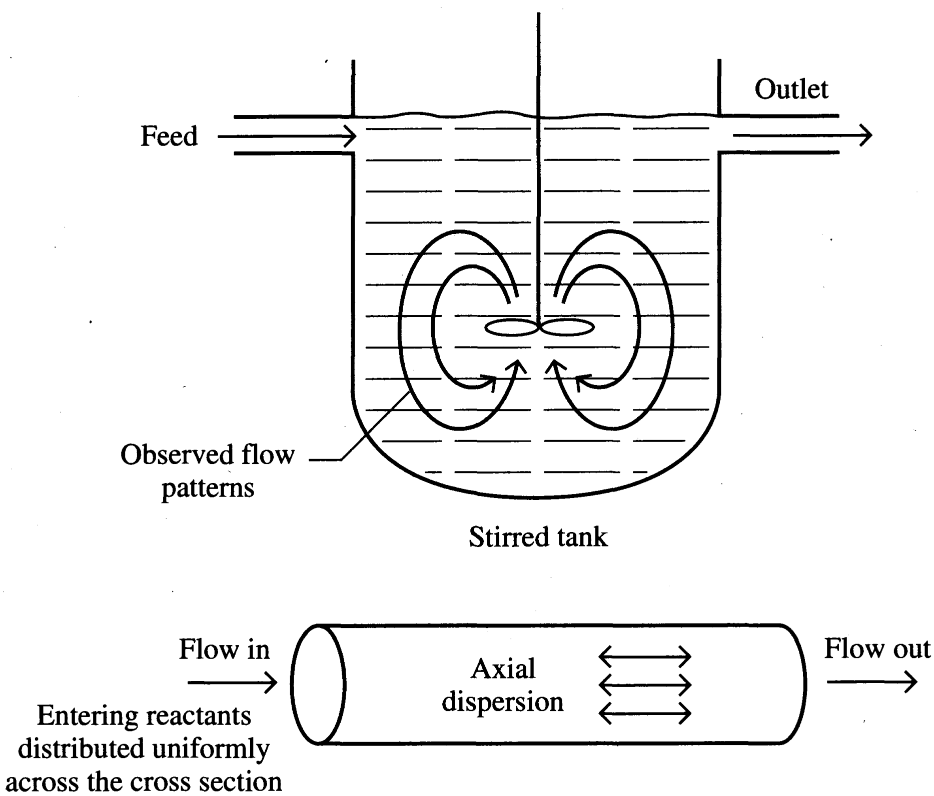


FIGURE 2.1
Flow patterns in a stirred tank (lumped parameter system) and a tubular reactor (distributed parameter system).

An engineer typically strives to treat discrete variables as continuous even at the cost of achieving a suboptimal solution when the continuous variable is rounded off. Consider the variation of the cost of insulation of various thickness as shown in Figure E1.1. Although insulation is only available in 0.5-in. increments, continuous approximation for the thickness can be used to facilitate the solution to this optimization problem.

2.2 HOW TO BUILD A MODEL

For convenience of presentation, model building can be divided into four phases: (1) problem definition and formulation, (2) preliminary and detailed analysis, (3) evaluation, and (4) interpretation application. Keep in mind that model building is an iterative procedure. Figure 2.2 summarizes the activities to be carried out,

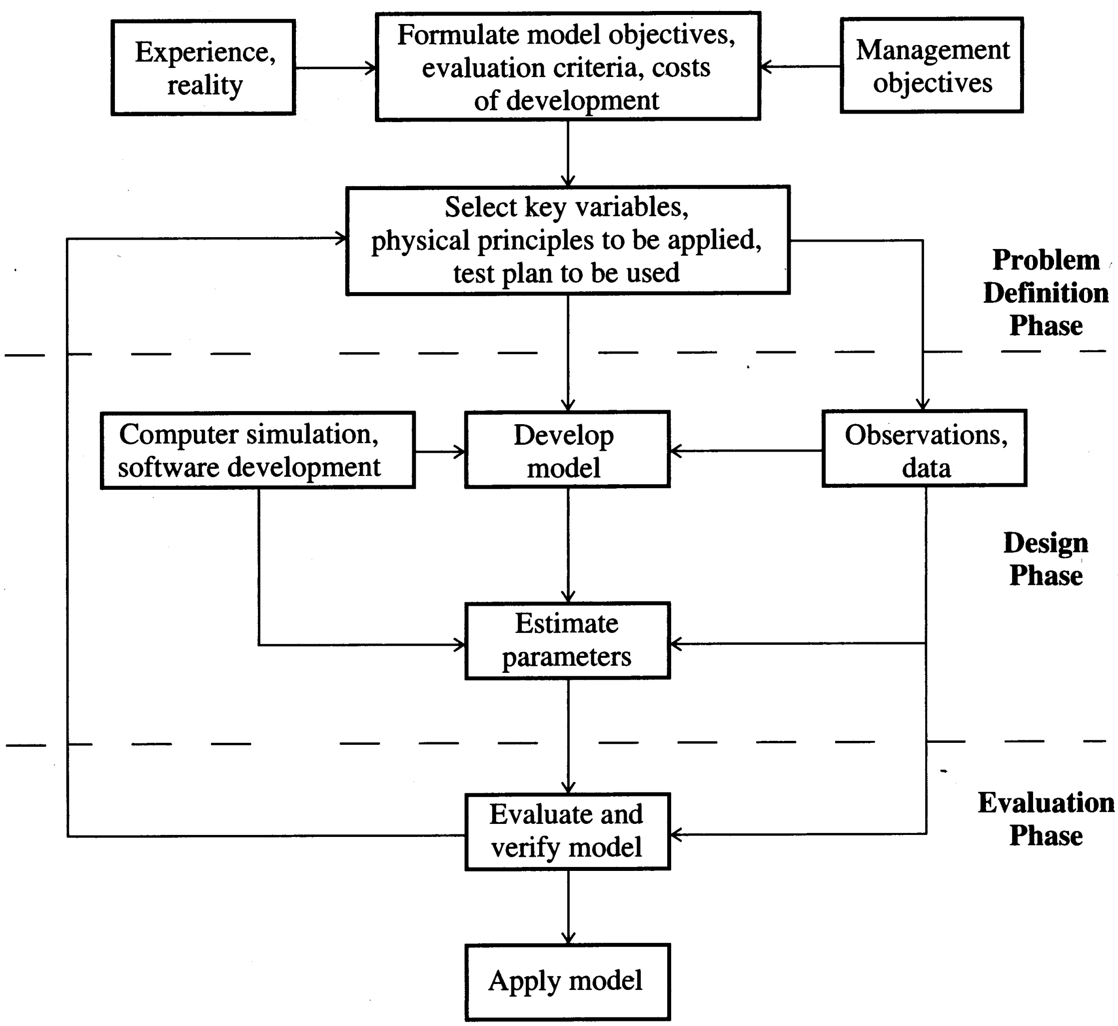


FIGURE 2.2
Major activities in model building prior to application.

which are discussed in detail later on. The content of this section is quite limited in scope; before actually embarking on a comprehensive model development program, consult textbooks on modeling (see References).

Problem definition and formulation phase

In this phase the problem is defined and the important elements that pertain to the problem and its solution are identified. The degree of accuracy needed in the model and the model's potential uses must be determined. To evaluate the structure and complexity of the model, ascertain

1. The number of independent variables to be included in the model.
2. The number of independent equations required to describe the system (sometimes called the "order" of the model).
3. The number of unknown parameters in the model.

In the previous section we addressed some of these issues in the context of physical versus empirical models. These issues are also intertwined with the question of model verification: what kinds of data are available for determining that the model is a valid description of the process? Model building is an iterative process, as shown by the recycling of information in Figure 2.2.

Before carrying out the actual modeling, it is important to evaluate the economic justification for (and benefits of) the modeling effort and the capability of support staff for carrying out such a project. Primarily, determine that a successfully developed model will indeed help solve the optimization problem.

Design phase

The design phase includes specification of the information content, general description of the programming logic and algorithms necessary to develop and employ a useful model, formulation of the mathematical description of such a model, and simulation of the model. First, define the input and output variables, and determine what the "system" and the "environment" are. Also, select the specific mathematical representation(s) to be used in the model, as well as the assumptions and limitations of the model resulting from its translation into computer code. Computer implementation of the model requires that you verify the availability and adequacy of computer hardware and software, specify computer input–output media, develop program logic and flowsheets, and define program modules and their structural relationships. Use of existing subroutines and databases saves you time but can complicate an optimization problem for the reasons explained in Chapter 15.

Evaluation phase

This phase is intended as a final check of the model as a whole. Testing of individual model elements should be conducted during earlier phases. Evaluation of the model is carried out according to the evaluation criteria and test plan established in the problem definition phase. Next, carry out sensitivity testing of the model inputs and parameters, and determine if the apparent relationships are physically meaningful. Use actual data in the model when possible. This step is also referred to as diagnostic checking and may entail statistical analysis of the fitted parameters (Box et al., 1978).

Model validation requires confirming logic, assumptions, and behavior. These tasks involve comparison with historical input–output data, or data in the literature, comparison with pilot plant performance, and simulation. In general, data used in formulating a model should not be used to validate it if at all possible. Because model evaluation involves multiple criteria, it is helpful to find an expert opinion in the verification of models, that is, what do people think who know about the process being modeled?

No single validation procedure is appropriate for all models. Nevertheless, it is appropriate to ask the question: What do you want the model to do? In the best of all possible worlds, you want the model to predict the desired process performance with suitable accuracy, but this is often an elusive goal.

2.3 SELECTING FUNCTIONS TO FIT EMPIRICAL DATA

A model relates the output (the dependent variable or variables) to the independent variable(s). Each equation in the model usually includes one or more coefficients that are presumed constant. The term *parameter* as used here means coefficient and possibly input or initial condition. With the help of experimental data, we can determine the *form* of the model and subsequently (or simultaneously) estimate the value of some or all of the parameters in the model.

2.3.1 How to Determine the Form of a Model

Models can be written in a variety of mathematical forms. Figure 2.3 shows a few of the possibilities, some of which were already illustrated in Section 2.1. This section focuses on the simplest case, namely models composed of algebraic equations, which constitute the bulk of the equality constraints in process optimization. Emphasis here is on estimating the coefficients in simple models and not on the complexity of the model.

Selection of the form of an empirical model requires judgment as well as some skill in recognizing how response patterns match possible algebraic functions. Optimization methods can help in the selection of the model structure as well as in the estimation of the unknown coefficients. If you can specify a quantitative criterion that defines what "best" represents the data, then the model can be improved by adjusting its form to improve the value of the criterion. The best model presumably exhibits the least error between actual data and the predicted response in some sense.

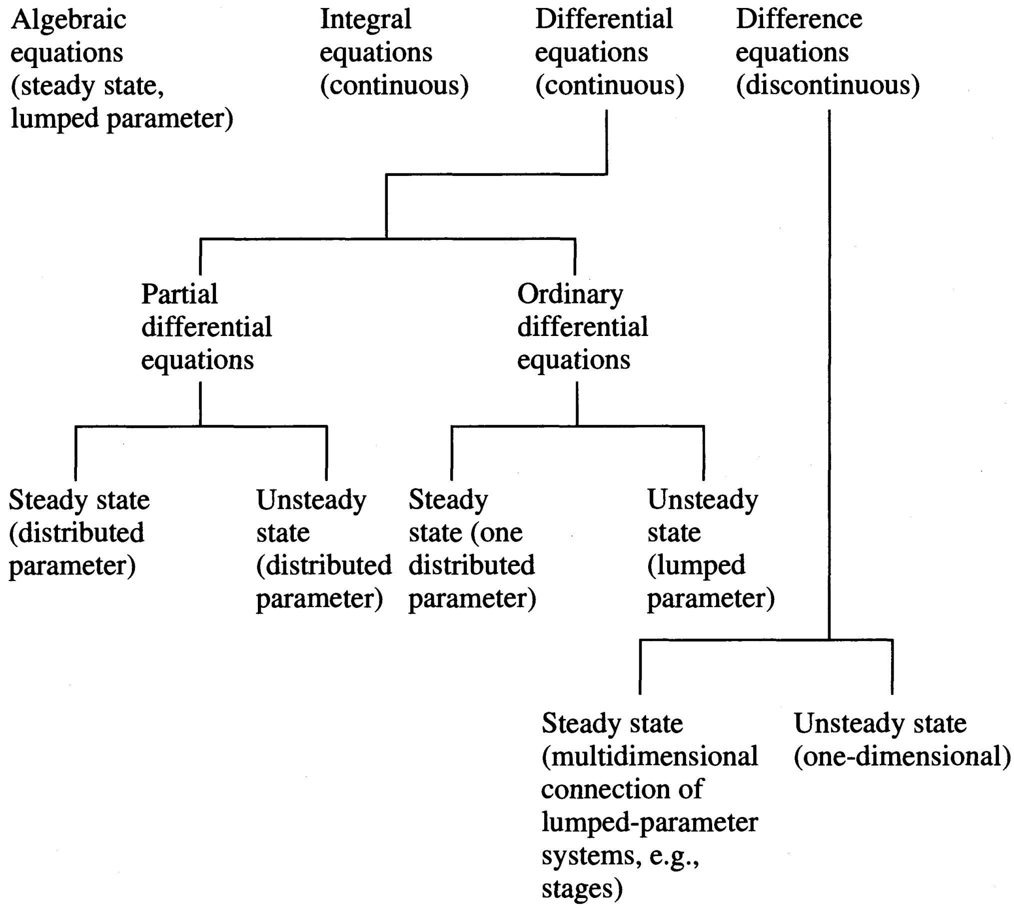


FIGURE 2.3
Typical mathematical forms of models.

Typical relations for empirical models might be

$y = a_0 + a_1x_1 + a_2x_2 + \cdots$	linear in the variables and coefficients
$y = a_0 + a_{11}x_1^2 + a_{12}x_1x_2 + \cdots$	linear in the coefficients, nonlinear in the variables (x_1, x_2)
$G(s) = \dfrac{1}{a_0 + a_1s + a_2s^2}$	nonlinear in all the coefficients
$\mathrm{Nu} = a(\mathrm{Re})^b$	nonlinear in the coefficient b (Nu: Nusselt number; Re: Reynolds number)

When the model is linear in the coefficients, they can be estimated by a procedure called *linear regression*. If the model is nonlinear in the coefficients, estimating them is referred to as *nonlinear regression*. In either case, the simplest adequate model (with the fewest number of coefficients) should be used.

Graphical presentation of data assists in determining the form of the function of a single variable (or two variables). The response y versus the independent variable x can be plotted and the resulting form of the model evaluated visually. Figure 2.4 shows experimental heat transfer data plotted on log–log coordinates. The plot

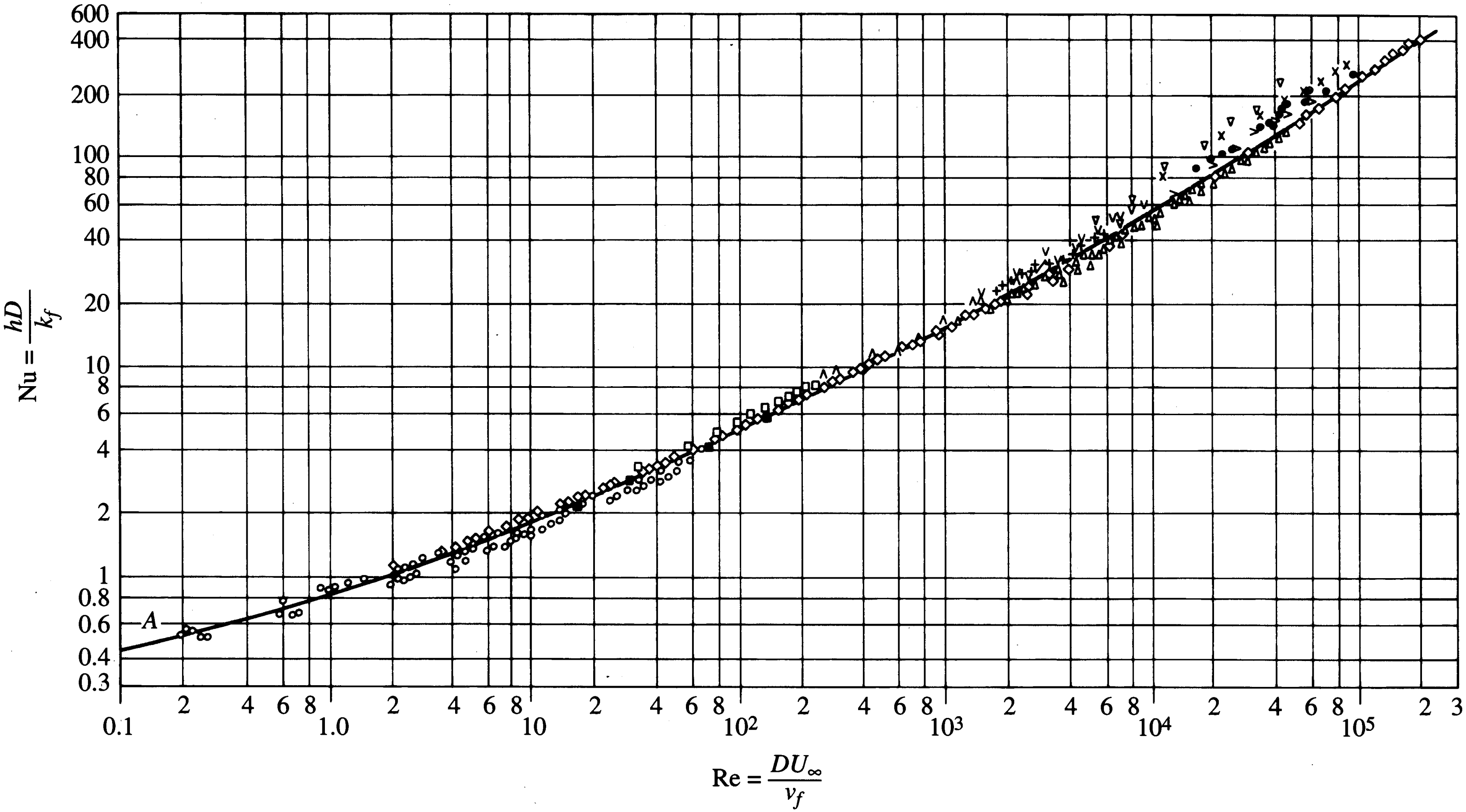


FIGURE 2.4
Average Nusselt number (Nu) versus Reynolds number (Re) for a circular cylinder in air, placed normal to the flow (McAdams, 1954, with permission from McGraw-Hill Companies).

