Floudas, C. A.; and G. E. Paules. "A Mixed-Integer Nonlinear Programming Formulation for the Synthesis of Heat-Integrated Distillation Sequences." *Comput Chem Eng* **12:** 531–546 (1988).

Harding, S. T.; and C. A. Floudas. "Locating all Heterogeneous and Reactive Azeotropes in Multicomponent Mixtures." *Ind Eng Chem Res* **39** (6): 1576–1595 (2000).

Logsdon, J. S.; and L. T. Biegler. "Accurate Determination of Optimal Reflux Policies for the Maximum Distillate Problem in Batch Distillation." *Ind Eng Chem Res* **32** (4): 692–700 (1993).

Natarajan, V.; B. W. Bequette; and S. M. Cramer. "Optimization of Ion-Exchange Displacement Separations. I. Validation of an Iterative Scheme and its Use as a Methods Development Tool." *J Chromatogr* A. **876** (1 + 2): 51–62 (2000).

Viswanathan, J.; and I. E. Grossmann. "An Alternate MINLP Model for Finding the Number of Trays Required for a Specified Separation Objective." *Comput Chem Eng* **17:** 949–955 (1993).

Viswanathan, J.; and I. E. Grossmann. "Optimal Feed Locations and Number of Trays for Distillation Columns with Multiple Feeds." *Ind Eng Chem Res* **32:** 2942–2949 (1993).

Wajge, R. M.; and G. V. Reklaitis. "An Optimal Campaign Structure for Multicomponent Batch Distillation with Reversible Reaction." *Ind Eng Chem Res* **37** (5): 1910–1916 (1998).

Westerberg, A. W.; and O. Wahnschafft. "Synthesis of Distillation-Based Separation Processes." In *Advances in Chemical Engineering*, Vol. 23, *Process Synthesis*, J. L. Anderson, ed. Academic Press, New York (1996), pp. 63–170.

13

FLUID FLOW SYSTEMS

Example

OPTIMIZATION OF FLUID flow systems encompasses a wide-ranging scope of problems. In water resources planning the objective is to decide what systems to improve or build over a long time frame. In water distribution networks and sewage systems, the time frame may be quite long, but the water and sewage flows have to balance at the network nodes. In pipeline design for bulk carriers such as oil, gas, and petroleum products, specifications on flow rates and pressures (including storage) must be met by suitable operating strategies in the face of unusual demands. Simpler optimization problems exist in which the process models represent flow through a single pipe, flow in parallel pipes, compressors, heat exchangers, and so on. Other flow optimization problems occur in chemical reactors, for which various types of process models have been proposed for the flow behavior, including well-mixed tanks, tanks with dead space and bypassing, plug flow vessels, dispersion models, and so on. This subject is treated in Chapter 14.

Optimization (and modeling) of fluid flow systems can be put into three general classes of problems: (1) the modeling and optimization under steady-state conditions, (2) the modeling and optimization under dynamic (unsteady-state) conditions, and (3) stochastic modeling and optimization. All three classes of problems are complicated for large systems. Under steady-state conditions, the principal difficulties in obtaining the optimum for a large system are the complexity of the topological structure, the nonlinearity of the objective function, the presence of a large number of possibly nonlinear inequality constraints, and the large number of variables. We do not consider optimization of dynamic or stochastic processes in this chapter. Instead, we focus on relatively simple steady-state fluid flow processes using the following examples:

1. Optimal pipe diameter for an incompressible fluid (Example 13.1)
2. Minimum work of gas compression (Example 13.2)
3. Economic operation of a fixed-bed filter (Example 13.3)
4. Optimal design of a gas transmission line (Example 13.4)

EXAMPLE 13.1 OPTIMAL PIPE DIAMETER

Example 2.8 briefly discussed how to determine the optimal flow in a pipe. In this example we consider how the trade-off between the energy costs for transport and the investment charges for flow in a pipe determines the optimum diameter of a pipeline. With a few simplifying assumptions, you can derive an analytical formula for the optimal pipe diameter and the optimal velocity for an incompressible fluid with density ρ and viscosity μ. In developing this formula the investment charges for the pump itself are ignored because they are small compared with the pump operating costs, although these could be readily incorporated in the analysis if desired. The mass flow rate m of the fluid and the distance L the pipeline is to traverse are presumed known, as are ρ and μ. The variables whose values are unknown are D (pipe diameter), Δp (fluid pressure drop), and v (fluid velocity); the optimal values of the three variables are to be determined so as to minimize total annual costs. Not all of the variables are independent, as you will see.

Total annual costs comprise the sum of the pipe investment charges and the operating costs for running the pump. Let C_{inv} be the annualized charges for the pipe and C_{op} be the pump operating costs. We propose that

$$C_{\text{inv}} = C_1 D^n L \tag{a}$$

$$C_{\text{op}} = \frac{C_0 m \Delta p}{\rho \eta} \tag{b}$$

where n = an exponent from a cost correlation (assumed to be 1.3)
η = the pump efficiency
C_0 and C_1 = cost coefficients

C_1 includes the capitalization charge for the pipe per unit length, and C_0 corresponds to the power cost ($/kWh) due to the pressure drop. The objective function becomes

$$C = C_{\text{inv}} + C_{\text{op}} = C_1 D^n L + \frac{C_0 m \Delta p}{\rho \eta} \tag{c}$$

Note that Equation (*c*) has two variables: D and Δp. However, they are related through a fluid flow correlation as follows (part of the process model):

$$\Delta p = \frac{2 f \rho v^2 L}{D} \tag{d}$$

where f is the friction factor. Two additional unspecified variables exist in Equation (*d*), namely v and f. Both m and f are related to v as follows:

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

$$f = 0.046\,\text{Re}^{-0.2} = \frac{0.046 \mu^{0.2}}{D^{0.2} v^{0.2} \rho^{0.2}} \tag{f}$$

Equation (*e*) is merely a definition of the mass flow rate. Equation (*f*) is a standard correlation for the friction factor for turbulent flow. (Note that the correlation between f and the Reynold's number (Re) is also available as a graph, but use of data from a graph requires trial-and-error calculations and rules out an analytical solution.)

