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PROCESS ANALYSIS AND DESIGN FOR CHEMICAL ENGINEERS

istics not only to guard against possible systematic exclusion of certain types of structures but also to indicate insensitivity of the optimal structure to the particular heuristics used.

Rudd (1968) and Masso and Rudd (1969) illustrated their procedures by application to the synthesis of heat-exchanger networks, one of the categories to which programmed synthesis techniques are usually applied. The generation of process flowsheets, however, is more complex than the computer-aided synthesis of a subsystem such as a heat-exchanger network. The latter type of subsystem involves only the interconnection between specified kinds of processing equipment. The creation of a flowsheet involves, in addition, a determination of the tasks to be accomplished and the specification of the type of technology to execute these tasks in order to convert some particular raw materials into desired products. We shall return to this point in a later discussion of a computer-aided process synthesizer.

10-4 OPTIMIZATION METHODS FOR PROCESS SYNTHESIS

Various optimization and mathematical programming techniques are used to search for the optimal set among the alternative structural configurations and operating conditions. The number of combinations of equipment, temperature, pressure, concentrations, etc., is so large for even a small process plant that exhaustive enumeration of all cases and the calculation of the objective function for each case followed by direct selection of the optimum represents an impossible computational task. It is the purpose of the various optimization techniques not only to reach the optimal solution but also to reach it efficiently.

In optimization we seek to maximize or minimize a function of a number of variables with the variables subject to certain constraints. Until approximately 30 years ago the only mathematical methods available for handling optimization problems were classical differential and variational calculus. Since World War II there has been a rise in interest in optimization methods for dealing with problems not solvable by classical methods. Two classes of methods have been developed, optimum-seeking procedures and mathematical programming.

Although we now briefly discuss a number of optimization methods, a presentation of optimum-seeking procedures and mathematical programming in any depth is well beyond the scope of this book. A number of textbook treatments can be cited for study by the reader. Wilde (1964) presents single-variable and multivariable optimum-seeking procedures and also discusses the effects of experimental errors. In the work by Wilde and Beightler (1967) a unified theory of optimization is presented in a compact, readable form. Peters and Timmerhaus (1968) give a brief introduction to linear and dynamic programming to serve as a basis for further study and applications. Beightler and Phillips (1976) discuss the relatively new technique of geometric programming and present a number of applications. Avriel et al. (1973) is a more advanced treatise in which optimization methods and their applications to design are discussed.

10-5 OPTIMUM-SEEKING PROCEDURES

Optimum-seeking procedures are strategies to guide the search for the optimum of any function about which full knowledge is not available. Such functions obviously will arise when direct observations must be made on a physical system. In process synthesis optimum-seeking strategies can be used to guide us in the choice of values for the variables to permit an economic search of the response surface instead of performing an exhaustive evaluation over the entire response surface.

10-6 MATHEMATICAL PROGRAMMING

Mathematical programming developed as a branch of optimization theory to deal with maximization and minimization problems that arise in the decision sciences such as management science, operations research, and engineering design. It should not be confused with computer programming, although the solution of many algorithms arising in mathematical programming would not have been possible without the computer. We briefly describe several methods that are used in process synthesis, namely, linear programming, dynamic programming, geometric programming, and branch-and-bound methods.

Linear Programming

Linear programming is applicable to a large class of problems which involve linear objective functions subject to linear inequality and equality constraints. Linear-programming algorithms search the extreme points, which are the extremes of the region of feasible solutions. We shall see from a graphical solution to a simple linear optimization problem that the optimum solution occurs at an extreme point.

Example 10-1 A fertilizer-blending plant has a market for two grades of fertilizers, 10-8-5 and 7.5-10-15. (Fertilizers are specified by percentages of three major nutrient elements, N, P, K, where N is nitrogen, P is equivalent P_2O_5, and K is equivalent K_2O.) The expected profit on the first grade is \$20 per ton and \$30 per ton on the second grade. The plant has available 1500 tons of equivalent nitrogen, 1200 tons of equivalent P_2O_5, and 1500 tons of equivalent K_2O. How much of each grade of fertilizer should be made to realize maximum profit?

SOLUTION The problem statement can be cast into a linear optimization form, where x_1 and x_2 are the tons of first-grade and second-grade fertilizers,