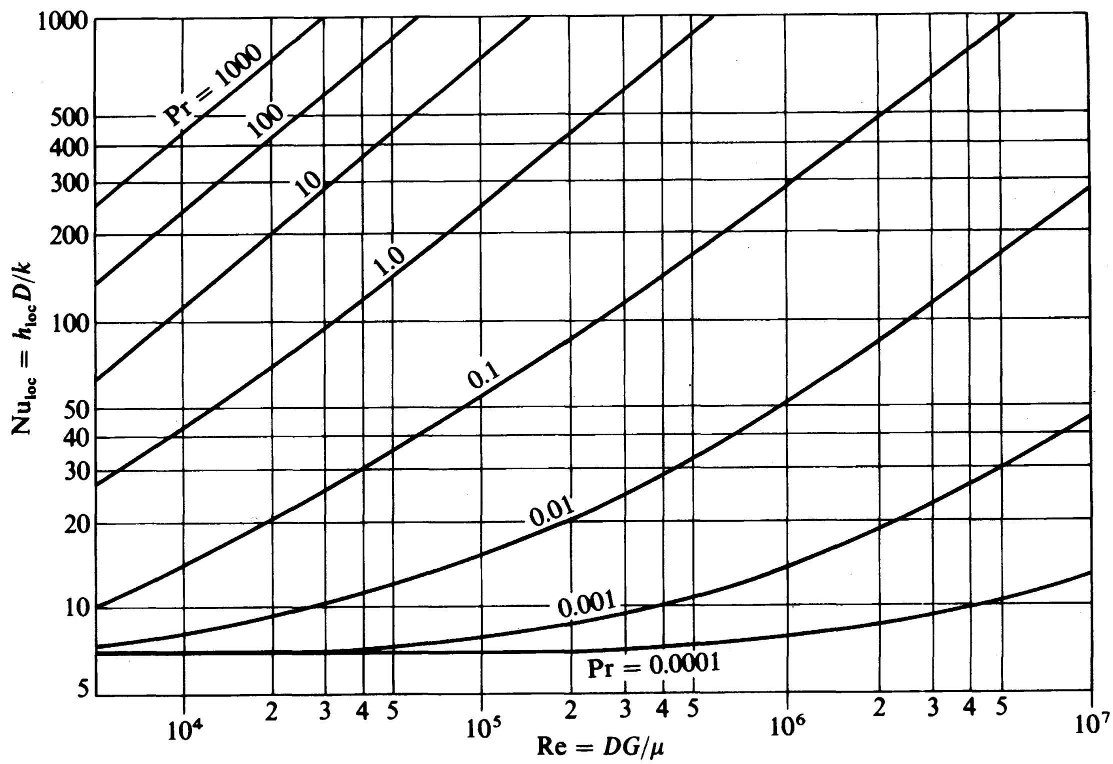
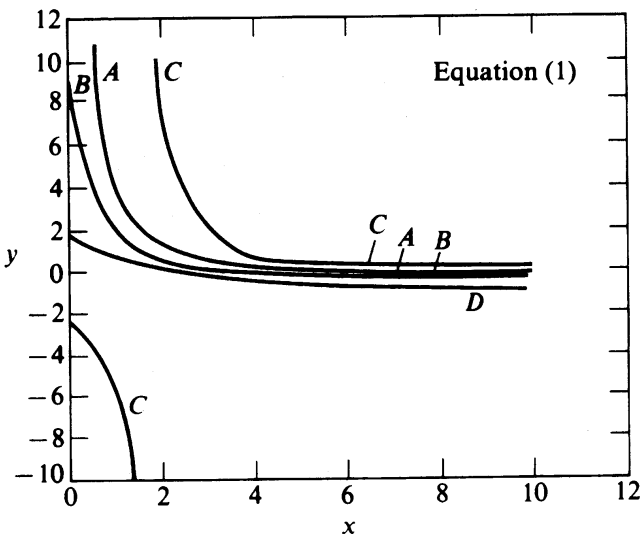


FIGURE 2.5
Predicted Nusselt numbers for turbulent flow with constant wall heat flux (*adapted with permission from John Wiley and Sons from Bird et al., 1964*). *Abbreviations*: Nu = Nusselt number; Re = Reynolds number; Pr = Prandtl number.

appears to be approximately linear over wide ranges of the Reynolds number (Re). A straight line in Figure 2.4 would correspond to log Nu = log a + b log Re or Nu = $a(\text{Re})^b$. Observe the scatter of experimental data in Figure 2.4, especially for large values of the Re.

If two independent variables are involved in the model, plots such as those shown in Figure 2.5 can be of assistance; in this case the second independent variable becomes a parameter that is held constant at various levels. Figure 2.6 shows a variety of nonlinear functions and their associated plots. These plots can assist in selecting relations for nonlinear functions of y versus x. Empirical functions of more than two variables must be built up (or pruned) step by step to avoid including an excessive number of irrelevant variables or missing an important one. Refer to Section 2.4 for suitable procedures.

Now let us review an example for selecting the form of a model to fit experimental data.



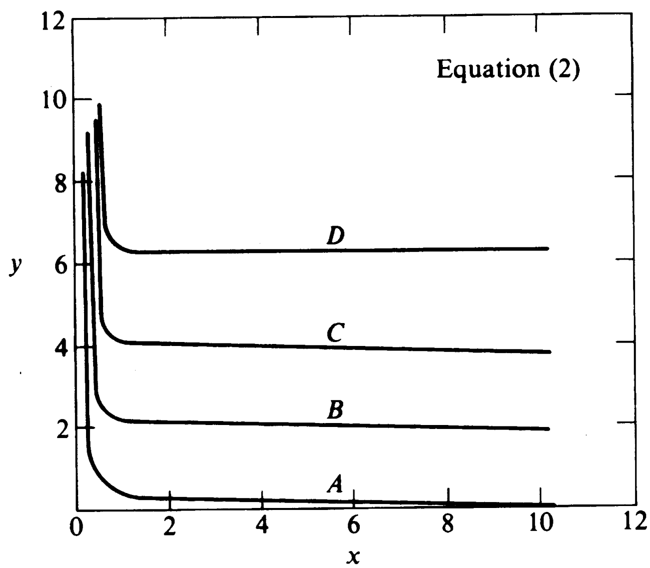
(1) $\frac{1}{y} = \alpha - \beta x$

A. $\frac{1}{y} = -0.1 - 0.3x$

B. $\frac{1}{y} = 0.1 - 0.3x$

C. $\frac{1}{y} = -0.5 - 0.3x$

D. $\frac{1}{y} = 0.5 + 0.3x$



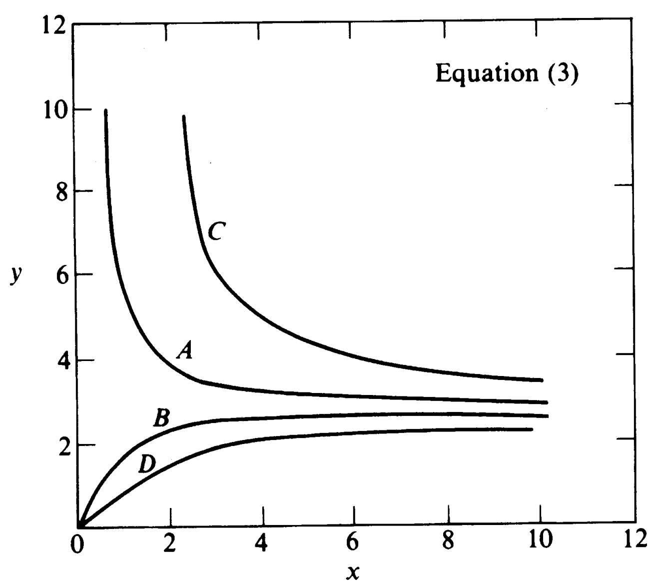
(2) $y = \alpha + \frac{\beta}{x}$

A. $y = -0.1 + \frac{0.3}{x}$

B. $y = 2 + \frac{0.3}{x}$

C. $y = 4 + \frac{0.3}{x}$

D. $y = 6 + \frac{0.3}{x}$



(3) $\frac{x}{y} = \alpha + \beta x$

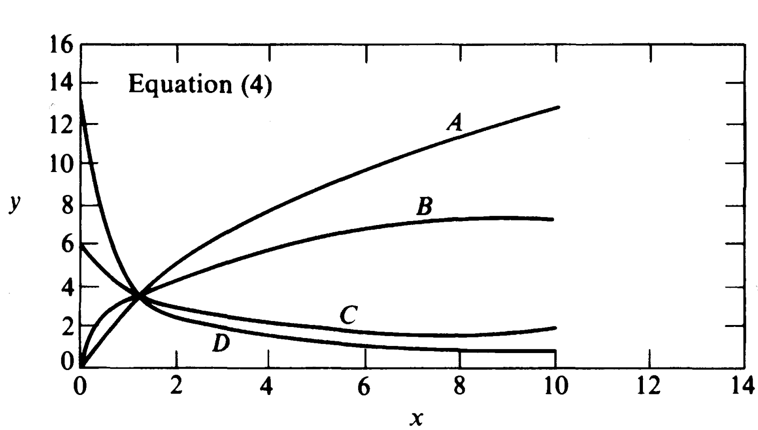
A. $\frac{x}{y} = -0.1 + 0.3x$

B. $\frac{x}{y} = 0.1 + 0.3x$

C. $\frac{x}{y} = -0.4 + 0.3x$

D. $\frac{x}{y} = 4 + 0.3x$

FIGURE 2.6
Functions of a single variable x and their corresponding trajectories. (*Continues*)



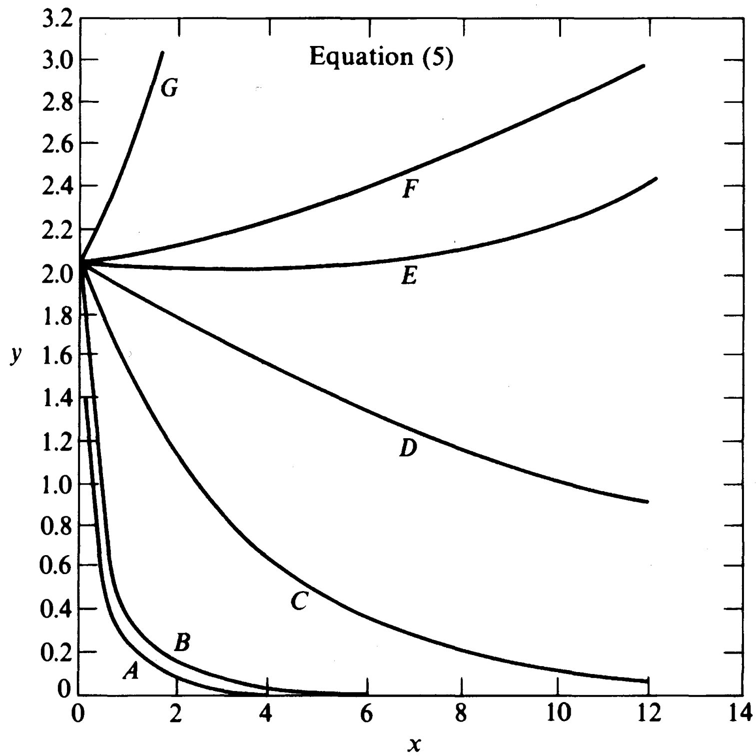
(4) $y = \alpha x^{\beta}$

A. $y = 4x^{0.5}$

B. $y = 4x^{0.3}$

C. $y = 4x^{-0.3}$

D. $y = 4x^{-0.5}$



(5) $y = \alpha \beta^{x}$

A. $y = 2(0.2)^x$

B. $y = 2(0.3)^x$

C. $y = 2(0.8)^x$

D. $y = 2(0.95)^x$

E. $y = 2(1.02)^x$

F. $y = 2(1.04)^x$

G. $y = 2(1.3)^x$

FIGURE 2.6 *(continued)*

EXAMPLE 2.3 ANALYSIS OF THE HEAT TRANSFER COEFFICIENT

Suppose the overall heat transfer coefficient of a shell-and-tube heat exchanger is calculated daily as a function of the flow rates in both the shell and tube sides (w_s and w_t, respectively). U has the units of Btu/(h)(°F)(ft^2), and w_s and w_t are in lb/h. Figures E2.3a and E2.3b illustrate the measured data. Determine the form of a semiempirical model of U versus w_s and w_t based on physical analysis.

Solution. You could elect to simply fit U as a polynomial function of w_s and w_t; there appears to be very little effect of w_s on U, but U appears to vary linearly with w_t (except at the upper range of w_t where it begins to level off). A more quantitative approach can be based on a physical analysis of the exchanger. First determine why w_s has no effect on U. This result can be explained by the formula for the overall heat transfer coefficient

$$\frac{1}{U} = \frac{1}{h_s} + \frac{1}{h_t} + \frac{1}{h_f} \tag{a}$$

where h_s = the shell heat transfer coefficient
h_t = the tube side heat transfer coefficient
h_f = the fouling coefficient

If h_t is small and h_s is large, U is dominated by h_t, hence changes in w_s have little effect, as shown in Figure E2.3a.

Next examine the data for U versus w_t in the context of Figure 2.6. For a reasonable range of w_t the pattern is similar to curve D in Equation (3) where

$$\frac{x}{y} = \alpha + \beta x \tag{b}$$

which can also be written as

$$\frac{1}{y} = \frac{\alpha}{x} + \beta \tag{c}$$

Note the similarity between Equations (c) and (a), where $x = h_t$ and $y = U$. From a standard heat transfer coefficient correlation (Gebhart, 1971), you can find that h_t also varies according to $K_t w_t^{0.8}$, where K_t is a coefficient that depends on the fluid physical properties and the exchanger geometry. If we lump $1/h_s$ and $1/h_f$ together into one constant $1/h_{sf}$, the semiempirical model becomes

$$\frac{1}{U} = \frac{1}{h_{sf}} + \frac{1}{K_t w_t^{0.8}}$$

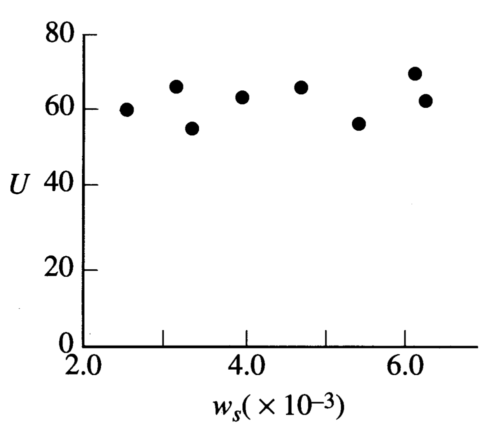


FIGURE E2.3*a*
Variation of overall heat transfer coefficient with shell-side flow rate $w_s = 8000$.

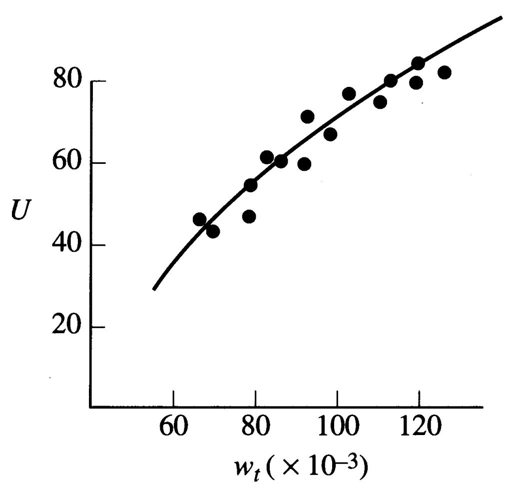


FIGURE E2.3*b*
Variation of overall heat transfer coefficient with tube-side flow rate w_t for $w_s = 4000$.

or

$$U = \frac{h_{sf} K_t w_t^{0.8}}{K_t w_t^{0.8} + h_{sf}} \tag{d}$$

The line in Figure E2.3b shows how well Equation (*d*) fits the data.

In the previous examples and figures we indicated that functions for two independent variables can be selected. When three (or more) independent variables occur, advanced analysis tools, such as experimental design (see Section 2.4) or principal component analysis (Jackson, 1991), are required to determine the structure of the model.

Once the form of the model is selected, even when it involves more than two independent variables, fitting the unknown coefficients in the model using linear or nonlinear regression is reasonably straightforward. We discuss methods of fitting coefficients in the next section.

2.3.2 Fitting Models by Least Squares

This section describes the basic idea of least squares estimation, which is used to calculate the values of the coefficients in a model from experimental data. In estimating the values of coefficients for either an empirical or theoretically based model, keep in mind that the number of data sets must be equal to or greater than the number of coefficients in the model. For example, with three data points of y versus x, you can estimate at most the values of three coefficients. Examine Figure 2.7. A straight line might represent the three points adequately, but the data can be fitted exactly using a quadratic model

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 \tag{2.2}$$

By introducing the values of a data point (Y_1, x_1) into Equation 2.2, you obtain one equation of Y_1 as a function of three unknown coefficients. The set of three data points therefore yields three linear equations in three unknowns (the coefficients) that can be solved easily.

To compensate for the errors involved in experimental data, the number of data sets should be greater than the number of coefficients p in the model. Least squares is just the application of optimization to obtain the "best" solution of the equations, meaning that the sum of the squares of the errors between the predicted and the experimental values of the dependent variable y for each data point x is minimized. Consider a general algebraic model that is linear in the coefficients.

$$y = \sum_{j=1}^{p} \beta_j x_j \tag{2.3}$$

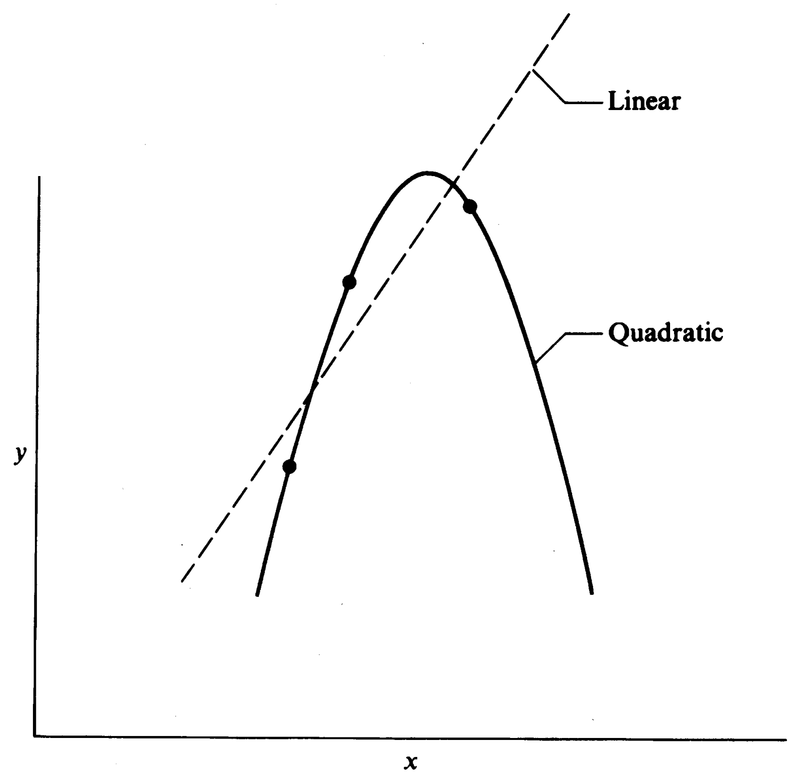


FIGURE 2.7
Linear versus quadratic fit for three data points.

There are p independent variables x_j, $j = 1, \ldots, p$. Independent here means controllable or adjustable, not functionally independent. Equation (2.3) is linear with respect to the β_j, but x_j can be nonlinear. Keep in mind, however, that the values of x_j (based on the input data) are just numbers that are substituted prior to solving for the estimates $\hat{\beta}_j$, hence nonlinear functions of x_j in the model are of no concern. For example, if the model is a quadratic function,

$$y = \beta_1 + \beta_2 x + \beta_3 x^2$$

we specify

$$x_1 = 1$$

$$x_2 = x$$

$$x_3 = x^2$$

and the general structure of Equation (2.3) is satisfied. In reading Section 2.4 you will learn that special care must be taken in collecting values of x to avoid a high degree of correlation between the x_i's.

Introduction of Equation (2.3) into a sum-of-squares error objective function gives

$$f = \sum_{i=1}^{n} \left(Y_i - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \tag{2.4}$$

The independent variables are now identified by a double subscript, the first index designating the data set (experiment) number ($i = 1, \ldots, n$) and the second the independent variables ($j = 1, p$).

Minimizing f with respect to the β's involves differentiating f with respect to $\beta_1, \beta_2, \ldots, \beta_p$ and equating the p partial derivatives to zero. This yields p equations that relate the p unknown values of the estimated coefficients $\hat{\beta}_1, \ldots, \hat{\beta}_p$:

$$\begin{array}{l}
\hat{\beta}_1 \sum_{i=1}^{n} x_{i1}x_{i1} + \hat{\beta}_2 \sum_{i=1}^{n} x_{i1}x_{i2} + \cdots + \hat{\beta}_p \sum_{i=1}^{n} x_{i1}x_{ip} = \sum_{i=1}^{n} Y_i x_{i1} \\
\hat{\beta}_1 \sum_{i=1}^{n} x_{i2}x_{i1} + \hat{\beta}_2 \sum_{i=1}^{n} x_{i2}x_{i2} + \cdots + \hat{\beta}_p \sum_{i=1}^{n} x_{i2}x_{ip} = \sum_{i=1}^{n} Y_i x_{i2} \\
\quad \vdots \\
\hat{\beta}_1 \sum_{i=1}^{n} x_{ip}x_{i1} + \hat{\beta}_2 \sum_{i=1}^{n} x_{ip}x_{i2} + \cdots + \hat{\beta}_p \sum_{i=1}^{n} x_{ip}x_{ip} = \sum_{i=1}^{n} Y_i x_{ip}
\end{array} \tag{2.5}$$

where $\hat{\beta}_i$ = the estimated value of β_i
x_{ij}'s = the experimental values of x_j
Y_i = the measured dependent variables

Note the symmetry of the summation terms in x_{ij} and that numbering of x_{ij}'s in the summations corresponds to matrix indices (rows, columns). This set of p equations in p unknowns can be solved on a computer using one of the many readily available routines for solving simultaneous linear equations.