To this point we isolated four variables: D, v, Δp, and f, and have introduced three equality constraints—Equations (*d*), (*e*), and (*f*)—leaving 1 degree of freedom (one independent variable). To facilitate the solution of the optimization problem, we eliminate three of the four unknown variables (Δp, v, and f) from the objective function using the three equality constraints, leaving D as the single independent variable. Direct substitution yields the cost equation

$$C = C_1 D^{1.3} L + 0.142 \frac{C_0}{\eta} m^{2.8} \mu^{0.2} \rho^{-2.0} D^{-4.8} L \tag{g}$$

Here, C_0 is selected with units {(\$/year)/[(lb_m)(ft^2/s^3)]}. We can now differentiate C with respect to D and set the resulting derivative to zero

$$\frac{dC}{dD} = 0 = 1.3C_1D^{0.3}L - 0.682\frac{C_0}{\eta g_c}m^{2.8}\mu^{0.2}\rho^{-2.0}D^{-5.8} \tag{h}$$

and solve for D^{opt}:

$$D^{opt} = 0.900\left(\frac{C_0}{C_1\eta g_c}\right)^{0.164} m^{0.459}\mu^{0.033}\rho^{-0.328} \tag{i}$$

Note that L does not appear in the result.

Equation (*i*) permits a quick analysis of the optimum diameter as a function of a variety of physical properties. From the exponents in Equation (*i*), the density and mass flow rate seem to be fairly important in determining D^{opt}, but the ratio of the cost factors is less important. A doubling of m changes the optimum diameter by a factor of 1.4, but a doubling of the density decreases D^{opt} by a factor of 1.25. The viscosity is also not too important. For very viscous fluids, larger diameters resulting in lower velocities are indicated, whereas gases (low density) give smaller diameters and higher velocities. The validity of Equation (*i*) for gases is questionable, because the variation of gas velocity with pressure must be taken into account.

Using Equation (*e*)

$$v = \frac{4m}{\pi\rho D^2} \tag{j}$$

we can discover how the optimum velocity varies as a function of m, ρ, and μ by substituting Equation (*i*) for D^{opt} into (*j*):

$$v^{opt} = C_2m^{0.082}\mu^{-0.066}\rho^{-0.344} \tag{k}$$

where C_2 is a consolidated constant. Consider the effect of ρ on the optimum velocity. Generally optimum velocities for liquids vary from 3 to 8 ft/s, whereas for gases the range is from 30 to 60 ft/s. Although D^{opt} is influenced noticeably by changes in m, v^{opt} is very insensitive to changes in m.

Suppose a flow problem with the following specifications is posed:

m = 50 lb/s
ρ = 60 lb/ft^3
μ = 6.72×10^{-4} lb/(ft)(s)
η = 0.6 (60% pump efficiency)
Purchased cost of electricity = \$0.05/kWh
8760 h/year of operation (100% stream factor)
C_1 = \$5.7 (D in ft); C_1D^n is an annualized cost expressed as \$/(ft)(year)
L = immaterial

The units in Equation (*g*) must be made consistent so that C is in dollars per year. For \$0.05/kWh, C_0 = \$0.5938 {(\$/year)/[lb_m)(ft^2)/s^3)]}. Substitution of the values specified into Equation (*i*) gives D^{opt} = 0.473 ft = 5.7 in. The standard pipe schedule

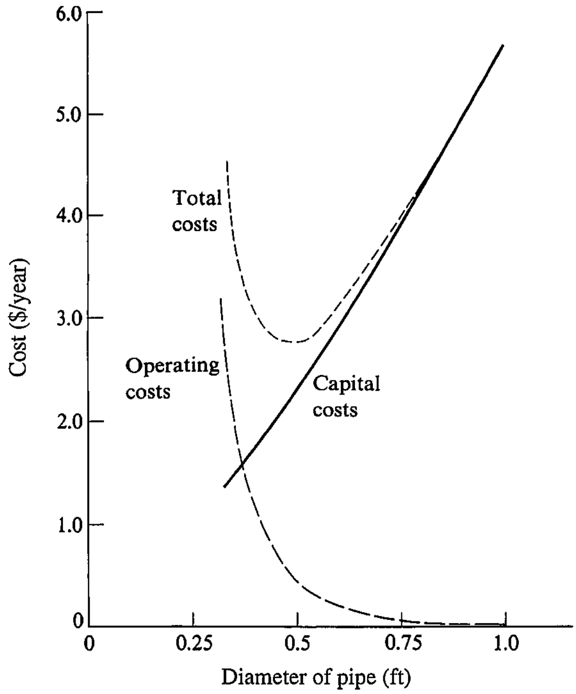


FIGURE E13.1
Investment, operating, and total costs for pipeline example (L = 1 ft).

40 size closest to D^{opt} is 6 in. For this pipe size (ID = 6.065 in.) the optimum velocity is 4.2 ft/s. (A schedule 80 pipe has an ID of 5.7561 in.) Figure E13.1 shows the respective contributions of operating and investment costs to the total value of C.

As the process model is made more accurate and complicated, you can lose the possibility of obtaining an analytical solution of the optimization problem. For example, if (1) the pressure losses through the pipe fittings and valves are included in the model, (2) the pump investment costs are included as a separate term with a cost exponent ($\bar{n}$) that is not equal to 1.0, (3) elevation changes must be taken into account, (4) contained solids are present in the flow, or (5) significant changes in density occur, the optimum diameter will have to be calculated numerically.

