
3

FORMULATION OF THE OBJECTIVE FUNCTION

3.1 Economic Objective Functions	84
3.2 The Time Value of Money in Objective Functions	91
3.3 Measures of Profitability	100
References	104
Supplementary References	104
Problems	105

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 :

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

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

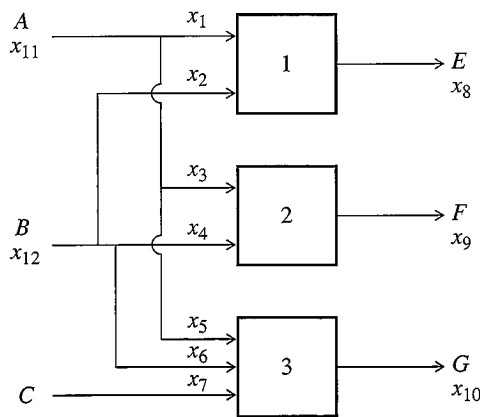


FIGURE E3.1

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	$\frac{1}{2}A, \frac{1}{6}B, \frac{1}{3}C$ (mass is conserved)	1.0	3.8

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

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

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

$$2\left(\frac{\pi D^2}{4}\right) + \pi DL = \frac{\pi D^2}{2} + \pi DL \quad (a)$$

(ends) (cylinder)

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

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

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

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

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

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

Hence, the problem has only one independent variable.

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

$$f_4 = \frac{\pi D^2}{2} + \frac{4V}{D} \quad (f)$$

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

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

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

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

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):

$$t = 0.0108D + 0.125 \quad (i)$$

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

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

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

$$f_6 = 0.0339D^2L + 0.435D^2 + 0.3927DL + 0.0376D^3 \quad (k)$$

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

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

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:

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

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 $(L/D)^{\text{opt}}$:

TABLE E3.2
Optimum (L/D)

Capacity (gal)	Design pressure (psi)		
	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 $(L/D)^{\text{opt}} = 3$ 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.

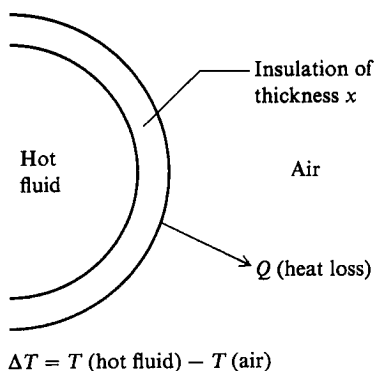
Next we consider an example in which both operating costs and capital costs are included in the objective function. The solution of this example requires that the two types of costs be put on some common basis, namely, dollars per year.

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

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

**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 coefficient, $\text{kJ}/(\text{h})(\text{m}^2)(\text{K})$

k = thermal conductivity of insulation, $\text{kJ}/(\text{h})(\text{m})(\text{K})$

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_i ($\$/10^6 \text{ kJ}$). 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 :

$$Q_0 - Q = h_c \Delta T A - \frac{\Delta T A}{x/k + 1/h_c} \quad (b)$$

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

$$f = (Q_0 - Q) \left(\frac{\text{kJ}}{\text{h}} \right) \cdot Y \left(\frac{\text{h}}{\text{year}} \right) \cdot H_i \left(\frac{\text{dollars}}{\text{kJ}} \right) \frac{1}{r} (\text{year}) - (C_0 + C_1 x) A (\text{dollars}) \quad (c)$$

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

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

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.

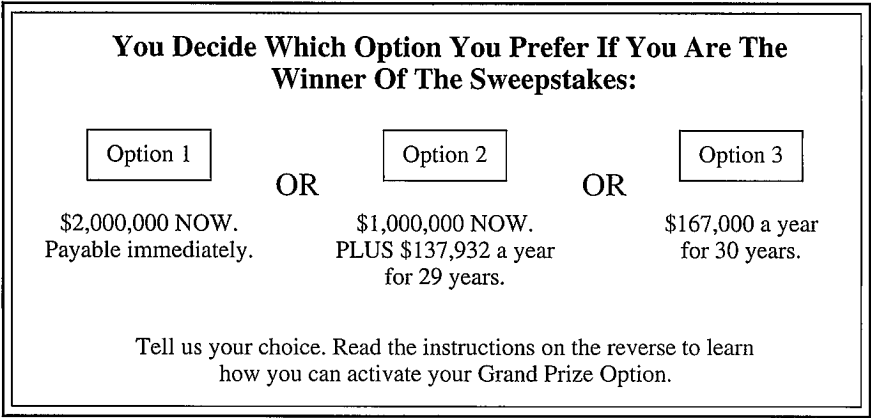


FIGURE 3.1
Options for potential sweepstakes winners. Which option provides the optimal value?