Equations (2.5) can be expressed in more compact form if matrix notation is employed (see Appendix A). Let the model be expressed in vector matrix notation as

$$\mathbf{Y} = \mathbf{x}\hat{\boldsymbol{\beta}} + \boldsymbol{\varepsilon} \tag{2.6}$$

where $\boldsymbol{\varepsilon}$ = the random error in the data
$\mathbf{Y}$ = the vector of measured dependent variables

$$\boldsymbol{\beta} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \cdot \\ \cdot \\ \cdot \\ \beta_p \end{bmatrix} \qquad \mathbf{Y} = \begin{bmatrix} Y_1 \\ Y_2 \\ \cdot \\ \cdot \\ \cdot \\ Y_n \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

The objective function to be minimized is

$$f = \boldsymbol{\varepsilon}^T\boldsymbol{\varepsilon} = (\mathbf{Y} - \mathbf{x}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{x}\boldsymbol{\beta}) \tag{2.7}$$

Equations 2.5 can then be expressed as

$$\mathbf{x}^T\mathbf{x}\hat{\boldsymbol{\beta}} = \mathbf{x}^T\mathbf{Y} \tag{2.8}$$

which has the formal solution via matrix algebra

$$\hat{\boldsymbol{\beta}} = (\mathbf{x}^T\mathbf{x})^{-1}\mathbf{x}^T\mathbf{Y} \tag{2.9}$$

Statistical packages and spreadsheets solve the simultaneous equations in (2.8) to estimate $\hat{\boldsymbol{\beta}}$ rather than computing the matrix inverse in Equation (2.9).

The next two examples illustrate the application of Equation 2.9 to fit coefficients in an objective function. The same procedure is used to fit coefficients in constraint models.

EXAMPLE 2.4 APPLICATION OF LEAST SQUARES TO DEVELOP A COST MODEL FOR THE COST OF HEAT EXCHANGERS

In the introduction we mentioned that it is sometimes necessary to develop a model for the objective function using cost data. Curve fitting of the costs of fabrication of heat exchangers can be used to predict the cost of a new exchanger of the same class with different design variables. Let the cost be expressed as a linear equation

$$C = \beta_1 + \beta_2 N + \beta_3 A$$

where β_1, β_2, and β_3 are constants
N = number of tubes
A = shell surface area

Estimate the values of the constants β_1, β_2, and β_3 from the data in Table E2.4. The regressors are $x_1 = 1$, $x_2 = N$, and $x_3 = A$.

Solution. The matrices to be used in calculating $\hat{\boldsymbol{\beta}}$ are as follows (each data set is weighted equally):

$$\mathbf{x} = \begin{bmatrix} 1 & 120 & 550 \\ 1 & 130 & 600 \\ 1 & 108 & 520 \\ 1 & 110 & 420 \\ 1 & 84 & 400 \\ 1 & 90 & 300 \\ 1 & 80 & 230 \\ 1 & 55 & 120 \\ 1 & 64 & 190 \\ 1 & 50 & 100 \end{bmatrix}$$

TABLE E2.4
Labor cost data for mild-steel floating-head exchangers (0–500 psig) working pressure

Labor cost ($)	Area (A)	Number of tubes (N)
310	120	550
300	130	600
275	108	520
250	110	420
220	84	400
200	90	300
190	80	230
150	55	120
140	64	190
100	50	100

Source: Shahbenderian, 1961.

$$(\mathbf{x}^T\mathbf{x}) = \begin{bmatrix} 10 & 891 & 3{,}430 \\ 891 & 86{,}241 & 349{,}120 \\ 3{,}430 & 349{,}120 & 1{,}472{,}700 \end{bmatrix}$$

$$(\mathbf{x}^T\mathbf{Y}) = \begin{bmatrix} 2{,}135 \\ 207{,}290 \\ 844{,}800 \end{bmatrix}$$

Equation (2.9) gives the best estimates of β_1, β_2, and β_3:

$$\hat{\beta}_1 = 38.177$$

$$\hat{\beta}_2 = 1.164$$

$$\hat{\beta}_3 = 0.209$$

Check to see if these coefficients yield a reasonable fit to the data in Table E2.4.

EXAMPLE 2.5 APPLICATION OF LEAST SQUARES IN YIELD CORRELATION

Ten data points were taken in an experiment in which the independent variable x is the mole percentage of a reactant and the dependent variable y is the yield (in percent):

x	y
20	73
20	78
30	85
40	90
40	91
50	87
50	86
50	91
60	75
70	65

Fit a quadratic model with these data and determine the value of x that maximizes the yield.

Solution. The quadratic model is $y = \beta_1 + \beta_2 x + \beta_3 x^2$. The estimated coefficients computed using Excel are

$$\hat{\beta}_1 = 35.66$$

$$\hat{\beta}_2 = 2.63$$

$$\hat{\beta}_3 = -0.032$$

The predicted optimum can be formed by differentiating

$$\hat{Y} = \hat{\beta}_1 + \hat{\beta}_2 x + \hat{\beta}_3 x^2$$

with respect to x and setting the derivative to zero to get

$$x^{\text{opt}} = \frac{-\hat{\beta}_2}{2\hat{\beta}_3} = 41.09$$

The predicted yield $\hat{Y}$ at the optimum is 88.8.

Certain assumptions underly least squares computations such as the independence of the unobservable errors ε_i, a constant error variance, and lack of error in the x's (Draper and Smith, 1998). If the model represents the data adequately, the residuals should possess characteristics that agree with these basic assumptions. The analysis of residuals is thus a way of checking that one or more of the assumptions underlying least squares optimization is not violated. For example, if the model fits well, the residuals should be randomly distributed about the value of y predicted by the model. Systematic departures from randomness indicate that the model is unsatisfactory; examination of the patterns formed by the residuals can provide clues about how the model can be improved (Box and Hill, 1967; Draper and Hunter, 1967).

Examinations of plots of the residuals versus $\hat{Y}_i$ or x_i, or a plot of the frequency of the residuals versus the magnitude of the residuals, have been suggested as numerical or graphical aids to assist in the analysis of residuals. A study of the signs of the residuals (+ or −) and sums of signs can be used. Residual analysis should include

1. Detection of an outlier (an extreme observation).
2. Detection of a trend in the residuals.
3. Detection of an abrupt shift in the level of the experiment (sequential observations).
4. Detection of changes in the error variance (usually assumed to be constant).
5. Examination to ascertain if the residuals are represented by a normal distribution (so that statistical tests can be applied).

When using residuals to determine the adequacy of a model, keep in mind that as more independent variables are added to the model, the residuals may become less informative. Each residual is, in effect, a weighted average of the ε_i's; as more unnecessary x_i's are added to a model, the residuals become more like one another, reflecting an indiscriminate average of all the ε's instead of primarily representing one ε_i. In carrying out the analysis of residuals, you will quickly discover that a graphical presentation of the residuals materially assists in the diagnosis because one aberration, such as a single extreme value, can simultaneously affect several of the numerical tests.

Nonlinear least squares

If a model is nonlinear with respect to the model parameters, then nonlinear least squares rather than linear least squares has to be used to estimate the model coefficients. For example, suppose that experimental data is to be fit by a reaction rate expression of the form $r_A = kC_A^n$. Here r_A is the reaction rate of component A, C_A is the reactant concentration, and k and n are model parameters. This model is *linear* with respect to rate constant k but is *nonlinear* with respect to reaction order n. A general nonlinear model can be written as

$$y = f(x_1, x_2, x_3, \ldots, \beta_1, \beta_2, \beta_3 \ldots) \tag{2.10}$$

where y = the model output
x_j's = model inputs
β_j's = the parameters to be estimated

We still can define a sum-of-squares error criterion (to be minimized) by selecting the parameter set β_j so as to

$$\min_{\beta_j} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 \tag{2.11}$$

where Y_i = the ith output measurement
$\hat{Y}_i$ = model prediction corresponding to the ith data point

The estimated coefficients listed for model 2 in Example 2.2 were obtained using nonlinear least squares (Bates and Watts, 1988).

As another example, consider the problem of estimating the gain K and time constants τ_i for first-order and second-order dynamic models based on a measured unit step response of the process $y(t)$. The models for the step response of these two processes are, respectively (Seborg et al., 1989),

$$y(t) = K(1 - e^{-t/\tau_1}) \tag{2.12}$$

$$y(t) = K\left(1 - \frac{\tau_1 e^{-t/\tau_1} - \tau_2 e^{-t/\tau_2}}{\tau_1 - \tau_2}\right) \tag{2.13}$$

where t = the independent variable (time)
y = the dependent variable

Although K appears linearly in both response equations, τ_1 in (2.12) and τ_1 and τ_2 in (2.13) appear nonlinearly, so that nonlinear least squares must be used to estimate their values. The specific details of how to carry out the computations will be deferred until we take up numerical methods of unconstrained optimization in Chapter 6.

2.4 FACTORIAL EXPERIMENTAL DESIGNS

Because variables in models are often highly correlated, when experimental data are collected, the $\mathbf{x}^T\mathbf{x}$ matrix in Equation 2.9 can be badly conditioned (see Appendix A), and thus the estimates of the values of the coefficients in a model can have considerable associated uncertainty. The method of factorial experimental design forces the data to be orthogonal and avoids this problem. This method allows you to determine the relative importance of each input variable and thus to develop a parsimonious model, one that includes only the most important variables and effects. Factorial experiments also represent efficient experimentation. You systematically plan and conduct experiments in which all of the variables are changed simultaneously rather than one at a time, thus reducing the number of experiments needed.

Because of the orthogonality property of factorial design, statistical tests are effective in discriminating among the effects of natural variations in raw materials, replicated unit operations (e.g., equipment in parallel), different operators, different batches, and other environmental factors. A proper orthogonal design matrix for collecting data provides independent estimates of the sums of squares for each variable as well as combinations of variables. Also the estimates of the coefficients have a lower variance than can be obtained with a nonorthogonal experimental design (Montgomery, 1997; Box et al., 1978). That is, you can have more confidence in the values calculated for β_i than would occur with a nonorthogonal design.

TABLE 2.1
Orthogonal experimental design

Experiment number	Response y	Scaled (coded) values of the independent variables z_1	z_2
1	Y_1	-1	-1
2	Y_2	1	-1
3	Y_3	-1	1
4	Y_4	1	1
5	Y_5	0	0

From a practical standpoint, the user of the model must decide which input variables should be studied because this will determine the number of tests that must be carried out (Drain, 1997). In a standard factorial design, 2^n tests are required, where n is the number of input variables to be studied. You must also decide how much each input variable should be changed from its nominal value, taking into account the sensitivity of the process response to a change in a given input variable, as well as the typical operating range of the process. The determination of the region of experimentation requires process knowledge. The experimental range should be chosen so that the resulting measurements of the response do not involve errors in the sensors that are greater than typical noise levels.

Suppose you want to fit the linear model $y = \beta_1 + \beta_2 z_1 + \beta_3 z_2$, where z_1 and z_2 are the independent variables. Let the values of z_1 and z_2 in the experiment be deliberately chosen by an *experimental orthogonal design* like that shown in Table 2.1.

The values of the coded independent variables correspond to the four corners of a square in the z_1 and z_2 space. The summations in Equation (2.5) simplify in this case ($x_1 = 1, x_2 = z_1, x_3 = z_2$):

$$\sum_{i=1}^{5} x_{i1}x_{i2} = \sum_{i=1}^{5} z_{1i} = 0 \quad \sum_{i=1}^{5} x_{i1}x_{i3} = \sum_{i=1}^{5} z_{2i} = 0 \quad \sum_{i=1}^{5} x_{i2}x_{i3} = \sum_{i=1}^{5} z_{1i}z_{2i} = 0$$

$$\sum_{i=1}^{5} x_{i1}x_{i1} = 5 \quad \sum_{i=1}^{5} x_{i2}x_{i2} = \sum_{i=1}^{5} z_{1i}^2 = 4 \quad \sum_{i=1}^{5} x_{i3}x_{i3} = \sum_{i=1}^{5} z_{2i}^2 = 4$$

For the experimental design in Table 2.1,

$$\mathbf{x}^T\mathbf{x} = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{Y} = \begin{bmatrix} y_1 + y_2 + y_3 + y_4 + y_5 \\ -y_1 + y_2 - y_3 + y_4 \\ -y_1 - y_2 + y_3 + y_4 \end{bmatrix}$$

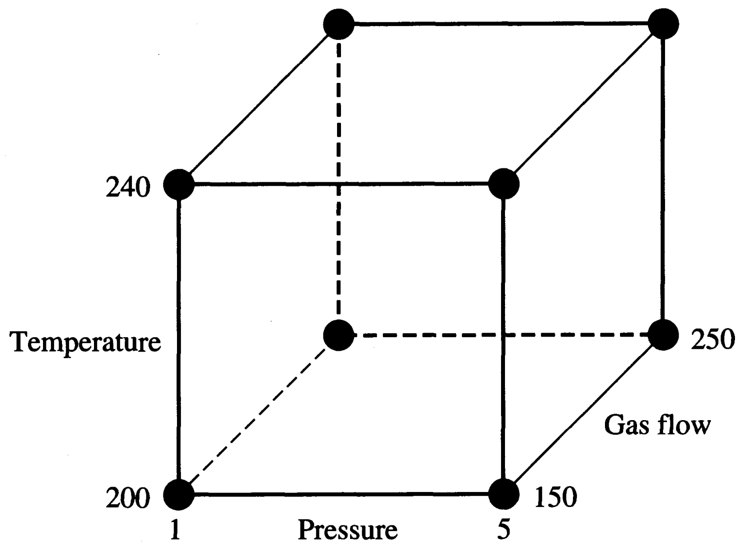


FIGURE E2.6
Orthogonal design for the variables temperature, pressure, and flowrate.

It is quite easy to solve Equation (2.9) now because these expressions are *uncoupled*; the inverse of $\mathbf{x}^T\mathbf{x}$ for Equation (2.13) can be obtained by merely taking the reciprocal of the diagonal elements.

EXAMPLE 2.6 IDENTIFICATION OF IMPORTANT VARIABLES BY EXPERIMENTATION USING AN ORTHOGONAL FACTORIAL DESIGN

Assume a reactor is operating at the reference state of 220°C, 3 atm pressure, and a gas flow rate of 200 kg/h. We can set up an orthogonal factorial design to model this process with a linear model $Y = \beta_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4$ so that the coded values of the x_i are 1, -1, and 0. Examine Figure E2.6. Suppose we select the changes in the operating conditions of ± 20°C for the temperature, ± 2 atm for the pressure, and ± 50 kg/h for flowrates. Let $x_1 = 1$; then x_2, x_3, and x_4, the coded variables, are calculated in terms of the proposed operating conditions as follows:

$$x_2 = \frac{t(°\mathrm{C}) - 220}{20}$$

$$x_3 = \frac{p(\mathrm{atm}) - 3}{2}$$

$$x_4 = \frac{m(\mathrm{kg/h}) - 200}{50}$$

Based on the design the following data are collected:

Y (yield)	x_2	x_3	x_4
20.500	−1	−1	−1
60.141	1	−1	−1
58.890	−1	1	−1
67.712	1	1	−1
22.211	−1	−1	1
61.541	1	−1	1
59.902	−1	1	1
69.104	1	1	1
77.870	0	0	0
78.933	0	0	0
70.100	0	0	0

The extra data at the (0, 0) point are used to obtain a measure of the error involved in the experiment.

Solution. The matrices involved are

$$\mathbf{x}^T\mathbf{x} = \begin{bmatrix} 11 & 0 & 0 & 0 \\ 0 & 8 & 0 & 0 \\ 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 8 \end{bmatrix} \qquad (\mathbf{x}^T\mathbf{x})^{-1} = \begin{bmatrix} 0.091 & 0 & 0 & 0 \\ 0 & 0.125 & 0 & 0 \\ 0 & 0 & 0.125 & 0 \\ 0 & 0 & 0 & 0.125 \end{bmatrix}$$

$$\mathbf{x}^T\mathbf{Y} = \begin{bmatrix} 646.9 \\ 96.99 \\ 91.21 \\ 5.51 \end{bmatrix}$$

With these matrices you can compute the estimates of $\hat{\beta}_i$ by solving Equation (2.9), yielding

$$\hat{Y} = 58.810 + 12.124x_2 + 11.402x_3 + 0.689x_4$$

In terms of the original variables

$$\hat{Y} = 58.810 + 12.124\left(\frac{t(°\text{C}) - 220}{20}\right) + 11.402\left(\frac{p(\text{atm}) - 3}{2}\right)$$

$$+ 0.689\left(\frac{m(\text{kg/h}) - 200}{50}\right)$$

$$= 58.810 + 0.6062(t - 220) + 5.701(p - 3) + 0.0138\,(m - 200)$$

It is clear from the size of the estimated coefficients that mass flowrate changes have a much smaller influence on the yield and thus, for practical purposes, could be eliminated as an important independent variable.

If the independent variables are orthogonal, deciding whether to add or delete variables or functions of variables in models is straightforward using stepwise least squares (regression), a feature available on many software packages. Stepwise regression consists of sequentially adding (or deleting) a variable (or function) of variables to a proposed model and then testing at each stage to see if the added (or deleted) variable is significant. The procedure is only effective when the independent variables are essentially orthogonal. The coupling of orthogonal experimental design with optimization of operating conditions has been called "evolutionary operation" by which the best operating conditions are determined by successive experiments (Box and Draper, 1969; Biles and Swain, 1980).

2.5 DEGREES OF FREEDOM

In Section 1.5 we briefly discussed the relationships of equality and inequality constraints in the context of independent and dependent variables. Normally in design and control calculations, it is important to eliminate redundant information and equations before any calculations are performed. Modern multivariable optimization software, however, does not require that the user clearly identify independent, dependent, or superfluous variables, or active or redundant constraints. If the number of independent equations is larger than the number of decision variables, the software informs you that no solution exists because the problem is overspecified. Current codes have incorporated diagnostic tools that permit the user to include all possible variables and constraints in the original problem formulation so that you do not necessarily have to eliminate constraints and variables prior to using the software. Keep in mind, however, that the smaller the dimensionality of the problem introduced into the software, the less time it takes to solve the problem.

The degrees of freedom in a model is the number of variables that can be specified independently and is defined as follows:

$$N_F = N_v - N_E \tag{2.14}$$

where N_F = degrees of freedom
N_v = total number of variables involved in the problem
N_E = number of independent equations (including specifications)

A degrees-of-freedom analysis separates modeling problems into three categories:

1. $N_F = 0$: *The problem is exactly determined.* If $N_F = 0$, then the number of independent equations is equal to the number of process variables and the set of equations may have a unique solution, in which case the problem is not an optimization problem. For a set of linear independent equations, a unique solution exists. If the equations are nonlinear, there may be no real solution or there may be multiple solutions.

2. $N_F > 0$: *The problem is underdetermined.* If $N_F > 0$, then more process variables exist in the problem than independent equations. The process model is said to be underdetermined, so at least one variable can be optimized. For linear models, the rank of the matrix formed by the coefficients indicates the number of independent equations (see Appendix A).
3. $N_F < 0$: *The problem is overdetermined.* If $N_F < 0$, fewer process variables exist in the problem than independent equations, and consequently the set of equations has no solutions. The process model is said to be overdetermined, and least squares optimization or some similar criterion can be used to obtain values of the unknown variables as described in Section 2.5.

EXAMPLE 2.7 MODEL FOR A SEPARATION TRAIN

Figure E2.7 shows the process flow chart for a series of two distillation columns, with mass flows and splits defined by $x_1, x_2, \ldots, x_5$. Write the material balances, and show that the process model comprises two independent variables and three degrees of freedom.