EXAMPLE 13.2 MINIMUM WORK OF COMPRESSION

In this example we describe the calculation of the minimum work for ideal compressible adiabatic flow using two different optimization techniques, (a) analytical, and (b) numerical. Most real flows lie somewhere between adiabatic and isothermal flow. For adiabatic flow, the case examined here, you cannot establish a priori the relationship between pressure and density of the gas because the temperature is unknown as a function of pressure or density, hence the relation between pressure and

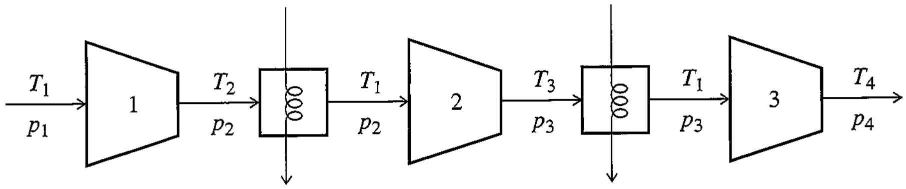


FIGURE E13.2

density is derived using the mechanical energy balance. If the gas is assumed to be ideal, and $k = C_p/C_v$ is assumed to be constant in the range of interest from p_1 to p_2, you can make use of the well-known relation

$$pV^k = \text{Constant} \tag{a}$$

in getting the theoretical work per mole (or mass) of gas compressed for a single-stage compressor (McCabe and colleagues, 1993)

$$W = \frac{kRT_1}{k-1}\left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} - 1\right] \tag{b}$$

where T_1 is the inlet gas temperature and R the ideal gas constant ($p_1\hat{V}_1 = RT_1$). For a three-stage compressor with intercooling back to T_1 between stages as shown in Figure E13.2, the work of compression from p_1 to p_4 is

$$\hat{W} = \frac{kRT_1}{k-1}\left[\left(\frac{p_2}{p_1}\right)^{(k-1)/k} + \left(\frac{p_3}{p_2}\right)^{(k-1)/k} + \left(\frac{p_4}{p_3}\right)^{(k-1)/k} - 3\right] \tag{c}$$

We want to determine the optimal interstage pressures p_2 and p_3 to minimize $\hat{W}$ keeping p_1 and p_4 fixed.

Analytical solution. We set up the necessary conditions using calculus and also test to ensure that the extremum found is indeed a minimum.

$$\frac{\partial \hat{W}}{\partial p_2} = 0 = RT_1[(p_1)^{(1-k)/k}(p_2)^{1/k} - (p_3)^{(k-1)/k}(p_2)^{(1-2k)/k}] \tag{d}$$

$$\frac{\partial \hat{W}}{\partial p_3} = 0 = RT_1[(p_2)^{(1-k)/k}(p_3)^{1/k} - (p_4)^{(k-1)/k}(p_3)^{(1-2k)/k}] \tag{e}$$

The simultaneous solution of Equations (d) and (e) yields the desired results

$$p_2^2 = p_1p_3 \qquad \text{and} \qquad p_3^2 = p_2p_4$$

so that the optimal values of p_2 and p_3 in terms of p_1 and p_4 are

$$p_2^* = (p_1^2p_4)^{1/3} \tag{f}$$

$$p_3^* = (p_4^2p_1)^{1/3} \tag{g}$$

With these conditions for pressure, the work for each stage is the same.

To check the sufficiency conditions, we examine the Hessian matrix of $\hat{W}$ (after substituting p_2^* and p_3^*) to see if it is positive-definite.

$$\nabla^2 W = RT_1\left(\frac{k-1}{k}\right)\cdot\begin{bmatrix} 2[(p_1^*)^{(1-5k)/3k}][(p_4^*)^{-(1+k)/3k}] & [(p_1^*)^{(1-4k)3k}][(p_4^*)^{-(1+2k)/3k}] \\ [(p_1^*)^{(1-4)/3k}][(p_2^*)^{-(1+2k)/3k}] & 2[(p_1^*)^{(1-3k)/3k}][(p_4^*)^{-(1+2k)/3k}] \end{bmatrix}$$

The two principal minors (the two diagonal elements) must be positive because p_1^* and p_4^* are both positive, and the determinant of $\nabla^2\hat{W}$

$$4\left[\frac{RT_1(k-1)}{k}\right]^2[(p_1^*)^{(2-8k)/3k}(p_4^*)^{-(2+4k)/3k}] -$$

$$\left[\frac{RT_1(k-1)}{k}\right]^2[(p_1^*)^{2-8k)/3k}(p_4^*)^{-(2+4k)/3k}] > 0$$

is also positive, hence $\nabla^2\hat{W}$ is positive-definite.

Numerical solution. Numerical methods of solution do not produce the general solution given by Equations (f) and (g) but require that specific numerical values be provided for the parameters and give specific results. Suppose that $p_1 = 100$ kPa and $p_4 = 1000$ kPa. Let the gas be air so that $k = 1.4$. Then $(k-1)/k = 0.286$. Application of the BFGS algorithm to minimize $\hat{W}$ in Equation (c) as a function of p_2 and p_3 starting with $p_2 = p_3 = 500$ yields

$p_2^* = 215.44$	compared with	$p_2^* = 215.44$ from Equation (f)
$p_3^* = 464.17$	compared with	$p_3^* = 464.16$ from Equation (g)

EXAMPLE 13.3 ECONOMIC OPERATION OF A FIXED-BED FILTER

Various rules of thumb exist for standard water filtration rates and cycle time before backwashing. Higher filtration rates may appear to be economically justified, however, when the filter loading is within conventional limits. In this example, we examine the issues involved for constant-rate filtration for a dual-media bed. Dual- and mixed-media beds result in increased production of water in a filter for two reasons. First, the larger grains (say charcoal approximately 1-mm size) as a top layer help reduce cake formation and deposition within the small (150-mm) top layer of the bed. Second, the head loss in the region of significant filtration is reduced.

With respect to the objective function for a filter, the total annual cost of filtration f is assumed to be the sum of the annualized capital costs f_c and the annual operating costs f_0. The annualized capital cost is related to the cross-sectional area of the filter by the relation

$$f_c = rbA^z \qquad (a)$$

where r = the capital recovery factor involving the discount rate and economic life of the filter

b = an empirical constant

z = an empirical exponent
A = the cross-sectional area of the filter

The cross-sectional area can be calculated by dividing the design flow rate by a quantity that is equal to the number of filter runs per day times the net water production per run per cross-sectional area:

$$A = \frac{q}{1440/[(V_f/Q) + t_b] \cdot (V_f - V_b)} \tag{b}$$

where q = the design flow rate in gal/day, L/day (dual units given here)
V_f = the volume of water filtered per unit area of bed per filter run in gal/ft^2, L/m^2
V_b = the volume of filtered water used for backwash per unit area of bed in gal/ft^2; L/m^2
Q = the filtration rate in gal/(min)(ft^2); L/(min)(m^2)
t_b = the filter down time for backwash, min
1440 = the number of minutes/day

For a constant filtration rate, the length of the filter run is given by $t_f = V_f/Q$.

