A Shortcoming of the Multilevel Optimization Technique

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We should like to point out that the method of multilevel optimization (*1, 2*) may not be generally applicable to chemical process design problems due to the mathematical character of commonly encountered objective functions. The method of multilevel optimization suggests that units in a chemical process be uncoupled and optimized individually, subject to equality constraints that require a match of products and feeds between units. In order to accomplish this, special objective functions, called subobjective functions, are defined for each uncoupled unit in the process. We demonstrate here that the subobjective function associated with an individual unit in a heat recovery network possesses a stationary point that is always a saddle point.

That a subobjective function can possess this characteristic detracts seriously from the utility of multilevel optimization in two ways. First, in contrast to a minimization problem, no general numerical techniques exist which locate saddle points. This difficulty is accentuated by the lack of *a priori* knowledge as to whether or not the stationary point is a saddle or a minimum, or whether it possibly changes from one to the other for different parameter values. This knowledge comes only at the expense of considerable analytical or calculational effort. The generalized Newton-Raphson method might be used to determine the point at which the gradient vanishes, but this approach suffers from convergence difficulties in multidimensional problems; moreover the method requires second derivatives of the objective function. Secondly, the algorithm proposed (*1, 2*) for coordinating the optimization of the uncoupled units to satisfy the equality constraints (the heart of mulilevel optimization) is not applicable if saddle surfaces are obtained. The authors do not at present know if this difficulty can be circumvented computationally in a manner that results in a practical method of optimization.

The absence of an extremum at the stationary point of the subobjective function may be illustrated by the following process design problem. The cold stream D of Figure 1 is to be heated from temperature T_0 to T_p. Three hot streams having flow rates a, b, c and temperatures t_a, t_b, t_c may be used for heating; here they are considered to have sufficient heat capacity and availability to accomplish the task. The distribution of the total heat load among the three exchangers is to be accomplished at the minimum cost of equipment, which is related to the total heat transfer surface area A by

$$C = \sum_{i=1}^{3} c_i = \sum_{i=1}^{3} \gamma_i A_i^{\alpha_i} \tag{1}$$

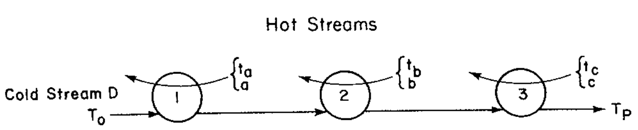

Fig. 1. Heat recovery process.

The parameters γ and α are positive constants; typically, $\alpha = 0.6$. It is easily demonstrated that with the representations for the heat exchangers considered here, a minimum cost solution exists for this problem and is unique.

The method of multilevel optimization suggests that the process be uncoupled as shown in Figure 2 with the enthalpies x_1, x_2, y_1, etc., of the stream entering and leaving each exchanger taken as independent variables. In this example, the enthalpies x_1 and z_2 are fixed because the flow rate and tempertures T_0 and T_p of stream D are specified. The optimization problem is thereby reduced to the minimization of the cost C through selection of the variables x_2, y_1, y_2, and z_1, subject, however, to the condition that the enthalpies match between units. In addition to these two equality constraints, inequality constraints must be appended to each unit to insure that the enthalpy change of stream D is non-negative and that the temperature driving force everywhere maintains the proper sign. These inequality constraints are not active, however, at the point of least cost of this process and are therefore not considered further here. Thus the optimization problem for the uncoupled process may be stated as:

$$\underset{x_2,\, y_1,\, y_2,\, z_1}{\text{Minimize}} \quad [c_1(x_2) + c_2(y_1, y_2) + c_2(z_1)]$$

Subject to:

$$x_2 = y_1 \qquad y_2 = z_1 \tag{2}$$

The solution to this constrained minimization problem may be found by determining the stationary point of the Lagrangian

$$L = \sum_{1}^{3} c_i - \lambda_1(x_2 - y_1) - \lambda_2(y_2 - z_1) \tag{3}$$

which may be expressed as follows in terms of subobjective functions l_i associated with each exchanger.