Solution. The balances for columns 1 and 2 are shown below:

Column 1

$$x_1 = x_2 + x_3 \quad \text{or} \quad x_1 - x_2 - x_3 = 0 \tag{a}$$

$$x_2 = .40x_1 \quad \text{or} \quad x_2 - 0.4x_1 = 0 \tag{b}$$

$$x_3 = .60x_1 \quad \text{or} \quad x_3 - 0.6x_1 = 0 \tag{c}$$

There are three equations and three unknowns.

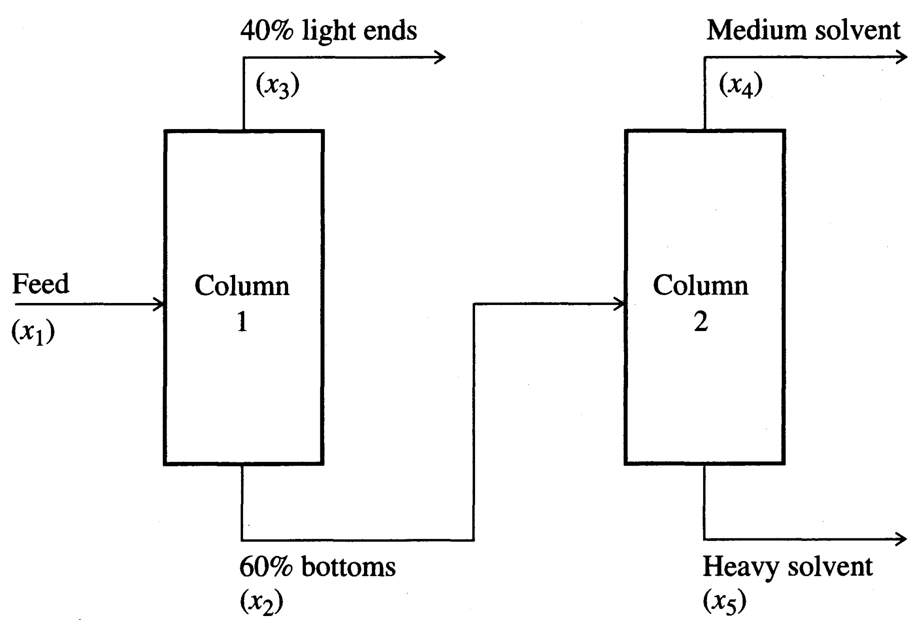


FIGURE E2.7
Train of distillation columns.

The coefficient matrix is

		Variables		
		x_1	x_2	x_3
Equations	(a)	1	−1	−1
	(b)	−0.4	1	0
	(c)	−0.6	0	1

The three equations are not independent. The rank of the coefficient matrix is 2, hence there are only two independent variables, and column 1 involves 1 degree of freedom.

Column 2 $\qquad x_2 = x_4 + x_5 \qquad$ or $\qquad x_2 - x_4 - x_5 = 0 \qquad$ (*d*)

There is one equation and three unknowns, so there are two degrees of freedom.Overall there are four equations (a), (b), (c), (d) and five variables.The coefficient matrix is

	x_1	x_2	x_3	x_4	x_5
(a)	1	−1	−1	0	0
(b)	−0.4	1	0	0	0
(c)	−0.6	0	1	0	0
(d)	0	1	0	−1	−1

Because the rank of the coefficient matrix is three, there are only three independent equations, so Equation (2.14) indicates that there are two degrees of freedom. You can reduce the dimensionality of the set of material balances by substitution of one equation into another and eliminating both variables and equations.

In some problems it is advantageous to eliminate obvious dependent variables to reduce the number of equations that must be included as constraints. You can eliminate linear constraints via direct substitution, leaving only the nonlinear constraints, but the resulting equations may be too complex for this procedure to have merit. The following example illustrates a pipe flow problem in which substitution leads to one independent variable.

EXAMPLE 2.8 ANALYSIS OF PIPE FLOW

Suppose you want to design a hydrocarbon piping system in a plant between two points with no change in elevation and want to select the optimum pipe diameter that minimizes the combination of pipe capital costs and pump operating costs. Prepare a model that can be used to carry out the optimization. Identify the independent and dependent variables that affect the optimum operating conditions. Assume the fluid properties (μ, ρ) are known and constant, and the value of the pipe length (L) and mass flowrate (m) are specified. In your analysis use the following process variables: pipe diameter (D), fluid velocity (v), pressure drop (Δp), friction factor (f).

Solution. Intuitively one expects that an optimum diameter can be found to minimize the total costs. It is clear that the four process variables are related and not independent, but we need to examine in an organized way how the equality constraints (models) affect the degrees of freedom.

List the equality constraints:

1. Mechanical energy balance, assuming no losses in fittings, no change in elevation, and so on.

$$\Delta p = \frac{2f\rho v^2 L}{D} \qquad (a)$$

2. Equation of continuity, based on plug flow under turbulent conditions.

$$m = \left(\frac{\rho \pi D^2}{4}\right) v \qquad (b)$$

3. A correlation relating the friction factor with the Reynolds number (Re).

$$f = f(\text{Re}) = f\left(\frac{Dv\rho}{\mu}\right)$$

The friction factor plot is available in many handbooks, so that given a value of Re, one can find the corresponding value of f. In the context of numerical optimization, however, using a graph is a cumbersome procedure. Because all of the constraints should be expressed as mathematical relations, we select the Blasius correlation for a smooth pipe (Bird et al., 1964):

$$f = 0.046\ \text{Re}^{-0.2} = \frac{0.046\mu^{0.2}}{D^{0.2}v^{0.2}\rho^{0.2}} \qquad (c)$$

The model involves four variables and three independent nonlinear algebraic equations, hence one degree of freedom exists. The equality constraints can be manipulated using direct substitution to eliminate all variables except one, say the diameter, which would then represent the independent variables. The other three variables would be dependent. Of course, we could select the velocity as the single independent variable of any of the four variables. See Example 13.1 for use of this model in an optimization problem.

2.6 EXAMPLES OF INEQUALITY AND EQUALITY CONSTRAINTS IN MODELS

As mentioned in Chapter 1, the occurrence of *linear inequality constraints* in industrial processes is quite common. Inequality constraints do not affect the count of the degrees of freedom unless they become active constraints. Examples of such constraints follow:

1. Production limitations arise because of equipment throughput restrictions, storage limitations, or market constraints (no additional product can be sold beyond some specific level).
2. Raw material limitations occur because of limitations in feedstock supplies; these supplies often are determined by production levels of other plants within the same company.
3. Safety or operability restrictions exist because of limitations on allowable operating temperatures, pressures, and flowrates.
4. Physical property specifications on products must be considered. In refineries the vapor pressure or octane level of fuel products must satisfy some specification. For blends of various products, you usually assume that a composite property can be calculated through the averaging of pure component physical properties. For N components with physical property values V_i and volume fraction y_i, the average property $\bar{V}$ is

$$\bar{V} = \sum_{i=1}^{N} V_i y_i$$

EXAMPLE 2.9 FORMULATION OF A LINEAR INEQUALITY CONSTRAINT FOR BLENDING

Suppose three intermediates (light naphtha, heavy naphtha, and "catalytic" oil) made in a refinery are to be blended to produce an aviation fuel. The octane number of the fuel must be at least 95. The octane numbers for the three intermediates are shown in the table.

	Amount blended (barrels/day)	Octane number
Light naphtha	x_1	92
Heavy naphtha	x_2	86
Catalytic oil	x_3	97

Write an inequality constraint for the octane number of the aviation fuel, assuming a linear mixing rule.

Solution. Assume the material balance can be based on conservation of volume (as well as mass). The production rate of aviation gas is $x_4 = x_1 + x_2 + x_3$. The volume-average octane number of the gasoline can be computed as

$$\frac{x_1}{x_1 + x_2 + x_3}(92) + \frac{x_2}{x_1 + x_2 + x_3}(86) + \frac{x_3}{x_1 + x_2 + x_3}(97) \geq 95 \qquad (a)$$

Multiplying Equation (a) by $(x_1 + x_2 + x_3)$ and rearranging, we get

$$-3x_1 - 9x_2 + 2x_3 \geq 0 \qquad (b)$$

This constraint ensures that the octane number specification is satisfied. Note that Equation (b) is linear.

EXAMPLE 2.10 LINEAR MATERIAL BALANCE MODELS

In many cases in which optimization is applied, you need to determine the allocation of material flows to a set of processes in order to maximize profits. Consider the process diagram in Figure E2.10.

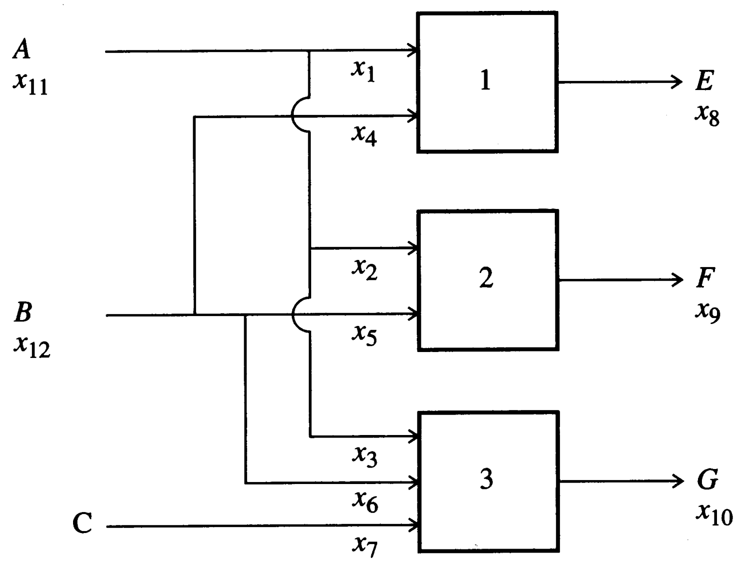


FIGURE E2.10
Flow diagram for a multiproduct plant.

Each product (E, F, G) requires different (stoichiometric) amounts of reactants according to the following mass balances:

Product	Reactants (1-kg product)
E	$\frac{2}{3}$ kg A, $\frac{1}{3}$ kg B
F	$\frac{2}{3}$ kg A, $\frac{1}{3}$ kg B
G	$\frac{1}{2}$ kg A, $\frac{1}{6}$ kg B, $\frac{1}{3}$ kg C

Prepare a model of the process using the mass balance equations.

Solution. Twelve mass flow variables can be defined for this process. Let x_1, x_2, x_3 be the mass input flows of A to each process. Similarly let x_4, x_5, x_6, and x_7 be the individual reactant flows of B and C, and define x_8, x_9, and x_{10} as the three mass product flows (E, F, G). Let x_{11} and x_{12} be the total amounts of A and B used as reactants (C is the same as x_7). Thus, we have a total of 12 variables.

The linear mass balance constraints that represent the process are:

$$A = x_{11} = x_1 + x_2 + x_3 \qquad (a)$$

$$B = x_{12} = x_4 + x_5 + x_6 \qquad (b)$$

$$x_1 = 0.667x_8 \qquad (c)$$

$$x_2 = 0.667x_9 \qquad (d)$$

$$x_3 = 0.5x_{10} \qquad (e)$$

$$x_4 = 0.333x_8 \qquad (f)$$

$$x_5 = 0.333x_9 \qquad (g)$$

$$x_6 = 0.167x_{10} \qquad (h)$$

$$x_7 = 0.333x_{10} \qquad (i)$$

With 12 variables and 9 independent linear equality constraints, 3 degrees of freedom exist that can be used to maximize profits. Note that we could have added an overall material balance, $x_{11} + x_{12} + x_7 = x_8 + x_9 + x_{10}$, but this would be a redundant equation since it can be derived by adding the material balances.

Other constraints can be specified in this problem. Suppose that the supply of A was limited to 40,000 kg/day, or

$$x_{11} \leq 40{,}000 \qquad (j)$$

If this constraint is inactive, that is, the optimum value of x_{11} is less than 40,000 kg/day, then, in effect, there are still 3 degrees of freedom. If, however, the optimization procedure yields a value of $x_{11} = 40{,}000$ (the optimum lies on the constraint, such as shown in Figure 1.2), then inequality constraint f becomes an equality constraint, resulting in only 2 degrees of freedom that can be used for optimization. You should recognize that it is possible to add more inequality constraints, such as constraints on materials supplies, in the model, for example,

$$x_{12} \leq 30{,}000 \qquad (k)$$

$$x_7 \leq 25{,}000 \qquad (l)$$

These can also become "active" constraints if the optimum lies on the constraint boundary. Note that we can also place inequality constraints on production of E, F, and G in order to satisfy market demand or sales constraints

$$x_8 \geq 20{,}000 \qquad (m)$$

$$x_9 \geq 25{,}000 \qquad (n)$$

$$x_{10} \geq 30{,}000 \qquad (o)$$

Now the analysis is much more complex, and it is clear that more potential equality constraints exist than variables if all of the inequality constraints become active. It is possible that optimization could lead to a situation where no degrees of freedom would be left—one set of the inequality constraints would be satisfied as equalities. This outcome means no variables remain to be optimized, and the optimal solution reached would be at the boundaries, a subset of the inequality constraints.

Other constraints that can be imposed in a realistic problem formulation include

1. Operating limitations (bottlenecks)—there could be a throughput limitation on reactants to one of the processes (e.g., available pressure head).
2. Environmental limitations—there could be some additional undesirable by-products H, such as the production of toxic materials (not in the original product list given earlier), that could contribute to hazardous conditions.

You can see that the model for a realistic process can become extremely complex; what is important to remember is that steps 1 and 3 in Table 1.1 provide an organized framework for identifying all of the variables and formulating the objective function, equality constraints, and inequality constraints. After this is done, you need not eliminate redundant variables or equations. The computer software can usually handle redundant relations (but not inconsistent ones).

REFERENCES

Bates, D. M.; and D. G. Watts. *Nonlinear Regression Analysis and Its Applications*. Wiley, New York (1988).
Biles, W. E.; and J. J. Swain. *Optimization and Industrial Experimentation*. Wiley-Interscience, New York (1980).
Bird, R. B.; W. E. Stewart; and E. N. Lightfoot. *Transport Phenomena*. Wiley, New York (1964).
Box, G. E. P.; and J. W. Hill. "Discrimination Among Mechanistic Models." *Technometrics* **9:** 57 (1967)
Box, G. E. P.; and N. R. Draper. *Evolutionary Operation*. Wiley, New York (1969).
Box, G. E. P.; W. G. Hunter, and J. S. Hunter. *Statistics for Experimenters*. Wiley-Interscience, New York (1978).
Deitz, D. "Modeling Furnace Performance." *Mech Eng* **119** (Dec), 16 (1997).
Drain, D. *Handbook of Experimental Methods for Process Improvements*. Chapman and Hall, International Thomson Publishing, New York (1997).
Draper, N. R.; and W. G. Hunter. "The Use of Prior Distribution in the Design of Experiments for Parameter Estimation in Nonlinear Situations." *Biometrika* **54:** 147 (1967).
Draper, N. R.; and H. Smith. *Applied Regression Analysis*, 3rd ed. Wiley, New York (1998).
Eykhoff, P. *System Identification*. Wiley-Interscience, New York (1974).
Jackson, J. E. *A User's Guide to Principal Components*. Wiley, New York (1991).
McAdams, W. H. *Heat Transmission*. McGraw-Hill, New York (1954).
Montgomery, D. C. *Design and Analysis of Experiments*, 4th ed. Wiley, New York (1997).
Seborg, D. E.; T. F. Edgar; and D. A. Mellichamp. *Process Dynamics and Control*. Wiley, New York (1989).
Shahbenderian, A. P. "The Application of Statistics to Cost Estimating." *Br Chem Eng* (January) **6:** 16 (1961).

SUPPLEMENTARY REFERENCES

Bendor, E. A. *An Introduction to Mathematical Modeling*. John Wiley, New York (1978).
Bequette, B. W. *Process Dynamics: Modeling, Analysis, and Simulation*. Prentice-Hall, Englewood Cliffs, NJ (1998).
Churchill, S. W. *The Interpretation and Use of Rate Data*. Scripta Publishing Company, Washington, D. C. (1974).
Davis, M. E. *Numerical Methods and Modeling for Chemical Engineers*. John Wiley, New York (1983).
Denn, M. M. *Process Modeling*. Pitman Publishing, Marshfield, MA (1986).
Friedly, J. C. *Dynamic Behavior of Processes*. Prentice-Hall, Englewood Cliffs, New Jersey (1972).

Luyben, W. L. *Process Modeling, Simulation, and Control for Chemical Engineers.* McGraw-Hill, New York (1990).

Montgomery, D. C.; G. C. Runger; and N. F. Hubele. *Engineering Statistcs.* Wiley, New York (1998).

Ogunnaike, T.; and W. H. Ray. *Process Dynamics, Modeling and Control.* Oxford University Press, New York (1994).

Rice, R. G.; and D. D. Duong. *Applied Mathematics and Modeling for Chemical Engineers.* Wiley, New York (1995).

Seider, W. D.; J. D. Seader; and D. R. Lewin. *Process Design Priciples.* Wiley, New York (1999).

Seinfeld, J. H.; and L. Lapidus. *Process Modeling, Estimation, and Identification.* Prentice-Hall, Englewood Cliffs, New Jersey (1974).

Wen, C. Y.; and L. T. Fan. *Models for Flow Systems and Chemical Reactors.* Marcel Dekker, New York (1975).

PROBLEMS

2.1 Classify the following models as linear or nonlinear

(a) Two-pipe heat exchanger (streams 1 and 2)

$$\frac{\partial T_1}{\partial t} + v\frac{\partial T_1}{\partial z} = \frac{2h_1}{S_1\rho_1 C_{p1}}(T_2 - T_1)$$

$$\frac{\partial T_2}{\partial t} = \frac{2h_1}{\rho_2 C_{p2} S_2}(T_2 - T_1)$$

$$BC\colon\ T_1(t,0) = a \qquad IC\colon\ T_1(0,z) = 0$$

$$T_2(t,0) = b \qquad T_2(0,z) = T_0$$

where T = temperature, C_p = heat capacity

t = time, S = area factor

BC = boundary conditions, IC = initial conditions

ρ = *density*

(b) Diffusion in a cylinder

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right)$$

$$C(0,r) = C_0$$

$$\frac{\partial C(t,0)}{\partial r} = 0$$

$$C(t,R) = C_0$$

where C = concentration r = radial direction
t = time D = constant

2.2 Classify the following equations as linear or nonlinear (y = dependent variable; x, z = independent variables)

(a) $y_1^2 + y_2^2 = a^2$

(b) $v_x \dfrac{\partial v_y}{\partial x} = \mu \dfrac{\partial^2 v_y}{\partial z^2}$

2.3 Classify the models in Problems 2.1 and 2.2 as steady state or unsteady state.

2.4 Classify the models in Problems 2.1 and 2.2 as lumped or distributed.

2.5 What type of model would you use to represent the process shown in the figure? Lumped or distributed? Steady state or unsteady state? Linear or nonlinear?

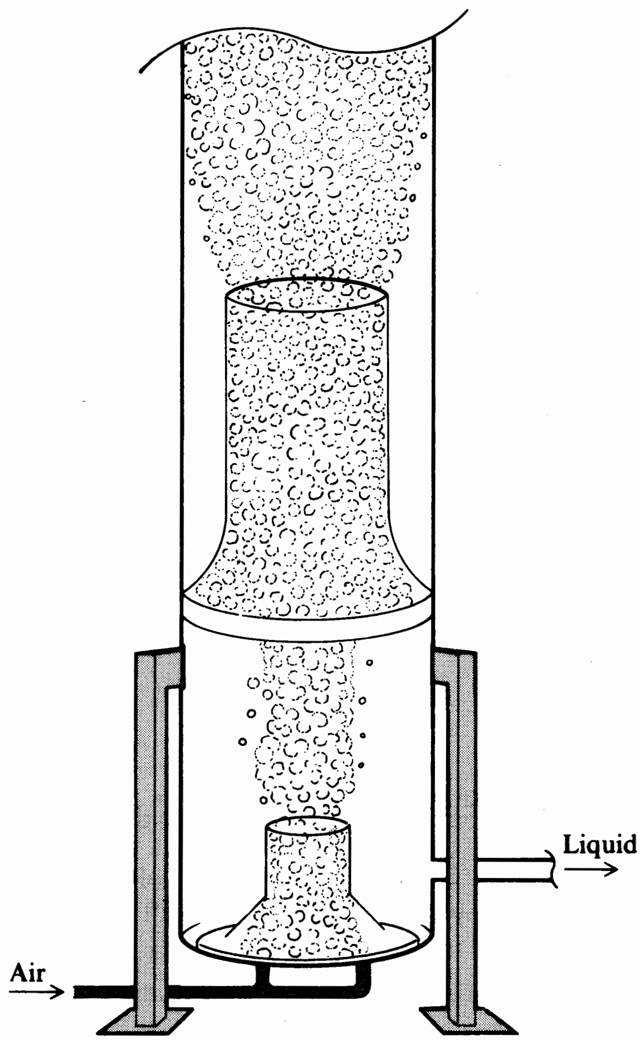


FIGURE P2.5
A wastewater treatment system uses five stacked venturi sections to ensure maximum oxygenation efficiency.