The water production per filter run V_f is based on a relation proposed by Letterman (1980) that assumes minimal surface cake formation by the time filtration is stopped because of head loss:

$$V_f = \frac{K_p D}{\beta C_0 n} \sum_{i=1}^{n} \log \frac{n \Delta H}{k_i D Q} \tag{c}$$

where K_p = a constant related to the density of the deposit within the bed
D = the overall depth of the bed, ft.
β = the overall fraction of the influent suspended solids removed during the entire filter run
C_0 = suspended solids concentration in the filter influent
n = the number of layers $i = 1, \ldots, n$ into which the filter is divided for use of Equation (c)
ΔH = the terminal pressure (head) loss for the bed, ft.
k_i = a function of the geometric mean grain diameter d_{gi} in layer i. For rounded grains, the Kozeny–Carmen equation can be used to estimate k_i: $k_i = 0.081\ d_{gi}^{-2}$, where d_{gi} is in millimeters.

Typical values are $n = 1$, $d_g = 1$ mm, $\Delta H = 10$ ft, $D = 3$ ft, and $(K_p/\beta C_0) = 700$.

The backwash flow rate is calculated from

$$q_b = \left(\frac{V_f}{V_f - V_b} - 1 \right) q \tag{d}$$

We assume the backwash water is not recycled.

We next summarize the annual operating costs of the filter because they are equal to the energy costs for pumping

$$f_0 = q_b \left[1.146 \times 10^{-3} C_E \left(\frac{h}{\eta} \right) \right] \tag{e}$$

where f_0 = dollars per year
h = the backwash pumping head in feet of water

C_E = the cost of electricity in dollars per kilowatt-hour
η = the pump efficiency
1.146×10^{-3} = the conversion factor

Let us now carry out a numerical calculation based on the following values for the filter parameters

$$h = 110 \text{ ft of water } (33.5 \text{ m})$$

$$\eta = 0.8$$

$$b = \frac{\$870}{(ft^2)^{0.86}}; \frac{\$6715}{(m^2)^{0.86}}$$

$$z = 0.86$$

$$r = 0.134 \text{ (12.5\% for 20 years) (year}^{-1})$$

$$C_E = 0.03/\text{kWh}$$

Substitution of these values into Equations (a) and (e) together with Equations (b) and (d) yields the total cost function

$$f\left(\frac{\$}{\text{year}}\right) = 116\left[\frac{10^6 q}{1440/[(V_f/Q) + t_b](V_f - V_b)}\right]^{0.86}_{0 \le q \le 10}$$

$$+ 4.73 \times 10^3\left[\frac{V_f}{V_f - V_b} - 1\right]q \qquad (f)$$

If the values of q, t_b, and V_b are specified, and Equation (c) is ignored, the total annual cost can be determined as a function of the water production V_f per bed area and the filtration rate Q.

Figure E13.3 shows f versus V_f, the water filtered per run, for q (in 10^6 units) = 10 Mgal/day (3.79×10 ML/day), t_b = 10 min, and V_b = 200 gal/ft² (8.15×10^3 L/m²)

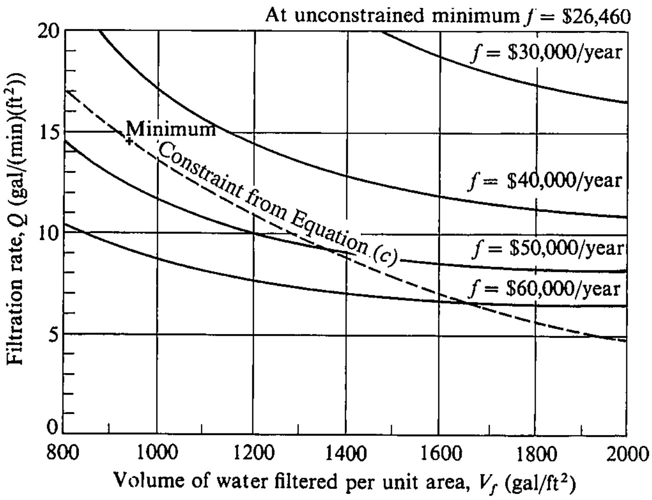


FIGURE E13.3

with Q gal/(min)(ft^2) as a parameter. The unconstrained solution is at the upper bounds on Q and V_f. Notice the flatness of f as V_f increases.

Equation (c) would be used in the design of the filter, hence Equation (c) imposes a constraint that must be taken into account. The optimal solution becomes $V_f = 940$ gal/ft^2 and $Q = 14.2$ gal/(min)(ft^2) with Equation (c) included in the problem (see Figure E13.3). A rule of thumb is 2 gal/(min)(ft^2) (Letterman, 1980), as compared with the optimal value of Q.

EXAMPLE 13.4 OPTIMAL DESIGN OF A GAS TRANSMISSION NETWORK

A gas-gathering and transmission system consists of sources of gas, arcs composed of pipeline segments, compressor stations, and delivery sites. The design or expansion of a gas pipeline transmission system involves capital expenditures as well as the continuing cost of operation and maintenance. Many factors have to be considered, including

1. The maximum number of compressor stations that would ever be required during a specified time horizon
2. The optimal locations of these compressor stations
3. The initial construction dates of the stations
4. The optimal solution for the expansion for the compressor stations
5. The optimal diameter sizes of the main pipes for each arc of the network
6. The minimum recommended thickness of the main pipes
7. The optimal diameter sizes, thicknesses, and lengths of any required parallel pipe loops on each arc of the network
8. The timing of constructions of the parallel pipe loops
9. The operating pressures of the compressors and the gas in the pipelines

In this example we describe the solution of a simplified problem so that the various factors involved are clear. Suppose that a gas pipeline is to be designed so that it transports a prespecified quantity of gas per time from point A to other points. Both the initial state (pressure, temperature, composition) at A and final states of the gas are known. We need to determine.

1. The number of compressor stations
2. The lengths of pipeline segments between compressor stations
3. The diameters of the pipeline segments
4. The suction and discharge pressures at each station.