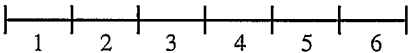


FIGURE 3.2
The time line with divisions corresponding to 6 time periods.

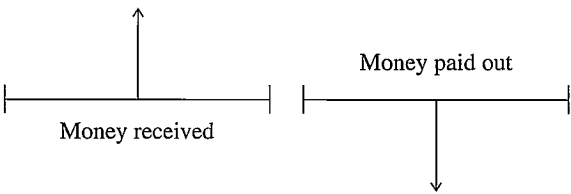
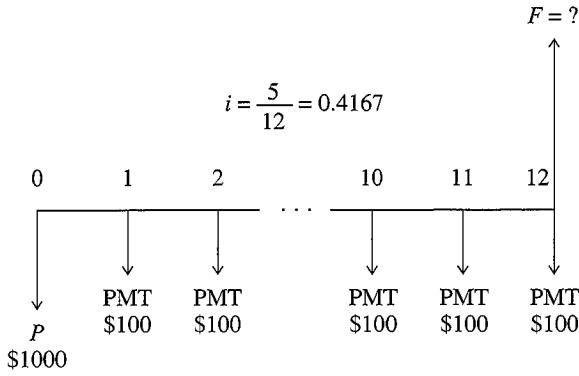


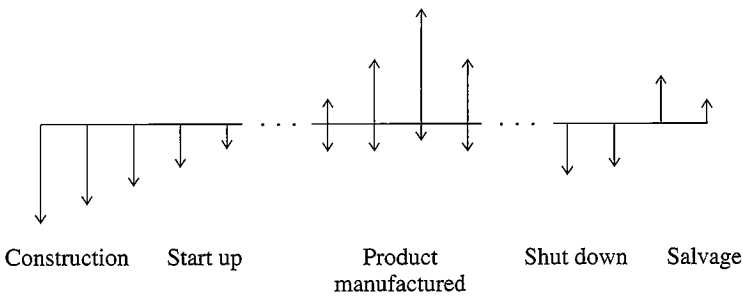
FIGURE 3.3
Representation of cash received and disbursed.

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

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

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

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

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

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

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 $k = 1, \dots, n$ in the future:

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

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

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

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

If $m = 1$,

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

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

Interest rate										
n	$i \rightarrow 1$	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

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

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

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

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 ft³/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.

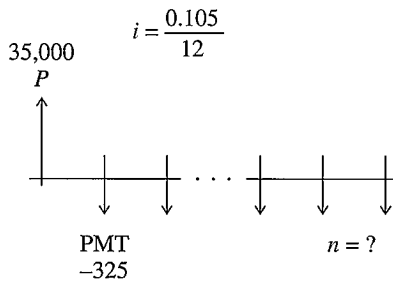


FIGURE E3.4a

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

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

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

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

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

In the example the data are

$$\begin{aligned} i &= \frac{0.105}{12} = 0.008750 & 1 + i &= 1.008750 \\ r &= \frac{325}{35,000} = 0.009286 & r/(r - i) &= 17.3333 \\ n &= \frac{2.85263}{0.008712} = 327.4 \text{ months} \end{aligned}$$

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 (fx) in the spreadsheet tool bar.
- 2. Choose financial function category (Figure E3.4b).
- 3. Select NPER.

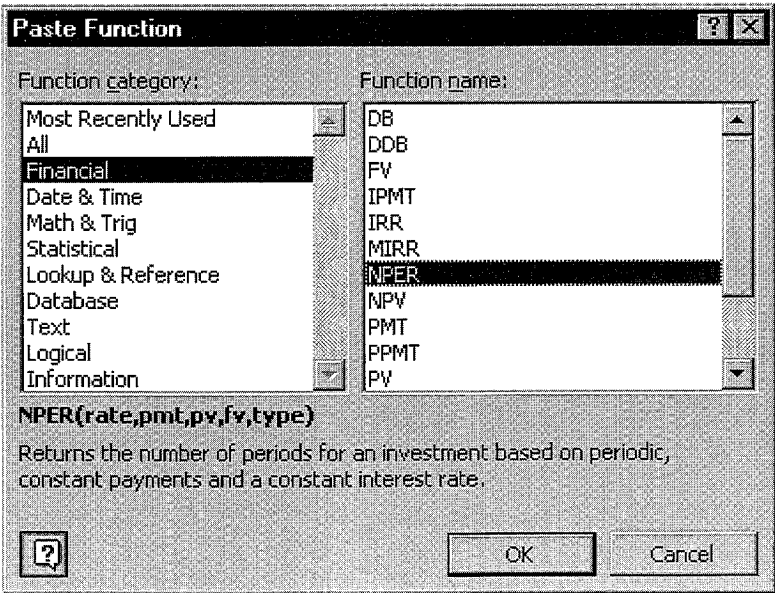


FIGURE E3.4b
Permission by Microsoft.