2.6 Determine the number of independent variables, the number of independent equations, and the number of degrees of freedom for the reboiler shown in the figure. What variables should be specified to make the solution of the material and energy balances determinate? (Q = heat transferred)

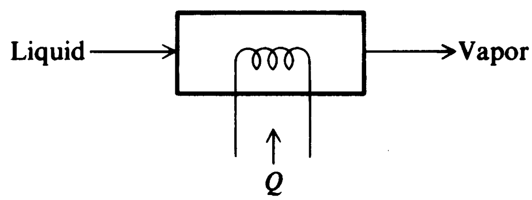


Figure P2.6

2.7 Determine the best functional relation to fit the following data sets:

(a)

x_i	Y_i
1	5
2	7
3	9
4	11

(b)

x_i	Y_i
2	94.8
5	87.9
8	81.3
11	74.9
14	68.7
17	64.0

(c)

x_i	Y_i
2	0.0245
4	0.0370
8	0.0570
16	0.0855
32	0.1295
64	0.2000
128	0.3035

(d)

x_i	Y_i
0	8290
20	8253
40	8215
60	8176
80	8136
100	8093

2.8 The following data have been collected:

x_i	Y_i
10	1.0
20	1.26
30	1.86
40	3.31
50	7.08

Which of the following three models best represents the relationship between Y and x?

$$y = e^{\alpha + \beta x}$$

$$y = e^{\alpha + \beta_1 x + \beta_2 x^2}$$

$$y = \alpha x^{\beta}$$

2.9 Given the following equilibrium data for the distribution of SO_3 in hexane, determine a suitable linear (in the parameters) empirical model to represent the data.

x_i pressure (psia)	Y_i weight fraction hexane
200	0.846
400	0.573
600	0.401
800	0.288
1000	0.209
1200	0.153
1400	0.111
1600	0.078

2.10 (a) Suppose that you wished to curve fit a set of data (shown in the table) with the equation

$$y = c_0 + c_1 e^{3x} + c_2 e^{-3x}$$

x_i	Y_i
0	1
1	2
2	2
3	1

Calculate c_0, c_1, and c_2 (show what summations need to be calculated). How do you find c_1 and c_2 if c_0 is set equal to zero?

(b) If the desired equation were $y = a_1 x e^{-a_2 x}$, how could you use least-squares to find a_1 and a_2?

2.11 Fit the following data using the least squares method with the equation:

$$y = c_0 + c_1 x$$

x_i	Y_i
0.5	0.6
1.0	1.4
2.1	2.0
3.4	3.6

Compare the results with a graphical (visual) estimate.

2.12 Fit the same data in Problem 2.11 using a quadratic fit. Repeat for a cubic model ($y = c_0 + c_1 x + c_2 x^2 + c_3 x^3$). Plot the data and the curves.

2.13 You are asked to get the best estimates of the coefficients b_0, b_1, and c in the following model

$$y = b_0 + b_1 e^{-cx}$$

given the following data.

Y_i	x_i
51.6	0.4
53.4	1.4
20.0	5.4
−4.2	19.5
−3.0	48.2
−4.8	95.9

Explain step by step how you would get the values of the coefficients.

2.14 Fit the following function for the density ρ as a function of concentration C, that is, determine the value of α in

$$\rho = \alpha + 1.33C$$

given the following measurements for ρ and C:

ρ (g/cm^3)	C (gmol/L)
3.31	1.01
4.69	1.97
5.92	3.11
7.35	4.00
8.67	4.95

2.15 (a) For the given data, fit a quadratic function of y versus x by estimating the values of all the coefficients.
(b) Does this set of data constitute an orthogonal design?

y	6.4	5.6	6.0	7.5	6.5	8.3	7.7	11.7	10.3	17.6	18.0
x	1.0	1.0	1.0	2.0	2.0	3.0	3.0	4.0	4.0	5.0	5.0

2.16 Data obtained from a preset series of experiments was

Temperature, T (°F)	**Pressure, p (atm)**	**Yield, Y (%)**
160	1	4
160	1	5
160	7	10
160	7	11
200	1	24
200	1	26
200	7	35
200	7	38

Fit the linear model $\hat{Y} = b_0 + b_1x_1 + b_2x_2$ using the preceding table. Report the estimated coefficients b_0, b_1, and b_2. Was the set of experiments a factorial design?

2.17 You are given data for Y versus x and asked to fit an empirical model of the form:

$$y = \alpha + \beta x$$

where β is a *known* value. Give an equation to calculate the best estimate of α.

2.18 A replicated two-level factorial experiment is carried out as follows (the dependent variables are yields):

Time (h)	Temperature (°C)	Yield (%)
1	240	24
5	240	42
1	280	3
5	280	19
1	240	24
5	240	46
1	280	5
5	280	21

Find the coefficients in a first-order model, $Y = \beta_0 + \beta_1 x_1 + \beta_2 x_2$. ($Y$ = yield, x_1 = time, x_2 = temperature.)

2.19 An experiment based on a hexagon design was carried out with four replications at the origin, producing the following data:

Factor levels			Design levels	
Yield (%)	Temperature (°C)	Time (h)	x_1	x_2
96.0	75	2.0	1.000	0
78.7	60	2.866	0.500	0.866
76.7	30	2.866	−0.500	0.866
54.6	15	2.0	−1.000	0
64.8	30	1.134	−0.500	−0.866
78.9	60	1.134	0.500	−0.866
97.4	45	2.0	0	0
90.5	45	2.0	0	0
93.0	45	2.0	0	0
86.3	45	2.0	0	0

Coding: $x_1 = \dfrac{\text{temperature} - 45}{30}$ $x_2 = \text{time} - 2$

Fit the full second-order (quadratic) model to the data.

2.20 A reactor converts an organic compound to product P by heating the material in the presence of an additive A. The additive can be injected into the reactor, and 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. In order to predict the yield of P, Y_p (lb mole product per lb mole feed), as a function of the mole fraction of A, X_A, and the steam addition S (in lb/lb mole feed), the following data were obtained.

Y_p	X_A	S
0.2	0.3	0
0.3	0	30
0.5	0	60

(a) Fit a linear model

$$Y_p = c_0 + c_1 X_A + c_2 S$$

that provides a least squares fit to the data.

(b) If we require that the model always must fit the point $Y_p = 0$ for $X_A = S = 0$, calculate c_0, c_1, and c_2 so that a least squares fit is obtained.

2.21 If you add a feed stream to the equilibrium stage shown in the figure, determine the number of degrees of freedom for a binary mixture (Q = heat transferred).

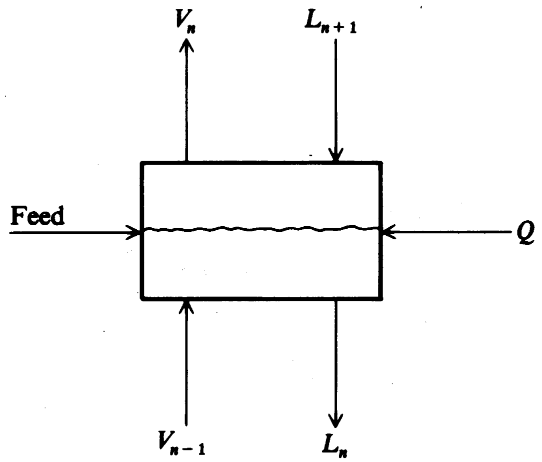


FIGURE P2.21

2.22 How many variables should be selected as independent variables for the furnace shown in the figure?

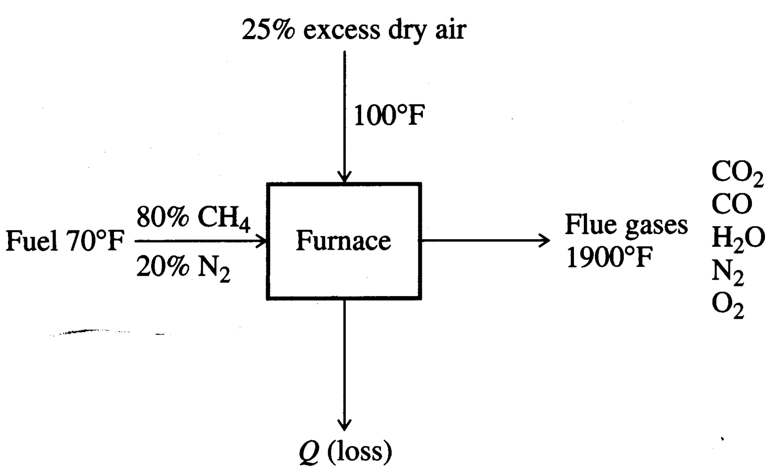


FIGURE P2.22

2.23 Determine the number of independent variables, the number of independent equations, and the number of degrees of freedom in the following process (A, B, and D are chemical species):

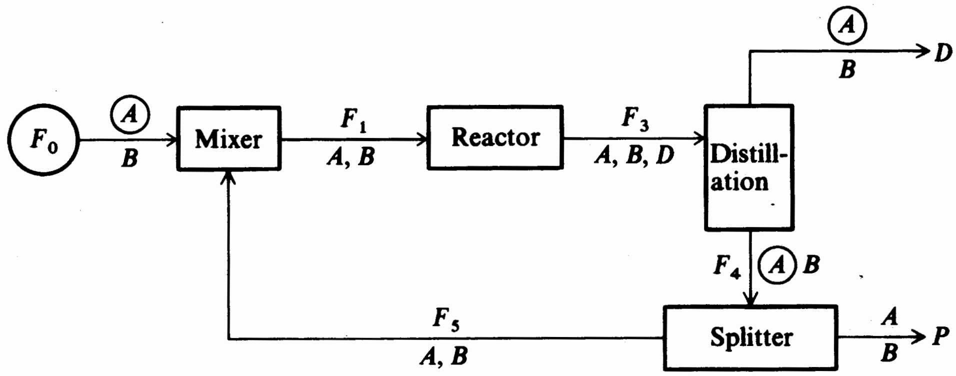


FIGURE P2.23

The encircled variables have known values. The reaction parameters in the reactor are known as the fraction split at the splitter between F_4 and F_5. Each stream is a single phase.

2.24 A waste heat boiler (see Fig. P2.24) is to be designed for steady-state operation under the following specifications.

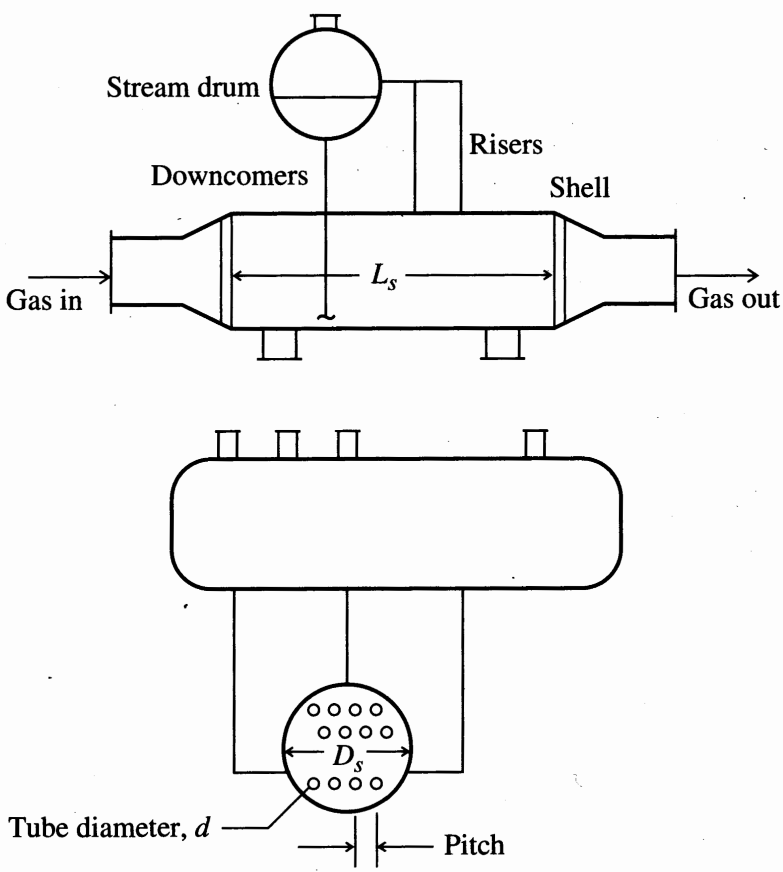


FIGURE P2.24

Total gas flow	25,000 kg/h
Gas composition	SO_2 (9%), O_2 (12%), N_2 (79%)
Gas temperatures	in = 1200°C; out = 350°C
Stream pressure outside tubes	250 kPa
Gas properties	$C_p = 0.24$ kcal/(g)(°C)
	$\mu = 0.14$ kg/(m)(h)
	$k = 0.053$ kcal/(m)(h)(°C)

Cost data are

Shell	\$2.50/kg
Tubes	\$150/m^2
Electricity	\$0.60/kWh
Interest rate	14%

Base the optimization on just the cost of the shell, tubes, and pumping costs for the gas. Ignore maintenance and repairs.

Formulate the optimization problem using only the following notation (as needed):

A	surface area of tubes, m^2
C_s	cost of shell, \$
C_t	cost of tubes, \$
C_{pi}	heat capacity of gas, kcal/(kg)(°C)
D	diameter of shell, m
d_o, d_i	tube outer and inner diameters, m
f	friction factor
g	acceleration due to gravity, m/s^2
h_i	gas side heat transfer coefficient inside the tubes, kcal/(m^2)(h)(°C)
i	interest rate, fraction
k	gas thermal conductivity, kcal/(m)(h)(°C)
L_s	length of shell, m
MW	molecular weight of gas
n	number of tubes
N	life of equipment, years
Q	duty of the boiler, kcal/h
T_1, T_2	gas temperature entering and leaving the boiler, °C
T	temperature in general
ρ_g	density of gas, kg/m^3
μ_g	viscosity of gas, kg/(m)(h)
V	gas velocity, m/s
W_g	gas flow, kg/h
W_s	weight of shell, tons
η	efficiency of blower
ΔP_g	gas pressure drop, kPa
Z	shell thickness, m

How many degrees of freedom are in the problem you formulated?

3

FORMULATION OF THE OBJECTIVE FUNCTION

THE FORMULATION OF objective functions is one of the crucial steps in the application of optimization to a practical problem. As discussed in Chapter 1, you must be able to translate a verbal statement or concept of the desired objective into mathematical terms. In the chemical industries, the objective function often is expressed in units of currency (e.g., U.S. dollars) because the goal of the enterprise is to minimize costs or maximize profits subject to a variety of constraints. In other cases the problem to be solved is the maximization of the yield of a component in a reactor, or minimization of the use of utilities in a heat exchanger network, or minimization of the volume of a packed column, or minimizing the differences between a model and some data, and so on. Keep in mind that when formulating the mathematical statement of the objective, functions that are more complex or more nonlinear are more difficult to solve in optimization. Fortunately, modern optimization software has improved to the point that problems involving many highly nonlinear functions can be solved.

Although some problems involving multiple objective functions cannot be reduced to a single function with common units (e.g., minimize cost while simultaneously maximizing safety), in this book we will focus solely on scalar objective functions. Refer to Hurvich and Tsai (1993), Kamimura (1997), Rusnak et al. (1993), or Steur (1986) for treatment of multiple objective functions. You can, of course, combine two or more objective functions by trade-off, that is, by suitable weighting (refer to Chapter 8). Suppose you want to maintain the quality of a product in terms of two of its properties. One property is the deviation of the variable y_i (i designates the sample number) from the setpoint for the variable, y_{sp}. The other property is the variability of y_i from its mean $\bar{y}$ (which during a transition may not be equal to y_{sp}). If you want to simultaneously use both criteria, you can minimize f:

$$f = w_1 \sum_i \left[y_{sp} - y_i \right]^2 + w_2 \sum_i \left[y_i - \bar{y} \right]^2 \tag{3.1}$$

where the w_i are weighting factors to be selected by engineering judgment. From this viewpoint, you can also view each term in the summations as being weighted equally.

This chapter includes a discussion of how to formulate objective functions involved in economic analysis, an explanation of the important concept of the time value of money, and an examination of the various ways of carrying out a profitability analysis. In Appendix B we cover, in more detail, ways of estimating the capital and operating costs in the process industries, components that are included in the objective function. For examples of objective functions other than economic ones, refer to the applications of optimization in Chapters 11 to 16.

3.1 ECONOMIC OBJECTIVE FUNCTIONS

The ability to understand and apply the concepts of cost analysis, profitability analysis, budgets, income-and-expense statements, and balance sheets are key skills that may be valuable. This section treats two major components of economic objective functions: capital costs and operating costs. Economic decisions are made at various levels of detail. The more detail involved, the greater the expense of preparing an economic study. In engineering practice you may need to prepare preliminary cost estimates for projects ranging from a small piece of equipment or a new product to a major plant retrofit or design.

To introduce the involvement of these two types of costs in an objective function, we consider three simple examples: The first involves only operating costs and income, the second involves only capital costs, and the third involves both.

EXAMPLE 3.1 OPERATING PROFITS AS THE OBJECTIVE FUNCTION

Let us return to the chemical plant of Example 2.10 with three products (E, F, G) and three raw materials (A, B, C) in limited supply. Each of the three products is produced in a separate process (1, 2, 3); Figure E3.1 illustrates the process.

Process data

Process 1: $A + B \rightarrow E$

Process 2: $A + B \rightarrow F$

Process 3: $3A + 2B + C \rightarrow G$

Raw material	Maximum available (kg/day)	Cost (¢/kg)
A	40,000	1.5
B	30,000	2.0
C	25,000	2.5

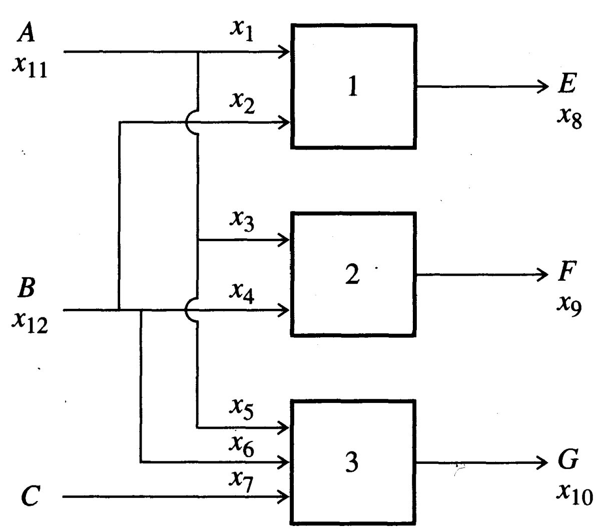


FIGURE E3.1
Flow diagram for a multiproduct plant.

Process	Product	Reactant requirements (kg/kg product)	Processing cost (product) (¢/kg)	Selling price (product) (¢/kg)
1	E	$\frac{2}{3}A, \frac{1}{3}B$	1.5	4.0
2	F	$\frac{2}{3}A, \frac{1}{3}B$	0.5	3.3
3	G	$\frac{1}{2}A, \frac{1}{6}B, \frac{1}{3}C$	1.0	3.8
		(mass is conserved)		

Formulate the objective function to maximize the total operating profit per day in the units of \$/day.