The criterion for the design will be the minimum total cost of operation per year including capital, operation, and maintenance costs. Note that the problem considered here does *not* fix the number of compressor stations, the pipeline lengths, the diameters of pipe between stations, the location of branching points, nor limit the configuration (branches) of the system so that the design problem has to be formulated as a nonlinear integer programming problem. Figure E13.4a illustrates a simplified pipeline that we use in defining and solving the problem.

Before presenting the details of the design problem, we need to distinguish between two related problem, one being of a higher degree of difficulty than the other. If the capital costs of the compressors are a linear function of horsepower as shown in line A in Figure E13.4b, the transmission line problem can be solved as a nonlinear programming problem by one of the methods discussed in Chapter 8. On the other

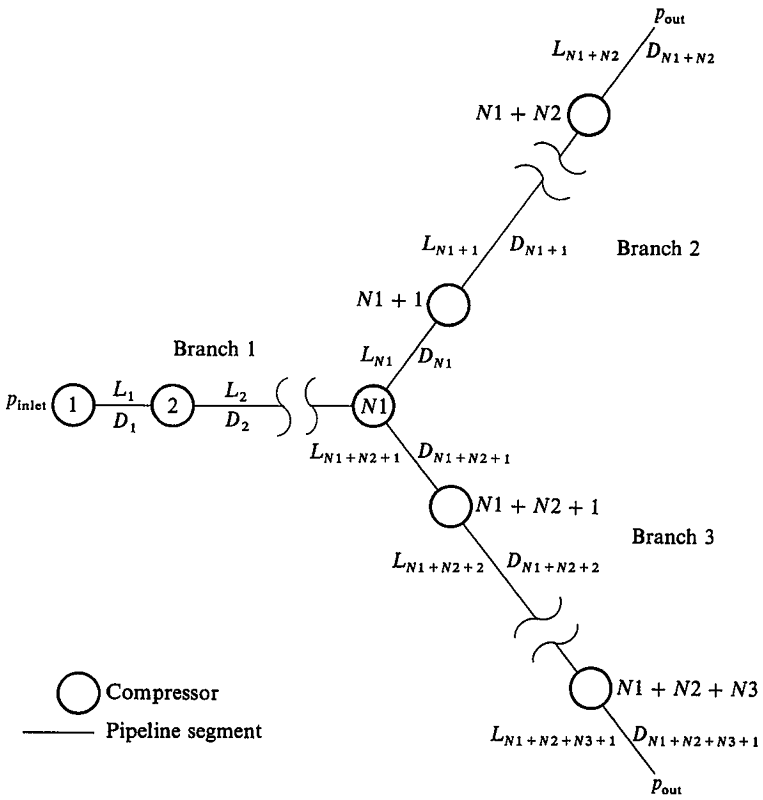


FIGURE E13.4a
Pipeline configuration with three branches.

hand, if the capital costs are a linear function of horsepower with a fixed capital outlay for zero horsepower as indicated by line B in Figure E13.4b, a condition that more properly reflects the real world, then the design problem becomes more difficult to solve and must be solved by a branch-and-bound algorithm combined with a nonlinear programming algorithm as discussed later on. The reason why the branch-and-bound method is avoided for the case involving line A is best examined after the mathematical formulation of the objective function (cost function) has been completed. We split the discussion of the transmission line problem into five parts: (1) the pipeline configuration, (2) the variables, (3) the objective function and costs, (4) the inequality constraints, and (5) the equality constraints.

The pipeline configuration. Figure E13.4a shows the configuration of the pipeline we are using in this example and the notation employed for the numbering system for the compressor stations and the pipeline segments. Each compressor station is represented by a node and each pipeline segment by an arc. N1, N2, and N3 represent the maximum number of possible stations in each of the three branches. Pressure increases at a compressor and decreases along the pipeline segment. The transmission

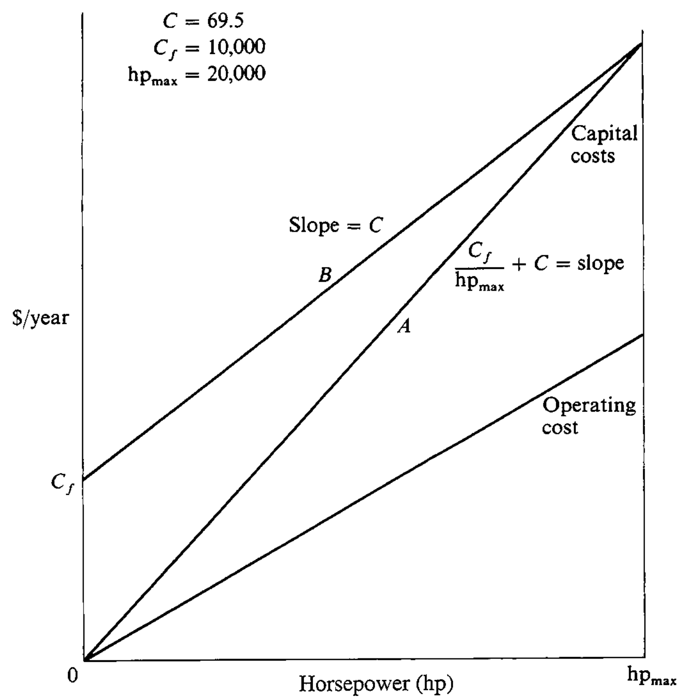


FIGURE E13.4b
Capital and operating costs of compressors.

system is presumed to be horizontal. Although a simple example has been selected to illustrate a transmission system, a much more complicated network can be accommodated that includes various branches and loops at the cost of additional computation time. For a given pipeline configuration each node and each arc are labeled separately. In total there are

- n total compressors $[n = \sum (N_i)]$
- $n - 1$ suction pressures (the initial entering pressure is known)
- n discharge pressures
- $n + 1$ pipeline segment lengths and diameters (note there are two segments issuing at the branch)

The variables. Each pipeline segment has associated with it five variables: (1) the flow rate Q; (2) the inlet pressure p_d (discharge pressure from the upstream compressor); (3) the outlet pressure p_s (suction pressure of the downstream compressor), (4) the pipe diameter D, and (5) the pipeline segment length L. Inasmuch as the mass flow rate is fixed, and each compressor is assumed to have gas consumed for operation of one-half of one percent of the gas transmitted, only the last four variables need to be determined for each segment.