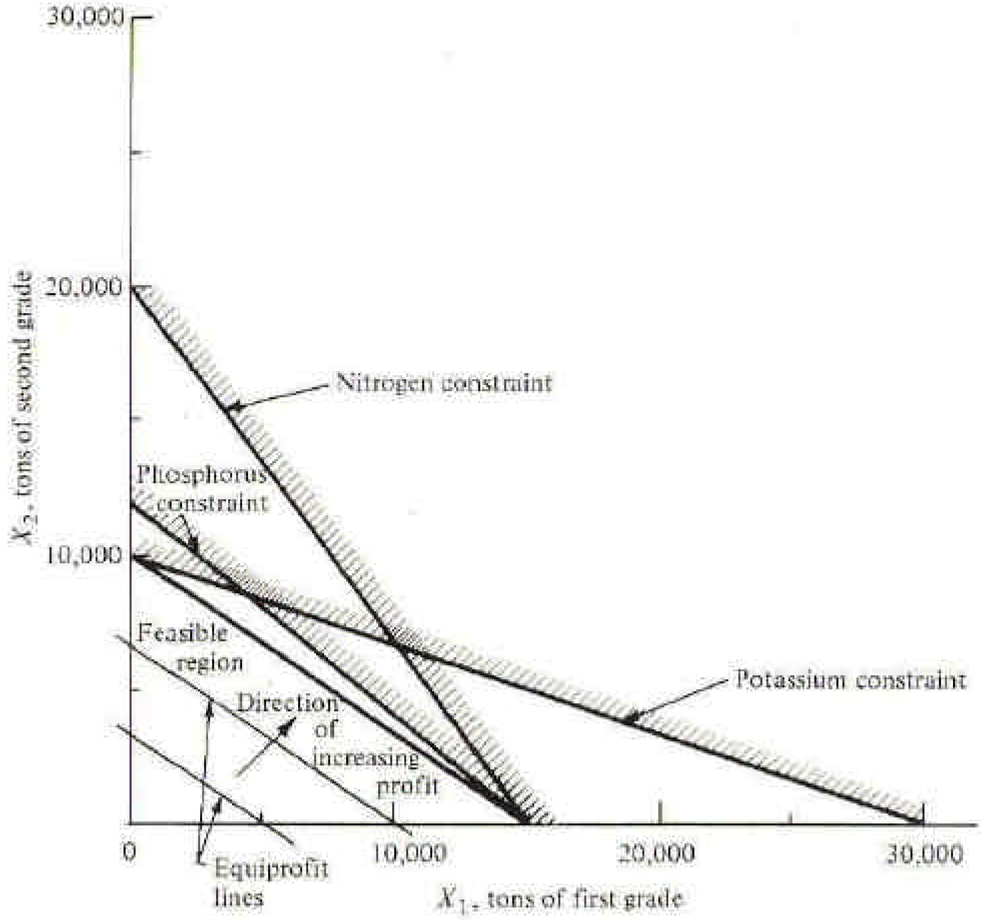

Figure 10-11 Graphical representation of fertilizer-optimization problem.

respectively,

$$\max P = 20x_1 + 30x_2$$

$$\text{Subject to } 0.1x_1 + 0.075x_2 \leq 1500 \text{ nitrogen constraint}$$

$$0.08x_1 + 0.10x_2 \leq 1200 \text{ phosphorus constraint}$$

$$0.05x_1 + 0.15x_2 \leq 1500 \text{ potassium constraint}$$

$$x_1, x_2 \geq 0$$

This is shown in graphical form in Fig. 10-11, which presents the linear constraints and equiprofit lines. It is obvious that the maximum profit will be reached at the extreme point where the equiprofit lines leave the feasible region at the intersection of the phosphorus and potassium constraints. The optimum production is 4286 tons of first-grade and 8571 tons of second-grade, yielding a maximum profit of $342,850. All the phosphorus and potassium would be used, but 429 tons of nitrogen would remain unused.

In general, the solution of a linear-programming problem requires a search only over the extreme points. Extremely efficient algorithms have been developed which take advantage of this property, and problems involving thousands of variables can be solved routinely and by rote. A generalization of linear programming is *convex programming*, in which the objective function and feasible-solution set are permitted to be convex.

Dynamic Programming

Dynamic programming can be used to transform an N-decision one-state initial-value optimization problem into a set of one-decision one-state problems. It transforms a large serial structure into a sequence of smaller problems and thus is reminiscent of process decomposition. The required computational effort is greatly reduced, but the technique requires that there be no recycle of information. A brief discussion of dynamic programming was presented in Chap. 9.

Geometric Programming

Geometric programming was developed for solving algebraic nonlinear programming problems subject to linear or nonlinear constraints. It can appear to be almost magical in its efficiency when, as can happen in certain cases, it can locate optima only by inspection of the exponents in the objective function. The optimal values of the independent variables are not sought directly by geometric programming. Instead, the optimal way to distribute the costs among the elements of the objective function is first sought. The optimal cost is then easily calculated. Only then does one determine the policy needed to reach the optimal cost.

As an example of geometric programming we shall use a hypothetical chemical plant postulated by Wilde and Beightler (1967). In this plant raw materials are mixed with a recycle stream from a recirculating compressor. The mixed stream is compressed and fed to a reactor followed by a separator. The product is one stream from the separator; the other stream is recycled to the mixer via the recirculating compressor. The annual cost figures are $1000x_1$ for the compressor; 10^4 for the mixer; $4 \times 10^9/x_1 x_2$ for the reactor; $10^5 x_2$ for the separator; and $1.5 \times 10^5 x_2$ for the recirculating compressor. x_1 is the operating pressure, and x_2 is the recycle ratio. The problem is then to choose x_1 and x_2 so as to minimize the annual cost y

$$\min y = 1000x_1 + \frac{4 \times 10^9}{x_1 x_2} + 2.5 \times 10^5 x_2$$

The classical method to determine the optimum conditions would be to differentiate the cost equation with respect to x_1 and x_2 and set the derivatives equal to zero. The asterisk in the following equations refers to the optimum.

$$\left(\frac{\partial y}{\partial x_1}\right)^* = 1000 - \frac{4 \times 10^9}{x_2^* x_1^{*2}} = 0$$

$$\left(\frac{\partial y}{\partial x_2}\right)^* = -\frac{4 \times 10^9}{x_1^* x_2^{*2}} + 2.5 \times 10^5 = 0$$