Solution The notation for the mass flow rates of reactants and products is the same as in Example 2.10.

The income in dollars per day from the plant is found from the selling prices ($0.04E + 0.033F + 0.038G$). The operating costs in dollars per day include

Raw material costs: $0.015A + 0.02B + 0.025C$

Processing costs: $0.015E + 0.005F + 0.01G$

Total costs in dollars per day $= 0.015A + 0.02B + 0.025C + 0.015E + 0.005F + 0.01G$

The daily profit is found by subtracting daily operating costs from the daily income:

$$
\begin{aligned}
f(\mathbf{x}) &= 0.025E + 0.028F + 0.028G - 0.015A - 0.02B - 0.025C \\
&= 0.025x_8 + 0.028x_9 + 0.028x_{10} - 0.015x_{11} - 0.02x_{12} - 0.025x_7
\end{aligned}
$$

Note that the six variables in the objective function are constrained through material balances, namely

$$
\begin{aligned}
x_{11} &= 0.667x_8 + 0.667x_9 + 0.5x_{10} \\
x_{12} &= 0.333x_8 + 0.333x_9 + 0.167x_{10} \\
x_7 &= 0.333x_{10}
\end{aligned}
$$

Also

$$
\begin{aligned}
0 \le x_{11} &\le 40{,}000 \\
0 \le x_{12} &\le 30{,}000 \\
0 \le x_7 &\le 25{,}000
\end{aligned}
$$

The optimization problem in this example comprises a linear objective function and linear constraints, hence linear programming is the best technique for solving it (refer to Chapter 7).

The next example treats a case in which only capital costs are to be optimized.

EXAMPLE 3.2 CAPITAL COSTS AS THE OBJECTIVE FUNCTION

Suppose you wanted to find the configuration that minimizes the capital costs of a cylindrical pressure vessel. To select the best dimensions (length L and diameter D) of the vessel, formulate a suitable objective function for the capital costs and find the optimal (L/D) that minimizes the cost function. Let the tank volume be V, which is fixed. Compare your result with the design rule-of-thumb used in practice, $(L/D)^{\text{opt}} = 3.0$.

Solution Let us begin with a simplified geometry for the tank based on the following assumptions:

1. Both ends are closed and flat.
2. The vessel walls (sides and ends) are of constant thickness t with density ρ, and the wall thickness is not a function of pressure.
3. The cost of fabrication and material is the same for both the sides and ends, and is S (dollars per unit weight).
4. There is no wasted material during fabrication due to the available width of metal plate.

The surface area of the tank using these assumptions is equal to

$$\underbrace{2\left(\frac{\pi D^2}{4}\right)}_{\text{(ends)}} + \underbrace{\pi DL}_{\text{(cylinder)}} = \frac{\pi D^2}{2} + \pi DL \qquad (a)$$

From assumptions 2 and 3, you might set up several different objective functions:

$$f_1 = \frac{\pi D^2}{2} + \pi DL \qquad \text{(units of area)} \qquad (b)$$

$$f_2 = \rho\left(\frac{\pi D^2}{2} + \pi DL\right)\cdot t \qquad \text{(units of weight)} \qquad (c)$$

$$f_3 = S\cdot\rho\cdot\left(\frac{\pi D_2}{2} + \pi DL\right)\cdot t \qquad \text{(units of cost in dollars)} \qquad (d)$$

Note that all of these objective functions differ from one another only by a multiplicative constant; this constant has no effect on the values of the independent variables at the optimum. For simplicity, we therefore use f_1 to determine the optimal values of D and L. Implicit in the problem statement is that a relation exists between volume and length, namely the constraint

$$V = \frac{\pi D^2}{4}\cdot L \qquad (e)$$

Hence, the problem has only one independent variable.

Next use (e) to remove L from (b) to obtain the objective function

$$f_4 = \frac{\pi D^2}{2} + \frac{4V}{D} \tag{f}$$

Differentiation of f_4 with respect to D for constant V, equating the derivative to zero, and solving the resulting equation gives

$$D^{\text{opt}} = \left(\frac{4V}{\pi}\right)^{1/3} \tag{g}$$

This result implies that $f_4 \sim V^{2/3}$, a relationship close to the classical "six-tenths" rule used in cost estimating. From (e), $L^{\text{opt}} = (4V/\pi)^{1/3}$; this yields a rather surprising result, namely

$$\left(\frac{L}{D}\right)^{\text{opt}} = 1 \tag{h}$$

The $(L/D)^{\text{opt}}$ ratio is significantly different from the rule of thumb stated earlier in the example, namely, $L/D = 3$; this difference must be due to the assumptions (perhaps erroneous) regarding vessel geometry and fabrication costs.

Brummerstedt (1944) and Happel and Jordan (1975) discussed a somewhat more realistic formulation of the problem of optimizing a vessel size, making the following modifications in the original assumptions:

1. The ends of the vessel are 2:1 ellipsoidal heads, with an area for the two ends of $2(1.16D^2) = 2.32D^2$.
2. The cost of fabrication for the ends is higher than the sides; Happel and Jordan suggested a factor of 1.5.
3. The thickness t is a function of the vessel diameter, allowable steel stress, pressure rating of the vessel, and a corrosion allowance. For example, a design pressure of 250 psi and a corrosion allowance of $\frac{1}{8}$ in. give the following formula for t in inches (in which D is expressed in feet):

$$t = 0.0108D + 0.125 \tag{i}$$

The three preceding assumptions require that the objective function be expressed in dollars since area and weight are no longer directly proportional to cost

$$f_5 = \rho[\pi DLS + (1.5S)(2.32D^2)]t \tag{j}$$

The unit conversion of t from inches to feet does not affect the optimum (L/D), nor do the values of ρ and S, which are multiplicative constants. The modified objective function, substituting Equation (i) in Equation (j), is therefore

$$f_6 = 0.0339D^2L + 0.435D^2 + 0.3927DL + 0.0376D^3 \tag{k}$$

The volume constraint is also different from the one previously used because of the dished heads:

$$V = \frac{\pi D^2}{4}\left(L + \frac{D}{3}\right) \tag{l}$$

Equation (l) can be solved for L and substituted into Equation (k). However, No analytical solution for D^{opt} by direct differentiation of the objective function is possible now because the expression for f_6, when L is eliminated, leads to a complicated polynomial equation for the objective function:

$$f_7 = 0.0432V + 0.5000\frac{V}{D} + 0.3041D^2 + 0.0263D^3 \tag{m}$$

When f_7 is differentiated, a fourth-order polynomial in D results; no simple analytical solution is possible to obtain the optimum value of D. A numerical search is therefore better for obtaining D^{opt} and should be based on f_7 (rather than examining $df_7/dD = 0$). However, such a search will need to be performed for different values of V and the design pressure, parameters which are embedded in Equation (i). Recall that Equations (i) and (m) are based on a design pressure of 250 psi. Happel and Jordan (1975) presented the following solution for $(L/D)^{opt}$:

TABLE E3.2
Optimum (L/D)

	Design pressure (psi)		
Capacity (gal)	**100**	**250**	**400**
2,500	1.7	2.4	2.9
25,000	2.2	2.9	4.3

In Chapter 5 you will learn how to obtain such a solution. Note that for small capacities and low pressures, the optimum L/D approaches the ideal case; examine Equation (h) considered earlier. It is clear from Table E3.2 that the rule of thumb that $(L/D)^{opt} = 3$ can be in error by as much as ± 50 percent from the actual optimum. Also, the optimum does not take into account materials wasted during fabrication, a factor that could change the answer.

Next we consider an example in which both operating costs and capital costs are included in the objective function. The solution of this example requires that the two types of costs be put on some common basis, namely, dollars per year.

EXAMPLE 3.3 OPTIMUM THICKNESS OF INSULATION

In specifying the insulation thickness for a cylindrical vessel or pipe, it is necessary to consider both the costs of the insulation and the value of the energy saved by adding the insulation. In this example we determine the optimum thickness of insulation for a large pipe that contains a hot liquid. The insulation is added to reduce heat losses from the pipe. Next we develop an analytical expression for insulation thickness based on a mathematical model.

The rate of heat loss from a large insulated cylinder (see Figure E3.3), for which the insulation thickness is much smaller than the cylinder diameter and the inside heat transfer coefficient is very large, can be approximated by the formula

$$Q = \frac{A\Delta T}{x/k + 1/h_c} \tag{a}$$

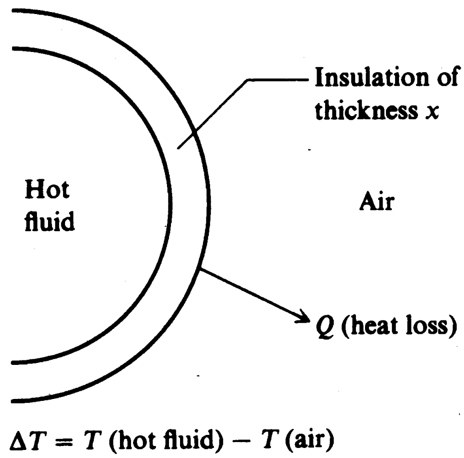


FIGURE E3.3
Heat loss from an insulated pipe

where ΔT = average temperature difference between pipe fluid and ambient surroundings, K
A = surface area of pipe, m^2
x = thickness of insulation, m
h_c = outside convective heat transfer coeffient, kJ/(h)(m^2)(K)
k = thermal conductivity of insulation, kJ/(h)(m)(K)
Q = heat loss, kJ/h

All of the parameters on the right hand side of Equation (*a*) are fixed values except for x, the variable to be optimized. Assume the cost of installed insulation per unit area can be represented by the relation $C_0 + C_1x$, where C_0 and C_1 are constants (C_0 = fixed installation cost and C_1 = incremental cost per foot of thickness). The insulation has a lifetime of 5 years and must be replaced at that time. The funds to purchase and install the insulation can be borrowed from a bank and paid back in five annual installments. Let r be the fraction of the installed cost to be paid each year to the bank. The value of r selected depends on the interest rate of the funds borrowed and will be explained in Section 3.2.

Let the value of the heat lost from the pipe be H_t (\$/10^6 kJ). Let Y be the number of hours per year of operation. The problem is to

1. Formulate an objective function to maximize the savings in operating cost, savings expressed as the difference between the value of the heat conserved less the annualized cost of the insulation.
2. Obtain an analytical solution for x^*, the optimum.

Solution If operating costs are to be stated in terms of dollars per year, then the capital costs must be stated in the same units. Because the funds required for the insulation are to be paid back in equal installments over a period of 5 years, the payment per year is $r(C_0 + C_1x)A$. The energy savings due to insulation can be calculated from the difference between $Q(x = 0) = Q_0$, and Q:

$$Q_0 - Q = h_c \Delta TA - \frac{\Delta TA}{x/k + 1/h_c} \qquad (b)$$

The objective function to be maximized is the present value of heat conserved in dollars less the annualized capital cost (also in dollars):

$$f = (Q_0 - Q)\left(\frac{\text{kJ}}{\text{h}}\right) \cdot Y\left(\frac{\text{h}}{\text{year}}\right) \cdot H_t\left(\frac{\text{dollars}}{\text{kJ}}\right)\frac{1}{r}\ (\text{year})$$

$$- (C_0 + C_1 x)A\,(\text{dollars}) \qquad (c)$$

Substitute Equation (*b*) into (*c*), differentiate f with respect to x, and solve for the optimum ($df/dx = 0$):

$$x^* = k\left\{\left(\frac{H_t Y\,\Delta T}{10^6 k C_1 r}\right)^{1/2} - \frac{1}{h_c}\right\} \qquad (d)$$

Examine how x^* varies with the different parameters in (*d*), and confirm that the trends are physically meaningful. Note that the heat transfer area A does not appear in Equation (*d*). Why? Could you formulate f as a cost minimization problem, that is, the sum of the value of heat lost plus insulation cost? Does it change the result for x^*? How do you use this result to select the correct commercial insulation size (see Example 1.1)?

Appendix B explains ways of estimating the capital and operating costs, leading to the coefficients in economic objective functions.

3.2 THE TIME VALUE OF MONEY IN OBJECTIVE FUNCTIONS

So far we have explained how to estimate capital and operating costs. In Example 3.3, we formulated an objective function for economic evaluation and discovered that although the revenues and operating costs occur in the future, most capital costs are incurred at the beginning of a project. How can these two classes of costs be evaluated fairly? The economic analysis of projects that incur income and expense over time should include the concept of the time value of money. This concept means that a unit of money (dollar, yen, euro, etc.) on hand now is worth more than the same unit of money in the future. Why? Because \$1000 invested today can earn additional dollars; in other words, the value of \$1000 received in the future will be less than the present value of \$1000.

For an example of the kinds of decisions that involve the time value of money, examine the advertisement in Figure 3.1. For which option do you receive the most value? Answers to this and similar questions sometimes may be quickly resolved using a calculator or computer without much thought. To understand the underlying assumptions and concepts behind the calculations, however, you need to account for cash flows in and out using the investment time line diagram for a project. Look at Figure 3.2.

You Decide Which Option You Prefer If You Are The Winner Of The Sweepstakes:

Option 1		Option 2		Option 3
$2,000,000 NOW. Payable immediately.	OR	$1,000,000 NOW. PLUS $137,932 a year for 29 years.	OR	$167,000 a year for 30 years.

Tell us your choice. Read the instructions on the reverse to learn how you can activate your Grand Prize Option.

FIGURE 3.1
Options for potential sweepstakes winners. Which option provides the optimal value?

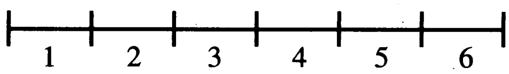


FIGURE 3.2
The time line with divisions corresponding to 6 time periods.

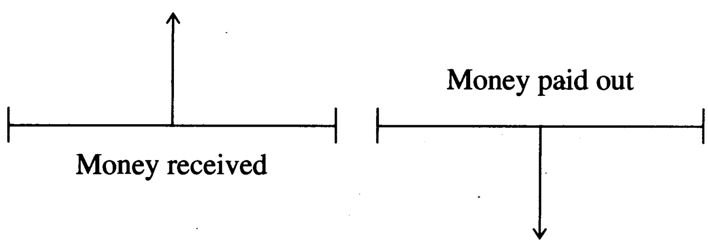


FIGURE 3.3
Representation of cash received and disbursed.

Figure 3.3 depicts money received (or income) with vertical arrows pointing upward; money paid out (or expenses) is depicted by vertical arrows pointing downward. With the aid of Figure 3.3 you can represent almost any complicated financial plan for a project. For example, suppose you deposit $1000 now (the present value P) in a bank savings account that pays 5.00 percent annual interest compounded monthly, and in addition you plan to deposit $100 per month at the end of each month for the next year. What will the future value F of your investments be at the end of the year? Figure 3.4 outlines the arrangement on the time line.

Note that cash flows corresponding to the accrual of interest are not represented by arrows in Figure 3.4. The interest rate per month is 0.4167, not 5.00 percent (the

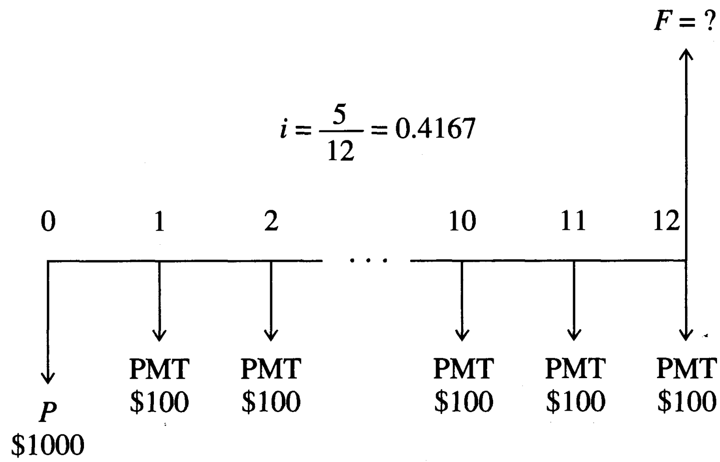


FIGURE 3.4
The transactions for the example placed on the time line.

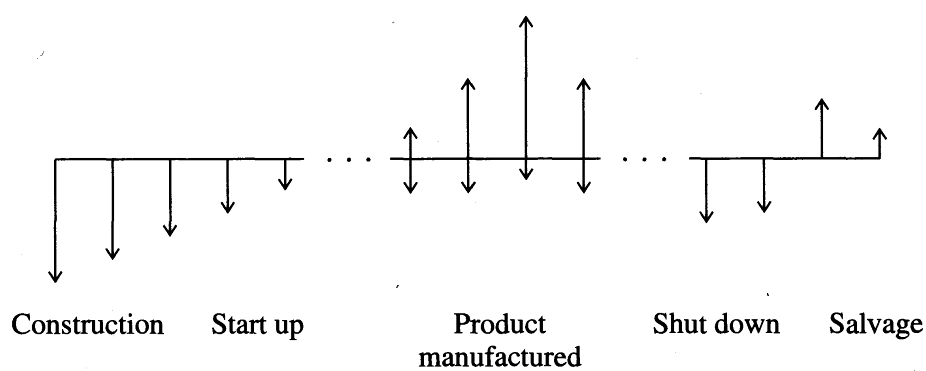


FIGURE 3.5
Cash flow transactions for a proposed plant placed on the time line.

annual interest rate). The number of compounding periods is $n = 12$. PMT is the periodic payment.

Figure 3.5 shows (using arrows only) some of the typical cash flows that might occur from the start to the end of a proposed plant. As the plant is built, the cash flows are negative, as is most likely the case during startup. Once in operation, the plant produces positive cash flows that diminish with time as markets change and competitors start up. Finally, the plant is closed, and eventually the equipment sold or scrapped.

It is easy to develop a general formula for investment growth for the case in which fractional interest i is compounded once per period (month, year). (*Note*: On most occasions we will cite i in percent, as is the common practice, even though in problem calculations i is treated as a fraction.) If P is the original investment (*present value*), then $P(1 + i)$ is the amount accumulated after one compounding period, say 1 year. Using the same reasoning, the value of the investment in successive years for discrete interest payments is

$$t = 2 \text{ years} \qquad F_2 = P(1+i) + iP(1+i) = P(1+i)^2 \tag{3.2a}$$

$$t = 3 \text{ years} \qquad F_3 = P(1+i)^2 + iP(1+i)^2 = P(1+i)^3 \tag{3.2b}$$

$$t = n \text{ years} \qquad F_n = P(1+i)^n \tag{3.2c}$$

The symbol F_n is called the *future worth* of the investment after year n, that is, the future value of a current investment P based on a specific interest rate i.

Equation (3.2c) can be rearranged to give present value in terms of future value, that is, the present value of one future payment F at period n

$$P = \frac{F_n}{(1+i)^n} \tag{3.3}$$

For continuous compounding Equation (3.2c) reduces to $F_n = Pe^{in}$. Refer to Garrett, Chapt. 5 (1989) for the derivation of this formula.

The following is a list of some useful extensions of Equation (3.3). Note that the factors involved in Equations (3.3)–(3.7) are F, P, i, and n, and given the values of any three, you can calculate the fourth. Software such as Microsoft Excel and hand calculators all contain programs to execute the calculations, many of which must be iterative.