The objective function. Because the problem is posed as a minimum cost problem, the objective function is the sum of the yearly operating and maintenance costs of the compressors plus the sum of the discounted (over 10 years) capital costs of the pipeline segments and compressors. Each compressor is assumed to be adiabatic with an inlet temperature equal to that of the surroundings. A long pipeline segment is assumed so that by the time gas reaches the next compressor it returns to the ambient temperature. The annualized capital costs for each pipeline segment depend on pipe diameter and length, but are assumed to be \$870/(in.)(mile)(year). The rate of work of one compressor is

$$W = (0.08531)Q\frac{k}{k-1}T_1\left[\left(\frac{p_d}{p_s}\right)^{z(k-1)/k} - 1\right] \qquad (a)$$

where $k = C_p/C_v$ for gas at suction conditions (assumed to be 1.26)
z = compressibility factor of gas at suction conditions (z ranges from 0.88 to 0.92)
p_s = suction pressure, psi
p_d = discharge pressure, psi
T_1 = suction temperature, °R (assumed 520°R)
Q = flow rate into the compressor, MMCFD (million cubic feet per day)
W = rate of work, horsepower.

Operation and maintenance charges per year can be related directly to horsepower and are estimated to be between 8.00 and 14.0 \$/(hp)(year), hence the total operating costs are assumed to be a linear function of compressor horsepower.

Figure E13.4b shows two different forms for the annualized capital cost of the compressors. Line A indicates the cost is a linear function of horsepower [\$70.00/(hp)(year)] with the line passing through the origin, whereas line B assumes a linear function of horsepower with a fixed initial capital outlay [\$70.00/(hp)(year) + \$10,000] to take into account installation costs, foundation, and so on. For line A, the objective function in dollars per year for the example problem is

$$f = \sum_{i=1}^{n}(C_0 + C_c)Q_i(0.08531)T_1\left(\frac{k}{k-1}\right)\left[\left(\frac{p_{d_i}}{p_{s_i}}\right)^{z(k-1)/k} - 1\right] + \sum_{j=1}^{m} C_s L_j D_j \qquad (b)$$

where n = number of compressors in the system
m = number of pipeline segments in the system ($= n + 1$)
C_0 = yearly operating cost \$/(hp)(year)
C_c = compressor capital cost \$/(hp)(year)
C_s = pipe capital cost \$/(in)(mile)(year)
L_j = length of pipeline segment j, mile
D_j = diameter of pipeline segment j, in.

You can now see why for line A a branch-and-bound technique is not required to solve the design problem. Because of the way the objective function is formulated, if the ratio $(p_d/p_s) = 1$, the term involving compressor i vanishes from the first summation in the objective function. This outcome is equivalent to the deletion of compressor i in the execution of a branch-and-bound strategy. (Of course the pipeline segments joined at node i may be of different diameters.) But when line B represents the compressor costs, the fixed incremental cost for each compressor in the system at zero horsepower (C_f) is *not* multiplied by the term in the square brackets of Equation (b). Instead, C_f is added in the sum of the costs whether or not compressor i is in the system, and a nonlinear programming technique cannot be used alone. Hence, if line B applies, a different solution procedure is required.

The inequality constraints. The operation of each compressor is constrained so that the discharge pressure is greater than or equal to the suction pressure

$$\frac{p_{d_i}}{p_{s_i}} \leq 1, \quad i = 1, 2, \ldots, n \tag{c}$$

and the compression ratio does not exceed some prespecified maximum limit K

$$\frac{p_{d_i}}{p_{s_i}} \geq K_i, \; i = 1, 2, \ldots, n \tag{d}$$

In addition, upper and lower bounds are placed on each of the four variables

$$p_{d_i}^{\min} \leq p_{d_i} \leq p_{d_i}^{\max} \tag{e}$$

$$p_{s_i}^{\min} \leq p_{s_i} \leq p_{s_i}^{\max} \tag{f}$$

$$L_i^{\min} \leq L_i \leq L_i^{\max} \tag{g}$$

$$D_i^{\min} \leq D_i \leq D_i^{\max} \tag{h}$$

The equality constraints. Two classes of equality constraints exist for the transmission system. First, the length of the system is fixed. With two branches, there are two constraints

$$\sum_{j=1}^{N1-1} L_j + \sum_{j=N1}^{N1+N2} L_j = L_1^*$$

$$\sum_{j=1}^{N1-1} L_j + \sum_{j=N1+N2+1}^{1N+N2+N3+1} = L_2^* \tag{i}$$

where L_k^* represents the length of a branch. Second, the flow equation, the Weymouth relation (GPSA handbook, 1972), must hold in each pipeline segment

$$Q_j = 871 D_j^{8/3}\left[\frac{p_d^2 - p_s^2}{L_j}\right]^{1/2} \tag{j}$$

where Q_j = a fixed number
p_d = the discharge pressure at the entrance of the segment
p_s = the suction pressure at the exit of the segment

To avoid problems in taking square roots, Equation (j) is squared to yield

$$(871)^2 D_j^{16/3}(p_d^2 - p_s^2) - L_j Q_j^2 = 0 \tag{k}$$

Solution strategy. As mentioned previously, if the capital costs in the problem are described by line A in Figure E13.4b, then the problem can be solved directly by a nonlinear programming algorithm. If the capital costs are represented by line B in Figure E13.4b, then nonlinear programming in conjunction with branch-and-bound enumeration must be used to accommodate the integer variable of a compressor being in place or not.

As explained in Chapter 9, a branch-and-bound enumeration is nothing more than a search organized so that certain portions of the possible solution set are deleted from consideration. A tree is formed of nodes and branches (arcs). Each branch in the tree represents an added or modified inequality constraint to the problem defined for the prior node. Each node of the tree itself represents a nonlinear optimization problem without integer variables.

With respect to the example we are considering, in Figure E13.4c, node 1 in the tree represents the original problem as posed by Equations (b)–(k), that is the problem in which the capital costs are represented by line A in Figure E13.4b. When the problem at node 1 is solved, it provides a lower bound on the solution of the problem involving the cost function represented by line B in Figure E13.4b. Note that line A always lies below line B. (If the problem at node 1 using line A had no feasible solution, the more complex problem involving line B also would have no feasible solution.) Although the solution of the problem at node 1 is feasible, the solution may not be feasible for the problem defined by line B because line B involves an initial fixed capital cost at zero horsepower.