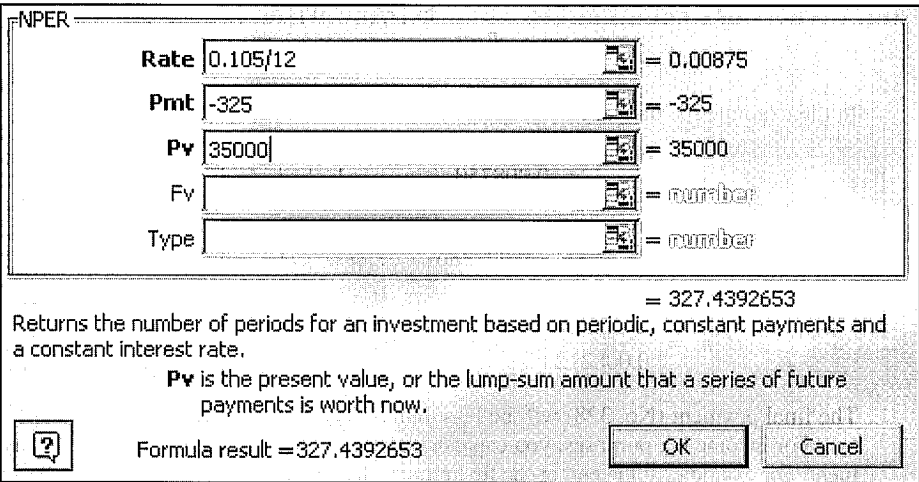


FIGURE E3.4c
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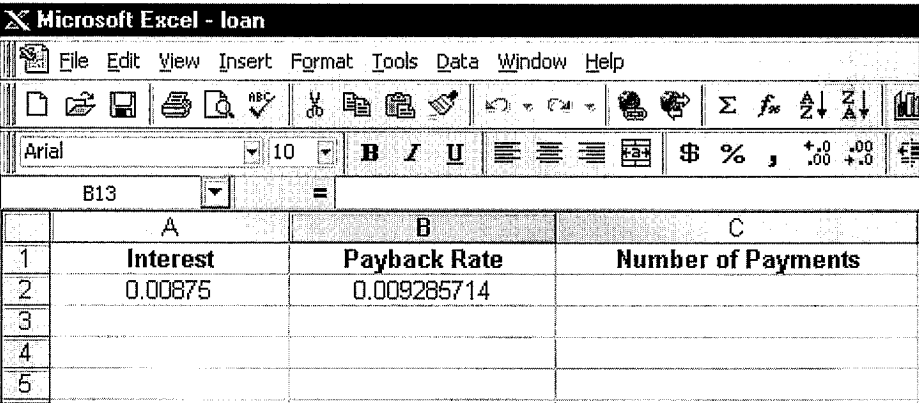


FIGURE E3.4d
Permission by Microsoft.

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.

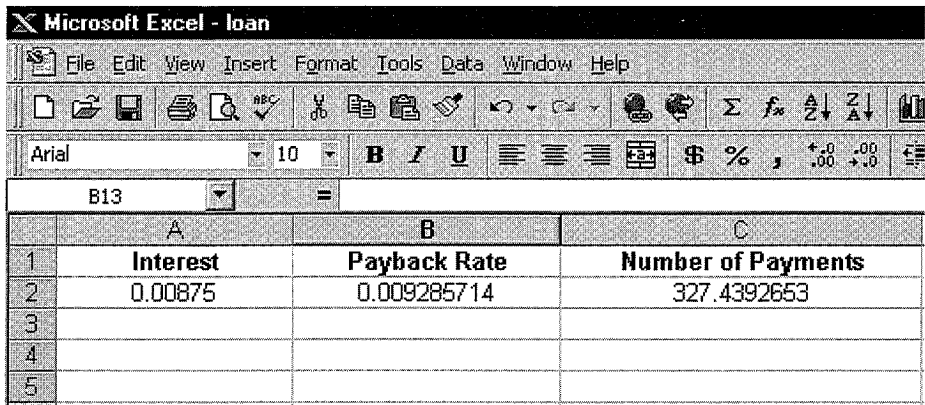


FIGURE E3.4e
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EXAMPLE 3.5 SELECTION OF THE CHEAPEST ANODES

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?