1. Present value of a series of payments F_k (not necessarily equal) at periods $k = 1, \ldots, n$ in the future:

$$P = \frac{F_1}{(1+i)} + \frac{F_2}{(1+i)^2} + \cdots + \frac{F_{n-1}}{(1+i)^{n-1}} + \frac{F_n}{(1+i)^n} \tag{3.4}$$

$$= \sum_{k=1}^{n} \frac{F_k}{(1+i)^k} \tag{3.4a}$$

2. Present value of a series of uniform future payments each of value 1 starting in period m and ending with period n:

$$P = \sum_{k=m}^{n} \frac{1}{(1+i)^k} = \left[-\left(\frac{1+i}{i}\right)\left(\frac{1}{1+i}\right)^k\right]_m^{n+1} = \frac{1}{i(1+i)^{m-1}} - \frac{1}{i(1+i)^n}$$

$$= \frac{(1+i)^{n-m+1} - 1}{i(1+i)^n}$$

If $m = 1$,

$$P = \sum_{k=1}^{n} \frac{1}{(1+i)^k} = \frac{(1+i)^n - 1}{i(1+i)^n} \tag{3.5}$$

3. Future value of a series of (not necessarily equal) payments P_k:

$$F = \sum_{k=1}^{n} P_k (1 + i)^{n-k+1} \tag{3.6}$$

4. Future value of a series of uniform future payments each of value 1 starting in period m and ending in period n:

$$F = (1 + i)^n \sum_{k=m}^{n} \frac{1}{(1 + i)^k} = \frac{(1 + i)^{n-m+1} - 1}{i} \tag{3.7}$$

If $m = 1$ so that $k = 1$, the equivalent of Equation (3.7) is

$$F = (1 + i)^n \sum_{k=1}^{n} \frac{1}{(1 + i)^k} = \frac{(1 + i)^n - 1}{i}$$

The right-hand side of Equation (3.5) is known as the "capital recovery factor" or "present worth factor," and the inverse of the right-hand side is known as the "repayment multiplier" r.

$$r = \frac{i(1 + i)^n}{(1 + i)^n - 1} \tag{3.8}$$

Tables of the repayment multiplier are listed in handbooks and some textbooks. Table 3.1 gives r over some limited ranges as a function of n and i.

TABLE 3.1

Values for the fraction $r = \dfrac{i(1 + i)^n}{(1 + i)^n - 1}$

	Interest rate									
n	$i \to 1$	2	4	6	8	10	12	14	16	18
1	1.010	1.020	1.040	1.060	1.080	1.100	1.120	1.140	1.160	1.180
2	0.507	0.515	0.530	0.545	0.561	0.576	0.592	0.607	0.623	0.639
3	0.340	0.347	0.360	0.374	0.388	0.402	0.416	0.431	0.445	0.460
5	0.206	0.212	0.225	0.237	0.251	0.264	0.277	0.291	0.305	0.320
10	0.106	0.111	0.123	0.136	0.149	0.163	0.177	0.192	0.207	0.222
15	0.072	0.078	0.090	0.103	0.117	0.132	0.147	0.163	0.179	0.196
20	0.055	0.061	0.074	0.087	0.102	0.117	0.134	0.151	0.169	0.187
25	0.045	0.051	0.064	0.078	0.094	0.110	0.128	0.145	0.164	0.183
30	0.039	0.045	0.058	0.073	0.089	0.106	0.124	0.143	0.162	0.181
40	0.030	0.037	0.051	0.067	0.084	0.102	0.121	0.141	0.160	0.180
50	0.026	0.032	0.047	0.063	0.082	0.101	0.120	0.140	0.160	0.180
75	0.019	0.026	0.042	0.061	0.080	0.100	0.120	0.140	0.160	0.180
100	0.016	0.023	0.041	0.060	0.080	0.100	0.120	0.140	0.160	0.180

Key: n = number of years i = interest rate, %

For uniform (equal) future payments each of value F, Equation (3.5) becomes

$$P = \frac{F}{r} \quad \text{or} \quad r = \frac{F}{P} \tag{3.9}$$

If the interest is calculated continuously, rather than periodically, the equivalent of Equation (3.5) is (with the uniform payments of value F)

$$P = F\frac{e^{in} - 1}{i(e^{in})} \tag{3.10}$$

The inverse of the right-hand side of Equation (3.6) is known in economics as the "sinking fund deposit factor," that is, how much a borrower must periodically deposit with a trustee to eventually pay off a loan.

Now let us look at some examples that illustrate the application of the concepts and relations discussed earlier.

EXAMPLE 3.4 PAYING OFF A LOAN

You borrow \$35,000 from a bank at 10.5% interest to purchase a multicone cyclone rated at 50,000 ft^3/min. If you make monthly payments of \$325 (at the end of the month), how many payments will be required to pay off the loan?

Solution The diagram on the time line in Figure E3.4a shows the cash flows. Because the payments are uniform, we can use Equation (3.5), but use \$325 per month rather than \$1.

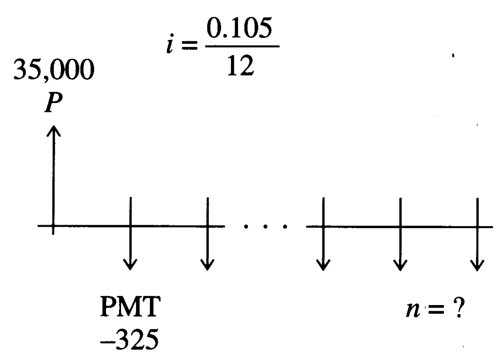


FIGURE E3.4a

$$35{,}000 - 325\left[\frac{(1 + i)^n - 1}{i(1 + i)^n}\right] = 0 \tag{a}$$

Equation (a) can be solved for n (months). Use Equation (3.8) to simplify the procedure.

$$r = \frac{i(i + 1)^n}{(1 + i)^n - 1}$$

$$(i + 1)^n = \frac{r}{r - i}$$

$$n = \frac{\ln\left[r/(r-1)\right]}{\ln(1+i)} \tag{b}$$

In the example the data are

$$i = \frac{0.105}{12} = 0.008750 \qquad 1 + i = 1.008750$$

$$r = \frac{325}{35{,}000} = 0.009286 \qquad r/(r - i) = 17.3333$$

$$n = \frac{2.85263}{0.008712} = 327.4 \text{ months}$$

The final payment (No. 328) will be less than \$325.00, namely \$143.11.

For income tax purposes, you can calculate the principal and interest in each payment. For example, at the end of the first month, the interest paid is \$35,000 (0.008750) = \$306.25 and the principal paid is \$325.00 − \$306.25 = \$18.75, so that the principal balance for the next month's interest calculation is \$34,981.25. Iteration of this procedure (best done on a computer) yields the "amortization schedule" for the loan.

You can carry out the calculations using the Microsoft Excel function key (found by clicking on the "insert" button in the toolbar):

1. Click on the function key (f_x) in the spreadsheet tool bar.
2. Choose financial function category (Figure E3.4b).
3. Select NPER.

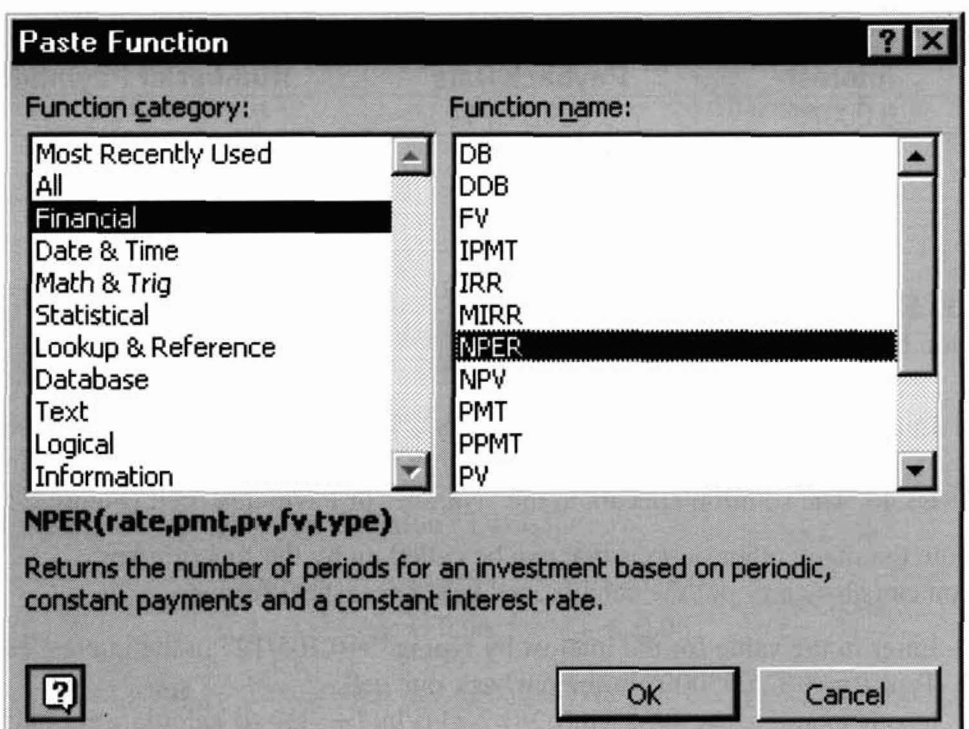


FIGURE E3.4b
Permission by Microsoft.

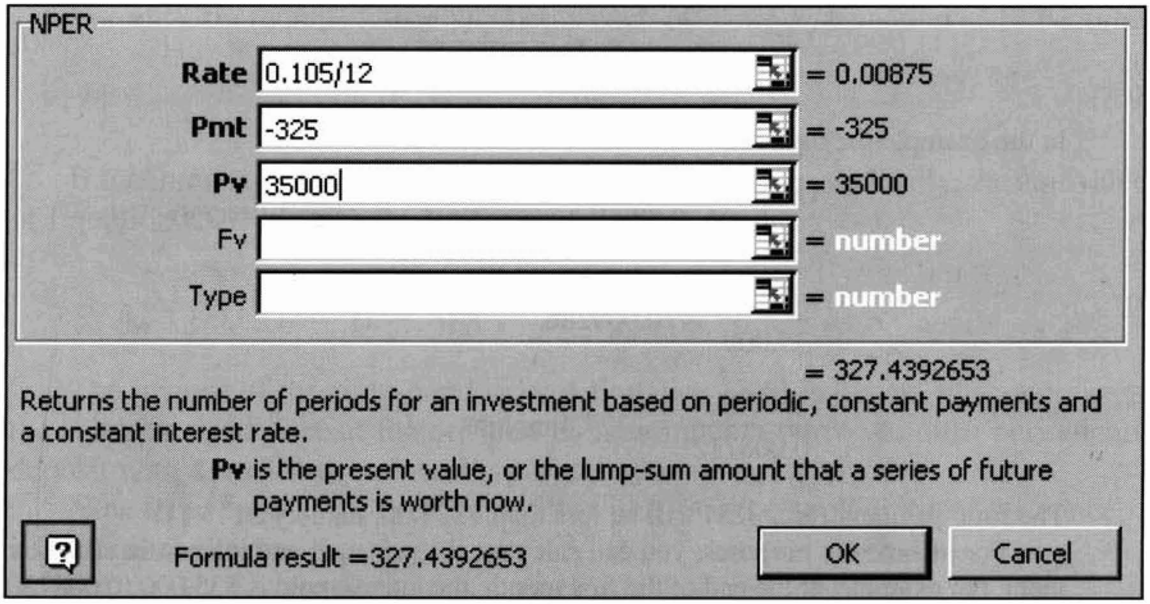


FIGURE E3.4c
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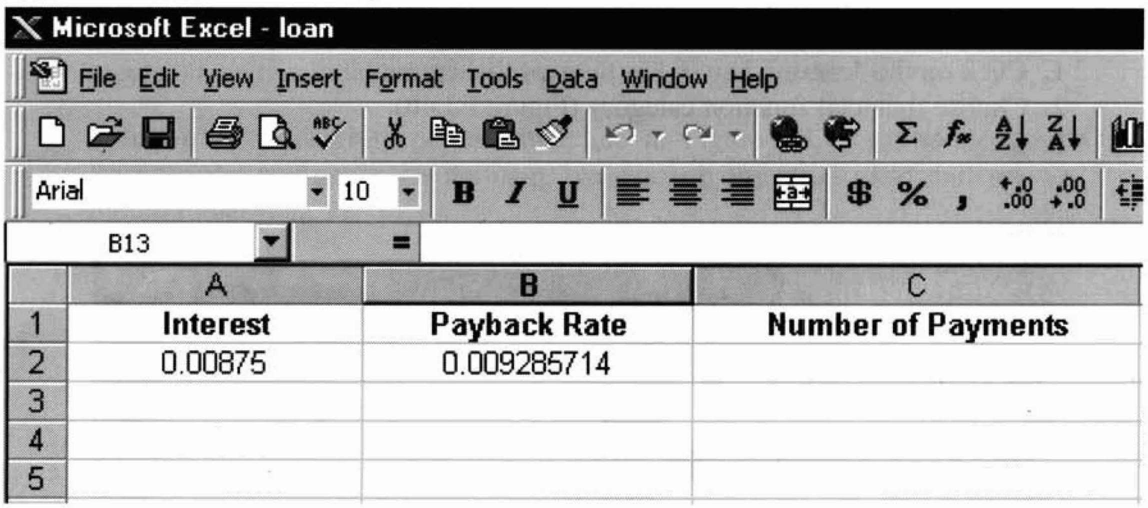

FIGURE E3.4d
Permission by Microsoft.

4. Enter correct values for payment (−\$325), rate (0.105/12), and present value (\$35,000) (Figure E3.4c), and click on "OK" to get the screen shown in Figure E3.4d. The solution appears in the "Number of Payments" cell (Figure E3.4e).

Note the many other options that can be called up by the function key.
You can also carry out the calculations in a spreadsheet format.

1. Enter in the value for the interest by typing "=0.105/12" in the interest cell.
2. Type "= −325/35000" in the payback rate cell.
3. In our example we type "ln(b2/(b2-a1))/ln(1+a1)" to calculate the number of payments.

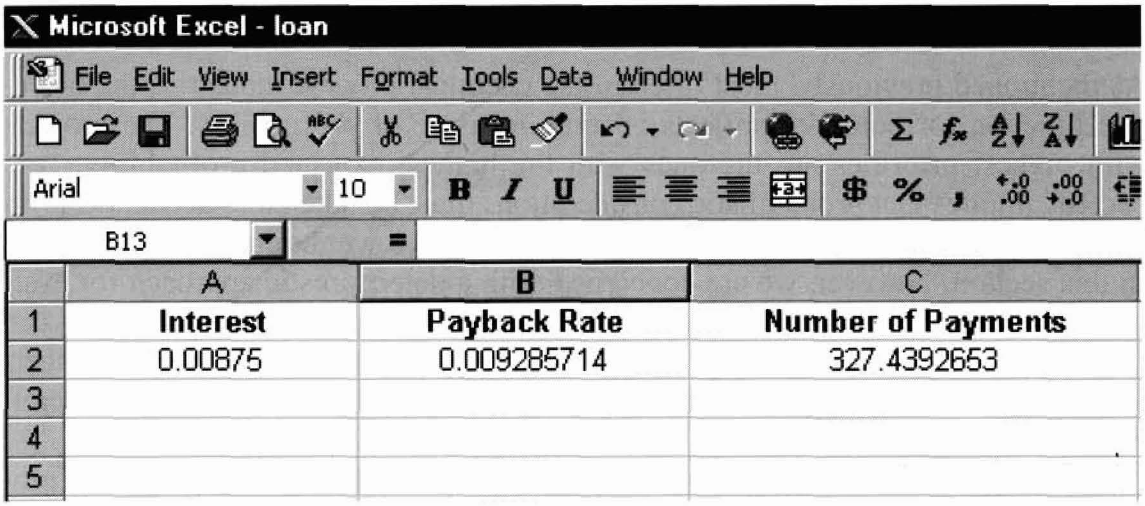

FIGURE E3.4e
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EXAMPLE 3.5 SELECTION OF THE CHEAPEST ANODES

Ordinary anodes for an electrochemical process last 2 years and then have to be replaced at a cost of \$20,000. An alternative choice is to buy impregnated anodes that last 6 years and cost \$56,000 (see Figure E3.5). If the annual interest rate is 6 percent per year, which alternative would be the cheapest?

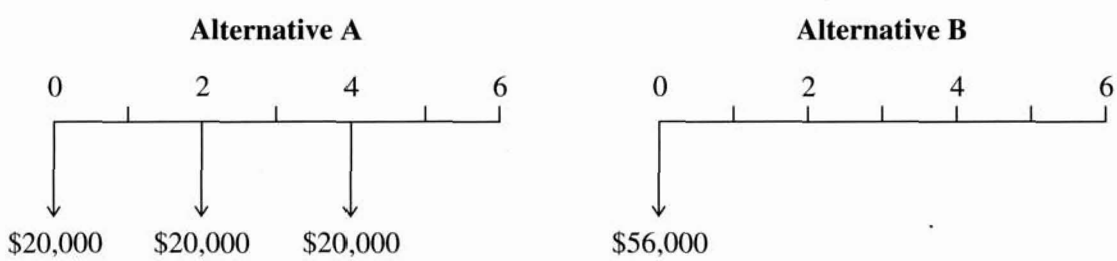

FIGURE E3.5

Solution We want to calculate the present value of each alternative. The present value of alternative A using Equation (3.4) is

$$P = \frac{-\$20{,}000}{1} + \frac{-\$20{,}000}{(1 + 0.06)^2} + \frac{-\$20{,}000}{(1 + 0.06)^4} = -\$53{,}642$$

The present value of alternative B is $-\$56{,}000$. Alternative A gives the largest (smallest negative) present value.

3.3 MEASURES OF PROFITABILITY

As mentioned previously, most often in the chemical process industries the objective function for potential projects is some measure of profitability. The projects with highest priorities are the ones with the highest expected profitability; "expected" implies that probabilistic considerations must be taken into account (Palvia and Gordon, 1992), such as calculating the upper and lower bounds of a prediction. In this section, however, we are concerned with a deterministic approach for evaluating profitability, keeping in mind that different definitions of profitability can lead to different priority rankings. Analyses are typically carried out in spreadsheets to generate a variety of possibilities that allow the projects to be ranked as a prelude to decision making.

Among the numerous measures of economic performance that have been proposed, two of the simplest are

1. Payback period (PBP)—how long a project must operate to break even; ignores the time value of money.

$$\text{PBP} = \frac{\text{Cost of investment}}{\text{Cash flow per period}}$$

Example: For an investment of \$20,000 with a return of \$500 per week the PBP is

$$\frac{\$20{,}000}{\$500} = 40 \text{ weeks}$$

2. Return on investment (ROI)—a simple yield calculation without taking into account the time value of money

$$\text{ROI (in percent)} = \frac{\text{Net income (after taxes) per year}}{\text{Cost of investment}} \times 100$$

Example: Given the net return of \$6000 (per year) for an initial investment of \$45,000, the ROI is

$$\frac{\$6000}{\$45{,}000} \times 100 = 13.3\%/\text{year}$$

Two other measures of profitability that take into account the time value of money are

1. Net present value (NPV).
2. Internal rate of return (IRR).

NPV takes into account the size and profitability of a project, but the IRR measures only profitability. If a company has sufficient resources to consider several small projects, given a prespecified amount of investment, a number of high-value IRRs usually provide a higher overall NPV than a single large project.

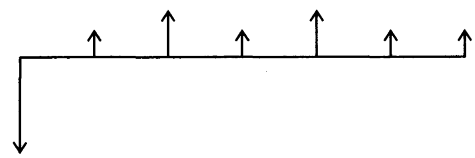

FIGURE 3.6
Cash flows used in calculating net present value (NPV) and internal rate of return (IRR) for a typical capital investment project.

Figure 3.6 designates the cash flows that might occur for a cash investment in a project. NPV is calculated by adding the initial investment (represented as a negative cash flow) to the present value of the anticipated future positive (and negative) cash flows. Equation (3.4) showed how to calculate NPV.

- If the NPV is positive, the investment increases the company's assets: The investment is financially attractive.
- If the NPV is zero, the investment does not change the value of the company's assets: The investment is neutral.
- If the NPV is negative, the investment decreases the company's assets: The investment is not financially attractive.

The higher the NPV among alternative investments with the same capital outlay, the more attractive the investment.

IRR is the rate of return (interest rate, discount rate) at which the future cash flows (positive plus negative) would equal the initial cash outlay (a negative cash flow). The value of the IRR relative to the company standards for internal rate of return indicates the desirability of an investment:

- If the IRR is greater than the designated rate of return, the investment is financially attractive.
- If the IRR is equal to the designated rate of return, the investment is marginal.
- If the IRR is less than the designated rate of return, the investment is financially unattractive.

Table 3.2 compares some of the features of PBP, NPV, and IRR.

Numerous other measures of profitability exist, and most companies (and financial professionals) use more than one. Cut-off levels are placed on the measures of profitability so that proposals that fall below the cut-off level are not deemed worthy of consideration. Those that fall above the cut-off level can be ranked in order of profitability and examined in more detail.