After solving the problem at node 1, a decision is made to partition on one of the three integer variables; $N1$, $N2$, or $N3$. The partition variable is determined by the following heuristic rule.

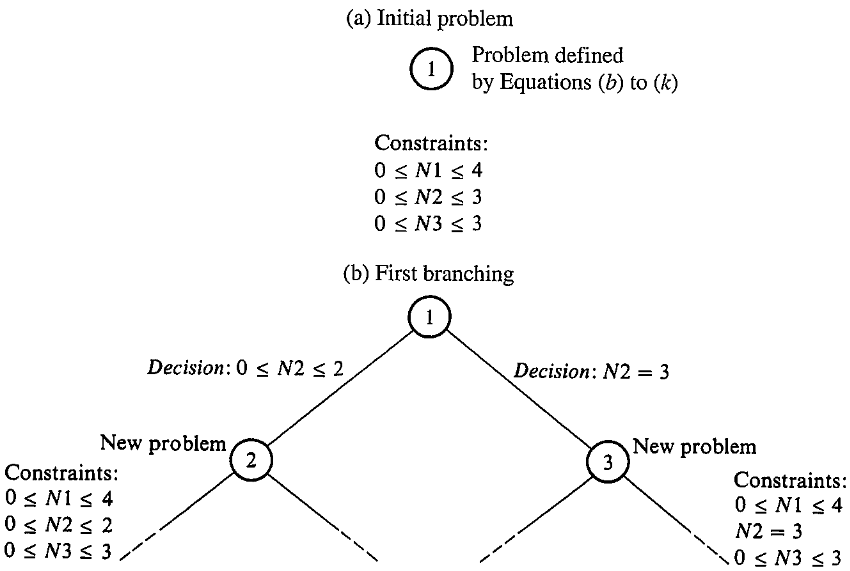


FIGURE E13.4c
Partial tree and branches for the example design problem.

> The smallest average compression ratio of all the branches in the transmission system is calculated by adding all the compression ratios in each branch and dividing by the number of compressors in the branch. The number of compressors in the branch that has smallest ratio becomes the partition variable.

Based on this rule, the partition variable was calculated to be $N2$.

After selection of the partition variable, the next step is to determine how the variable should be partitioned. It was decided to check each compressor in the branch of the transmission line associated with the partition variable, and if any compressor operated at less than 10 percent of capacity, it was assumed the compressor was not necessary in the line. (If all operate at greater than 10 percent capacity, the compressor with the smallest compression ratio was deleted.) For example, with $N2$ selected as the partition variable, and one of the three possible compressors in branch 2 of the gas transmission network operating at less than 10 percent of capacity, the first partition would lead to the tree shown in Figure E13.4c; $N2$ would either be 3 or would be $0 \le N2 \le 2$. Thus at each node in the tree, the upper or lower bound on the number of compressors in each branch of the pipeline is readjusted to be tighter.

The nonlinear problem at node 2 is the same as at node 1, with two exceptions. First, the maximum number of compressors permitted in branch 2 of the transmission line is now two. Second, the objective function is changed. From the lower bounds, we know the minimum number of compressors in each branch of the pipeline. For the lower bound, the costs related to line B in Figure E13.4b apply; for compressors in excess of the lower bound and up to the upper bound, the costs are represented by line A.

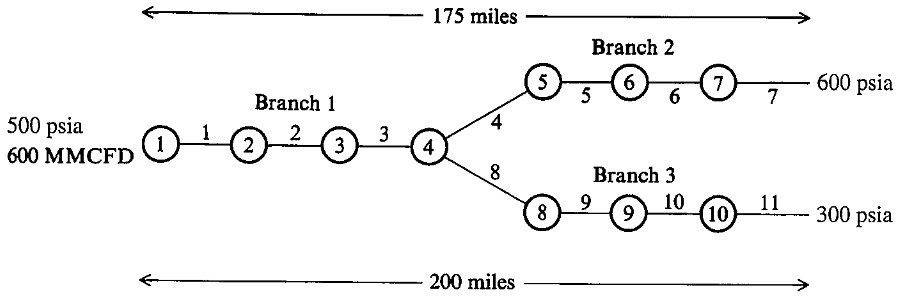
As the decision tree descends, the solution at each node becomes more and more constrained, until node r is reached, in which the upper bound and the lower bound for the number of compressors in each pipeline branch are the same. The solution at node r is feasible for the general problem but not necessarily optimal. Nevertheless, the important point is that the solution at node r is an upper bound on the solution of the general problem.

As the search continues through the rest of the tree, if the value of the objective function at a node is greater than that of the best feasible solution found to that stage in the search, then it is not necessary to continue down that branch of the tree. The objective function of any solution subsequently found in the branch is larger than the solution already found. Thus, we can fathom the node, that is, terminate the search down that branch of the tree.

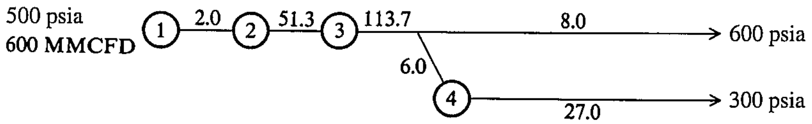
The next step is to backtrack up the tree and continue searching through other branches until all nodes in the tree have been fathomed. Another reason to fathom a particular node occurs when no feasible solution exists to the nonlinear problem at node r; then all subsequent nodes below node r are also infeasible.

At the end of the search, the best solution found is the solution to the general problem.