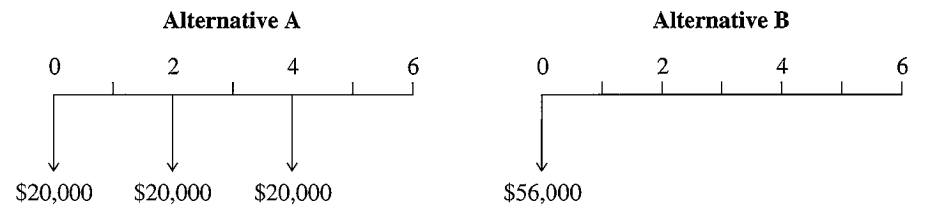


FIGURE E3.5

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

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

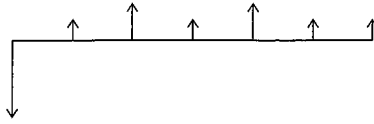
Example: Given the net return of \$6000 (per year) for an initial investment of \$45,000, the ROI is

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

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	Works with all cash flow patterns	Gives rate of return that is a familiar measure and indicates relative merits of a proposed investment
Commonly used and well understood	Easy to compute	Treats variable cash flows
	Gives correct ranking in most project evaluations	Does not require reinvestment rate assumption
Disadvantages		
Does not measure profitability	Is not always possible to specify a reinvestment rate for capital recovered	Implicitly assumes that capital recovered can be reinvested at the same rate
Ignores life of assets	Size of NPV (\$) sometimes fails to indicate relative profitability	Requires trial-and-error calculation
Does not properly consider the time value of money and distributed investments or cash flows		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:

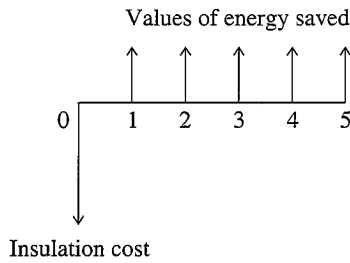


FIGURE E3.6
Cash flows for insulating a pipe.

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

$$C_1 x (\pi DL) \quad \text{in \$}$$

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 $L = 100\text{m}$. 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.

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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 upkeep 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		
<i>Glass-lined.</i> \$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.		
<i>Cast iron.</i> \$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?

Year	Cash flow, \$10 ³		
	<i>A</i>	<i>B</i>	<i>C</i>
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

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

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

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/ft² of heat

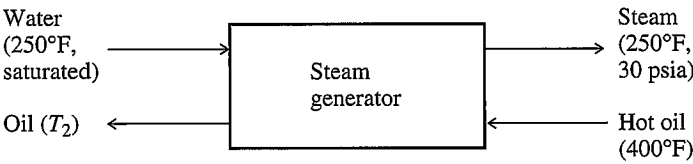


FIGURE P3.20
Steam generator flow diagram.

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.

	<i>A</i>	<i>B</i>	<i>C</i>	<i>D</i>	<i>E</i>
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
- Return on investment (ROI)
 - 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 $\pm 50\%$ changes in annual savings and the useful life.
- What is the present value P of your base case?
 - 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?
 - 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?

PART II

OPTIMIZATION THEORY AND METHODS

PART II DESCRIBES modern techniques of optimization and translates these concepts into computational methods and algorithms. Because the literature on optimization techniques is vast, we focus on methods that have proved effective for a wide range of problems. Optimization methods have matured sufficiently during the past 20 years so that fast and reliable methods are available to solve each important class of problem.

Seven chapters make up Part II of this book, covering the following areas:

1. Mathematical concepts (Chapter 4)
2. One-dimensional search (Chapter 5)
3. Unconstrained multivariable optimization (Chapter 6)
4. Linear programming (Chapter 7)
5. Nonlinear programming (Chapter 8)
6. Optimization involving discrete variables (Chapter 9)
7. Global optimization (Chapter 10)

The topics are grouped so that unconstrained methods are presented first, followed by constrained methods. The last two chapters in Part II deal with discontinuous (integer) variables, a common category of problem in chemical engineering, but one quite difficult to solve without great effort.

As optimization methods as well as computer hardware and software have improved over the past two decades, the degree of difficulty of the problems that can be solved has expanded significantly. Continued improvements in optimization algorithms and computer technology should enable optimization of large-scale nonlinear problems involving thousands of variables, both continuous and integer, some of which may be stochastic in nature.