In optimization you are interested in

1. Minimizing the payback period (PBP), or
2. Maximizing the net present value (NPV), or
3. Maximizing the internal rate of return (IRR)

TABLE 3.2
Comparisons of various methods used in economic analyses

Payback period (PBP)	Net present value (NPV)	Internal rate of return (IRR)
	Definition	
Number of years for the net after-tax income to recover the net investment without considering time value of money	Present worth of receipts less the present worth of disbursements	IRR equals the interest rate i such that the NPV of receipts less NPV of disbursements equals zero
	Advantages	
Measure of fluidity of an investment Commonly used and well understood	Works with all cash flow patterns Easy to compute Gives correct ranking in most project evaluations	Gives rate of return that is a familiar measure and indicates relative merits of a proposed investment Treats variable cash flows Does not require reinvestment rate assumption
	Disadvantages	
Does not measure profitability Ignores life of assets Does not properly consider the time value of money and distributed investments or cash flows	Is not always possible to specify a reinvestment rate for capital recovered Size of NPV ($) sometimes fails to indicate relative profitability	Implicitly assumes that capital recovered can be reinvested at the same rate Requires trial-and-error calculation Can give multiple answers for distributed investments

or optimizing another criterion of profitability. The decision variables are adjusted to reach an extremum. In most of the problems and examples in the subsequent chapters we have not included factors for the time value of money because we want to focus on other details of optimization. Nevertheless, the addition of such factors is quite straightforward.

EXAMPLE 3.6 CALCULATION OF THE OPTIMAL INSULATION THICKNESS

In Example 3.3 we developed an objective function for determining the optimal thickness of insulation. In that example the effect of the time value of money was introduced as an arbitrary constant value of r, the repayment multiplier. In this example, we treat the same problem, but in more detail. We want to determine the optimum insulation thickness for a 20-cm pipe carrying a hot fluid at 260°C. Assume that curvature of the pipe can be ignored and a constant ambient temperature of 27°C exists. The following information applies:

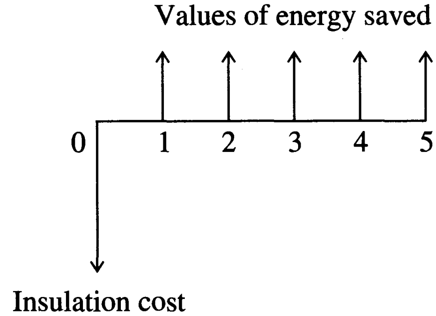

FIGURE E3.6
Cash flows for insulating a pipe.

Y	8000 operating hours/year
H_t	3.80/10^6 kJ fuel cost, 80% thermal efficiency (boiler)
k	0.80 kJ/(h)(m)(°C), insulation
C_1	\$34/cm insulation for 1 m^2 of area, cost of insulation
h_c	32.7 kJ/(h)(m^2)(°C), heat transfer coefficient (still air)
	Life of the insulation = 5 years
	Annual discount rate (i) = 14%
L	100 m, length of pipe

The insulation of thickness x can be purchased in increments of 1 cm (i.e., 1, 2, 3 cm, etc.). Equation (b) in Example 3.3 still applies. The value of the energy saved each year over 5 years is

$$Q_0 - Q = \Delta T(\pi DL)\left[h_c - \frac{1}{(x/k) + (1/h_c)}\right](Y)(H_t) \quad \text{in \$/year}$$

and the cost of the insulation is

$$C_1x(\pi DL) \quad \text{in \$}$$

at the beginning of the 5-year period. Figure E3.6 is the time line on which the cash flows are placed.

The basis for the calculations will be L = 100m. Because the insulation comes in 1-cm increments, let us calculate the net present value of insulating the pipe as a function of the independent variable x; vary x for a series of 1-, 2-, 3-cm (etc.) thick increments to get the respective internal rates of return, the payback period, and the return on investment. The latter two calculations are straightforward because of the assumption of five even values for the fuel saved. The net present value and internal rates of return can be compared for various thicknesses of insulation. The cost of the insulation is an initial negative cash flow, and a sum of five positive values represent the value of the heat saved. For example, for 1 cm insulation the net present value is (r = 0.291 from Table 3.1)

$$P_1 = -\$2135 + \frac{\$5281}{0.291} = \$16{,}013$$

A summary of the calculations is

Insulation thickness x (cm)	Insulation cost ($)	Value of fuel saved ($/year)	Payback period (years)	Return on investment (% per year)	Net present value ($)	Internal rate of return (%)
1	2,135	5,281	1.27	79	16,013	247
2	4,270	8,182	1.64	61	23,847	191
3	6,405	10,020	2.01	50	28,028	155
4	8,540	11,288	2.38	42	30,250	130
5	10,675	12,215	2.75	36	31,301	112
6	12,810	12,984	3.10	32	31,809	98
7	14,945	13,480	3.48	29	31,378	86

From Example 3.3, Equation E3.3(d) gives $x \approx 6.4$ cm as the optimal thickness corresponding to the net present value as the criterion for selection. Note that the optimal thickness chosen depends on the criterion you select.

Additional examples of the use of PBP, NPV, and IRR can be found in Appendix B. In Section B.5, we present a more detailed explanation of the various components that constitute the income and expense values that must be used in project evaluation.

REFERENCES

Brummerstedt, E. F. *Natl Pet News* **36:** R282, R362, R497 (1944).

Garrett, D. E. *Chemical Engineering Economics*. Van Nostrand-Reinhold, New York (1989).

Happel, J.; and D. G. Jordan. *Chemical Process Economics*, 2d ed. Marcel Dekker, New York (1975).

Hurvich, C.; and C. L. Tsai. "A Corrected Akaike Information Criterion for Vector Autoregressive Model Selection." *J Time Series Anal* **14**, 271–279 (1993).

Kamimura, R. "D-Entropy Minimization." In *Proceedings of the International Conference on Neural Networks*. Houston (1997).

Palvia, S. C.; and S. R. Gordon. "Tables, Trees, and Formulas in Decision Analysis." *Commun A C M* **35**, 104–113 (1992).

Rusnak, I.; A. Guez; and I. Bar-Kana. "Multiple Objective Approach to Adaptive Control of Linear Systems." In *Proceedings of the American Control Conference*. San Francisco, pp. 1101–1105 (1993).

Steur, R. E. *Multiple Criteria Optimization: Theory, Computation and Application*. Wiley, New York (1998).

SUPPLEMENTARY REFERENCES

Bhaskar, V.; S. K. Gupta; and A. K. Ray. "Applications of Multiobjective Optimization in Chemical Engineering." *Reviews in Chem Engr* **16** (1): 1–54 (2000).

Blank, L. T.; and A. J. Tarquin. *Engineering Economy*. McGraw-Hill, New York (1997).
Bowman, M. S. *Applied Economic Analysis for Technologists, Engineers, and Managers*. Prentice-Hall, Englewood Cliffs, NJ (1998).
Canada, J. R.; W. G. Sullivan; and J. A. White. *Capital Investment Analysis for Engineering and Management*. Prentice-Hall, Englewood Cliffs, NJ (1995).

PROBLEMS

3.1 If you borrow $100,000 from a lending agency at 10 percent yearly interest and wish to pay it back in 10 years in equal installments paid annually at the end of the year, what will be the amount of each yearly payment? Compute the principal and interest payments for each year.

3.2 Compare the present value of the two depreciation schedules listed below for $i = 0.12$ and $n = 10$ years. Depreciation is an expense and thus has a negative sign before each value. The present value also have a negative sign.

Year	(a)	(b)
1	−1000	−800
2	−1000	−1400
3	−1000	−1200
4	−1000	−1000
5	−1000	−1000
6	−1000	−1000
7	−1000	−900
8	−1000	−900
9	−1000	−900
10	−1000	−900

3.3 To provide for the college education of a child, what annual interest rate must you obtain to have a current investment of $5000 grow to become $10,000 in 8 years if the interest is compounded annually?

3.4 A company is considering a number of capital improvements. Among them is purchasing a small pyrolysis unit that is estimated to earn $15,000 per year at the end of each year for the next 5 years at which time the sellers agree to purchase the unit back for $550,000. Ignore tax effects, risk, and so on, and determine the present value of the investment based on an interest rate of 15.00% compounded annually. At the end of year 2 there will be an expense of $25,000 to replace the unit combustion chamber.

3.5 One member of your staff suggests that if your department spends just $10,000 to improve a process, it will yield cost savings of $3000, $5000, and $4000 over the next 3 years, respectively, for a total of $12,000. Your company policy is to have an internal rate of return of at least 15% on process improvements. What is the NPV of this proposed improvement?

3.6 You want to save for a cruise in the Caribbean. If you place in a savings account at 6% interest $200 at the beginning of the first year, $350 at the beginning of the next year, and

$250 at the beginning of the third year, how much will you have available at the end of the third year?

3.7 You open a savings account today (the middle of the month) with a $775 deposit. The account pays $6\frac{1}{4}\%$ interest (annual value) compounded semimonthly. If you make semimonthly deposits of $50 beginning next month, how long will it take for your account to reach $4000?

3.8 Looking forward to retirement, you wish to accumulate $60,000 after 15 years by making deposits in an account that pays $9\frac{3}{4}\%$ interest compounded semiannually. You open the account with a deposit of $3200 and intend to make semiannual deposits, beginning 6 months later, from your profit-sharing bonus paychecks. Calculate how much these deposits should be.

3.9 What is the present value of the tax savings on the annual interest payments if the loan payments consist of five equal monthly installments of principal and interest of $3600 on a loan of $120,000. The annual interest rate is 14.0%, and the tax rate is 40%. (Assume the loan starts at the first of July so that only five payments are made during the year on the first of each month starting August 1.)

3.10 The following advertisement appeared in the newspaper. Determine whether the statement in the ad is true or false, and show by calculations or explanation why your answer is correct.

> *A 15-year fixed-rate mortgage with annual payments saves you nearly 60 percent of the total interest costs over the life of the loan compared with a 30-year fixed-rate mortgage.*

3.11 You borrow $300,000 for 4 years at an interest rate of 10% per year. You plan to pay in equal annual, end-of-year installments. Fill in the following table.

Year	**Balance due at beginning of year, $**	**Principal payment, $**	**Interest payment, $**	**Total payment, $**
1				
2				
3				
4				

3.12 Consideration is being given to two plans for supplying water to a plant. Plan *A* requires a pipeline costing $160,000 with annual operation and unkeep costs of $2200, and an estimated life of 30 years with no salvage. Plan *B* requires a flume costing $34,000 with a life of 10 years, a salvage value of $5600, and annual operation and upkeep of $4500 plus a ditch costing $58,000, with a life of 30 years and annual costs for upkeep of $2500. Using an interest rate of 12 percent, compare the net present values of the two alternatives.

3.13 Cost estimators have provided reliable cost data as shown in the following table for the chlorinators in the methyl chloride plant addition. Analysis of the data and recommendations of the two alternatives are needed. Use present worth for $i = 0.10$ and $i = 0.20$.

	Chlorinators	
	Glass-lined	Cast iron
Installed cost	\$24,000	\$7200
Estimated useful life	10 years	4 years
Salvage value	\$4000	\$800
Miscellaneous annual costs as percent of original cost	10	20

Maintenance costs

Glass-lined. \$230 at the end of the second year, \$560 at the end of the fifth year, and \$900 at the end of each year thereafter.

Cast iron. \$730 each year.

The product from the glass-lined chlorinator is essentially iron-free and is estimated to yield a product quality premium of \$1700 per year. Compare the two alternatives for a 10-year period. Assume the salvage value of \$800 is valid at 10 years.

3.14 Three projects (*A, B, C*) all earn a total of \$125,000 over a period of 5 years (after-tax earnings, nondiscounted). For the cash-flow patterns shown in the table, predict by inspection which project will have the largest rate of return. Why?

	Cash flow, $\$10^3$		
Year	*A*	*B*	*C*
1	45	25	10
2	35	25	30
3	25	25	45
4	15	25	30
5	5	25	10

3.15 Suppose that an investment of \$100,000 will earn after-tax profits of \$10,000 per year over 20 years. Due to uncertainties in forecasting, however, the projected after-tax profits may be in error by ± 20 percent. Discuss how you would determine the sensitivity of the rate of return to an error of this type. Would you expect the rate of return to increase by 20 percent of its computed value for a 20-percent increase in annual after-tax profits (i.e., to \$12,000)?

3.16 The installed capital cost of a pump is \$200/hp and the operating costs are 4¢/kWh. For 8000 h/year of operation, an efficiency of 70 percent, and a cost of capital $i = 0.10$, for $n = 5$ years, determine the relative importance of the capital versus operating costs.

3.17 The longer it takes to build a facility, the lower its rate of return. Formulate the ratio of total investment I divided by annual cash flow C (profit after taxes plus depreciation) in terms of 1-, 2-, and 3-year construction periods if i = interest rate, and n = life of facility (no salvage value).

3.18 A chemical valued at \$0.94/lb is currently being dried in a fluid-bed dryer that allows 0.1 percent of the 4-million lb/year throughput to be carried out in the exhaust. An engineer is considering installing a \$10,000 cyclone that would recover the fines; extra pressure drop is no concern. What is the expected payback period for this investment? Maintenance costs are estimated to be \$300/year. The inflation rate is 8 percent, and the interest rate 15 percent.

3.19 To reduce heat losses, the exterior flat wall of a furnace is to be insulated. The data presented to you are

Temperature inside the furnace at the wall	500°F (constant)
Air temperature outside wall	Assume constant at 70°F
Heat transfer coefficients	
Outside air film (h)	4 Btu/(h)(ft^2)(°F)
Conductivity of insulation (k)	0.03 Btu/(hr)(ft)(°F)
Cost of insulation	\$0.75/(ft^2) (per inch of thickness)
Values of energy saved	\$0.60/10^6 Btu
Hours of operation	8700/year
Interest rate	30% per year for capital costs

Note that the overall heat transfer coefficient U is related to h and k by

$$\frac{1}{U} = \frac{1}{h} + \frac{t}{(12)(k)}$$

where t is the thickness in inches of the insulation, and the heat transfer through the wall is $Q = UA\,(T_{\text{furnace}} - T_{\text{wall}})$, where T is in °F. Ignore any effect of the uninsulated part of the wall.

What is the minimum cost for the optimal thickness of the insulation? List specifically the objective function, all the constraints, and the optimal value of t. Show each step of the solution. Ignore the time value of money for this problem.

3.20 We want to optimize the heat transfer area of a steam generator. A hot oil stream from a reactor needs to be cooled, providing a source of heat for steam production. As shown in Figure P3.20, the hot oil enters the generator at 400°F and leaves at an unspecified temperature T_2; the hot oil transfers heat to a saturated liquid water stream at 250°F, yielding steam (30 psi, 250°F). The other operating conditions of the exchanger are

$$U = 100 \text{ Btu/(h) (ft}^2\text{)(°F)} \qquad \text{overall heat transfer coefficient}$$

$$w_{\text{oil}} C_{p_{\text{oil}}} = 7.5 \times 10^4 \text{ Btu/(°F)(h)}$$

We ignore the cost of the energy of pumping and the cost of water and only consider the investment cost of the heat transfer area. The heat exchanger cost is \$25/ft^2 of heat

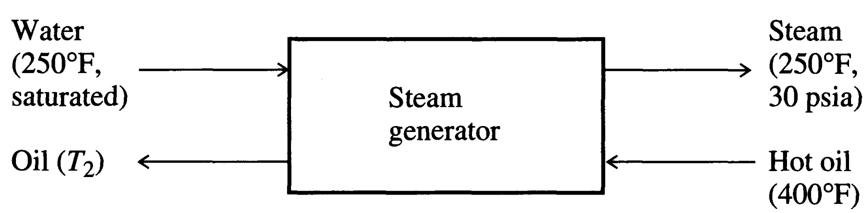

FIGURE P3.20
Steam generator flow diagram.

transfer surface. You can expect a credit of $\$2/10^6$ Btu for the steam produced. Assume the exchanger will be in service 8000 h/year. Find the outlet temperature T_2 and heat exchanger area A that maximize the profitability, as measured by (a) return on investment (ROI) and (b) net present value.

3.21 In *Chemical Engineering* (Jan. 1994, p. 103) the following explanation of internal rate of return appeared:

> Internal return rate. *The* internal return rate *(IRR), also known as the* discounted cash flow return rate, *is the iteratively calculated discounting rate that would make the sum of the annual cash flows, discounted to the present, equal to zero. As shown in Figure 2, the IRR for Project Chem-A is 38.3%/yr. Note that this single fixed point represents the zero-profitability situation. It does not vary with the cost of capital (discount rate), although the profitability should increase as the cost of capital decreases. There is no way that the IRR can be related to the profitability of a project at meaningful discount rates because of the nonlinear nature of the discounting step.*

What is correct and incorrect about this explanation? Be brief!

3.22 Refer to Problem 3.5. The same staff member asks if the internal rate of return on the proposed project is close to 15%. Calculate the IRR.

3.23 The cost of a piece of equipment is \$30,000. It is expected to yield a cash return per month of \$1000. What is the payback period?

3.24 After retrofitting an extruder, the net additional income after taxes is expected to be \$5000 per year. The remodeling cost was \$50,000. What is the return on investment in percent?

3.25 Your minimum acceptable rate of return (MARR) is 18%, the project life is 10 years, and no alternatives have a salvage value. The following mutually exclusive alternatives have been proposed. Rank them, and recommend the best alternative.

	A	*B*	*C*	*D*	*E*
Capital investment, \$	38,000	50,000	55,000	60,000	70,000
Net annual earnings, \$	11,000	14,100	16,300	16,800	19,200
IRR, %	26.1	25.2	26.9	25.0	24.3

3.26 You have four choices of equipment (as shown in the following table) to solve a pollution control problem. The choices are mutually exclusive and you must pick one. Assuming a useful life of 10 years for each design, no market value, and a pretax minimum acceptable rate of return (MARR) of 15% per year, rank them and recommend a choice.

Alternative	D_1	D_2	D_3	D_4
Capital investment, \$1000	600	760	1,240	1,600
Annual expenses, \$1000	780	728	630	574
P (present value), \$1000	−\$4,515	−\$4,414	−\$4,402	−\$4,481

3.27 A company invests $1,000,000 in a new control system for a plant. The estimated annual reduction in cost is calculated to be $162,000 in each of the next 10 years. What is the

(a) Return on investment (ROI)

(b) Internal rate of return (IRR)

Ignore income tax effects and depreciation to simplify the calculations.

3.28 The following table gives a comparison of costs for two types of heaters to supply heat to an oil stream in a process plant at a rate of 73,500,000 Btu/h:

	Oil convection	**Rotary air preheater**
Heat input in 10^6 Btu/h	114.0	96.5
Thermal efficiency, %	64.5	76.1
Total fuel cost (at $1.33/per 10^6 Btu) for 1 year	$1,261,000	$1,068,000
Power at $0.06/kWh for 1 year		48,185
Capital cost (installed), $	$1,888,000	$2,420,000

Assume that the plant in which this equipment is installed will operate 10 years, that a tax rate of 34%/year is applicable, and that a charge of 10% of the capital cost per year for depreciation will be employed over the entire 10-year period, that fixed charges including maintenance incurred by installation of this equipment will amount to 10%/year of the investment, and that a minimum acceptable return rate on invested capital after taxes and depreciation is 15%. Determine which of the two alternative installations should be selected, if any.

3.29 You are proposing to buy a new, improved reboiler for a distillation column that will save energy. You estimate that the initial investment will be $140,000, annual savings will be $25,000 per year, the useful life will be 12 years, and the salvage value at the end of that time will be $40,000. You are ignoring taxes and inflation, and your pretax constant dollar minimum acceptable rate of return (MARR) is 10% per year. Your boss wants to see a sensitivity diagram showing the present worth as a function of ±50% changes in annual savings and the useful life.

(a) What is the present value P of your base case?

(b) You calculate the P of −50% annual savings to be −$42,084 and the P for +50% annual savings to be $128,257. The P at −50% life is −$8,539. What is the P at +50% life?

(c) Sketch the P sensitivity diagram for these two variables [P vs the change in the base (in %)]. To which of the two variables is the decision most sensitive?