Computational results. Figure E13.4d and Table E13.4A show the solution to the example design problem outlined in Figure E13.4a using the cost relation of line A in Figure E13.4b. The maximum number of compressors in branches 1, 2, and 3 were set at 4, 3, and 3, respectively. The input pressure was fixed at 500 psi at a flow rate of 600 MMCFD, and the two output pressures were set at 600 psi and 300 psi, respectively, for branches 2 and 3. The total length of branches 1 plus 2 was constrained to be 175 miles, whereas the total length of branches 1 plus 3 was constrained



(a) Initial configuration (arcs are numbered sequentially)



(b) Optimal configuration with optimal pipeline lengths (in miles) shown on the arcs

FIGURE E13.4d
Initial gas transmission system and final optimal system using the costs of line *A*, Figure E13.4b.

at 200 miles. The upper bound on the diameter of the pipeline segments in branch 1 was set at 36 inches, the upper bound on the diameters of the pipeline segments in branches 2 and 3 at 18 in., and the lower bound on the diameters of all pipeline segments at 4 in. A lower bound of 2 miles was placed on each pipeline segment to ensure that the natural gas was at ambient conditions when it entered a subsequent compressor in the pipeline.

Figure E13.4d compares the optimal gas transmission network with the original network. From a nonfeasible starting configuration with 10-mile-long pipeline segments, the nonlinear optimization algorithm reduced the objective function from the first feasible state of 1.399×10^7 dollars/year to 7.289×10^6 dollars/year, a savings of close to \$7 million. Of the ten possible compressor stations, only four remained in the final optimal network. Table E13.4a lists the final state of the network. Note that because the suction and discharge pressures for the pipeline segments in branch 2 are identical, compressors 4, 5, 6, and 7 do not exist in the optimal configuration, nor do 9 and 10 in branch 3.

The same problem represented by Figure E13.4a was solved again but using the costs represented by line *B* instead of line *A* in Figure E13.4b. Figure E13.4e and Table E13.4B present the results of the computations. It is interesting to note that compressor 3 remains in the final configuration but with a compression ratio of 1, that is, compressor 3 is not doing any work. This means that it is cheaper to have two

TABLE E13.4A
Values of operating variables for the optimal network configuration using the costs of line *A*, Figure E13.4b

Pipeline segment	Discharge pressure (psi)	Suction pressure (psi)	Pipe diameter (in.)	Length (mile)	Flow rate (MMCFD)
1	719.1	715.4	35.0	2.0	597.0
2	1000.0	889.3	32.4	51.3	594.0
3	1000.0	735.8	32.4	113.7	591.0
4	735.7	703.8	18.0	2.0	294.0
5	703.8	670.6	18.0	2.0	292.6
6	670.6	636.1	18.0	2.0	291.1
7	636.1	600.0	18.0	2.0	289.7
8	735.8	703.8	18.0	2.0	294.0
9	685.2	859.1	18.0	2.0	292.6
10	859.1	832.5	18.0	2.0	291.1
11	832.5	300.0	18.0	27.0	289.7

Compressor station	Compression ratio	Capital cost ($/year)
1	1.44	70.00
2	1.40	70.00
3	1.00	70.00
4	1.00	70.00
5	1.00	70.00
6	1.00	70.00
7	1.00	70.00
8	1.26	70.00
9	1.00	70.00
10	1.00	70.00

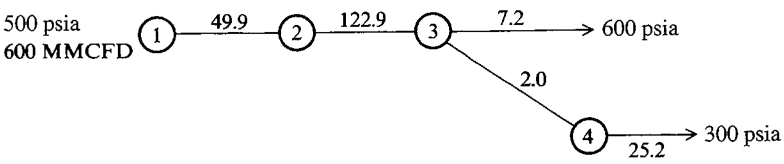


FIGURE E13.4e
Optimal configuration using the costs of line *B* in Figure E13.4b.

pipeline segments in branch 1 and two compressors each operating at about one-half capacity, plus a penalty of $10,000, than to have one pipeline segment and one compressor operating at full capacity. Compressor 3 doing no work represents just a branch in the line plus a cost penalty.

TABLE E13.4B

Values of operating variables for the optimal network configuration using the costs of line *B*, Figure E13.4b

Pipeline segment	Discharge pressure (psi)	Suction pressure (psi)	Pipe diameter (in.)	Length (mile)	Flow rate (MMCFD)
1	954.5	837.2	32.3	49.9	597.0
2	1000.0	699.7	32.3	122.9	594.0
3	699.7	600.0	15.2	2.2	295.5
4	699.7	665.7	18.0	2.0	295.5
5	952.2	300.0	16.9	25.2	294.0

Compressor station	Compression ratio	Capital cost ($/year)
1	1.91	69.50
2	1.19	69.50
3	1.00	69.50
4	1.43	69.50

REFERENCES

Gas Processor Suppliers Association. *Engineering Data Book.* 1972.

Letterman, R. D. "Economic Analysis of Granular Bed Filtration." *Trans Am Soc Civil Engrs* **106:** 279 (1980).

McCabe, W. L.; J. C. Smith; and P. Harriott. *Unit Operations of Chemical Engineering*, 5th ed. McGraw-Hill, New York (1993).

SUPPLEMENTARY REFERENCES

Bejan, A. "Maximum Power from Fluid Flow." *Int J Heat Mass Transfer* **39:** 1175–1181 (1996).

Carroll, J. A.; and R. N. Horne. "Multivariate Optimization of Production Systems." *J Petrol Tech* **44:** 782–789 (July, 1992).

Currie, J. C.; J. F. Novotrak; B. T. Ashdee; and C. J. Kennedy. "Optimize Reservoir Management: Mixed Linear Programming." *J Petrol Tech* 1351–1355 (December, 1997).

Heinemann, R. F.; and S. L. Lyons. "Next Generation Reservoir Optimization." *World Oil* **219:** 47–50 (1998).

Nishikiori, N.; R. A. Redner; and D. R. Doty. "An Improved Method for Gas Lift Allocation Optimization." *J Energy Resour Tech* **117:** 87–92 (1995).

Pan, Y.; and R. N. Horne. "Multivariate Optimization of Field Development Scheduling and Well-Placement Design." *J Petrol Tech* 83–86 (December, 1998).

Ramirez, W. F. *Application of Optimal Control to Enhanced Oil Recovery*. Elsevier, Amsterdam (1998).

Sung, W.; D. Huh; and J. Lee. "Optimization of Pipeline Networks with a Hybrid MCSTCD Networking Model." *SPE Prod Fac* **13**(3): 213–219 (1998).

14

CHEMICAL REACTOR DESIGN AND OPERATION

Example