$$L = \{c_1(x_2) - \lambda x_2\} + \{c_2(y_1, y_2) + \lambda_1 y_1 - \lambda_2 y_2\} + \{c_3(z_1) + \lambda_2 z_1\} \tag{4}$$

$$L = l_1(x_2, \lambda_1) + l_2(y_1, y_2, \lambda_1, \lambda_2) + l_3(z_1, \lambda_2) \tag{5}$$

The necessary conditions for the minimum of C are

$$\nabla_v L = \mathbf{0} = \nabla_v l_1 + \nabla_v l_2 + \nabla_v l_3 \tag{6}$$

$$\nabla_\lambda L = \mathbf{0} \tag{7}$$

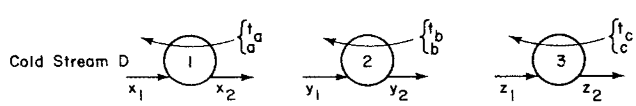

Fig. 2. Uncoupled heat recovery process showing the enthalpy variables used in the multilevel optimization method.

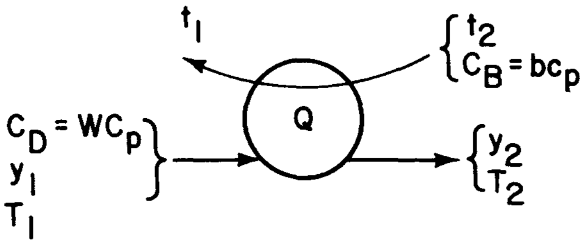

Fig. 3. Diagram showing notation for a single exchanger.

where the vector $\mathbf{v} = \text{col}\ (x_2, y_1, y_2, z_1)$ and the vector $\boldsymbol{\lambda} = \text{col}\ (\lambda_1, \lambda_2)$. Because the subobjective functions l_i are each functions of independent variables associated with a particular exchanger only, a necessary condition equivalent to Equation (6) is

$$\nabla_v l_1 = \nabla_v l_2 = \nabla_v l_3 = 0 \qquad (6a)$$

That is, the subobjective function for each exchanger must be stationary with respect to the variables associated with that exchanger only.

The determination of the stationary point of each subobjective function is direct if the function l_i has an extremum at that point. In the cases so far treated by the method of multilevel optimization, this situation has been assumed (*1, 2*). In the case considered here, it may be shown by an examination of the sufficient condition for a minimum that the stationary point of l_2, for example, is never an extremum.

The sufficient condition for a function to be a minimum at a stationary point is that the Hessian **H** be positive definite at that point. An entirely equivalent statement, and the one employed here, is that all eigenvalues of **H** be strictly positive. The Hessian for l_2 is defined as

$$\mathbf{H}_2 \equiv \begin{bmatrix} \dfrac{\partial^2 c_2}{\partial Q^2} & \dfrac{\partial^2 c_2}{\partial Q \partial y_1} \\ \dfrac{\partial^2 c_2}{\partial y_1 \partial Q} & \dfrac{\partial^2 c_2}{\partial y_1^2} \end{bmatrix} \equiv \begin{bmatrix} d_1 & e \\ e & d_2 \end{bmatrix} \qquad (8)$$

and the conditions assuring that both eigenvalues be strictly positive are

$$d_1 > 0, \quad d_2 > 0 \qquad (9)$$

$$\Delta \equiv (d_1 d_2 - e^2) > 0 \qquad (10)$$

In the above, the heat duty $Q = y_2 - y_1$ in Exchanger 2 has been substituted for the variable y_2.

The elements d_1, d_2, and e of the Hessian may be determined from Equation (1) and the following relations, which are suitable for the determination of heat exchange area. Figure 3 identifies the notation used here.

$$Q = C_D(T_2 - T_1) = C_B(t_2 - t_1)$$
$$Q = y_2 - y_1$$
$$T_1 = y_1/C_D$$

$$A = \frac{Q}{U \Delta T_m}$$

$$\Delta T_m = \frac{(t_2 - T_2) - (t_1 - T_1)}{\ln \dfrac{(t_2 - T_2)}{(t_1 - T_1)}}, \quad r \equiv \frac{C_D}{C_B} \neq 1$$

Without loss of generality, it is convenient to take $r > 1$; identical conclusions hold when $r < 1$. For $r = 1$, a separate analysis must be made with $\Delta T_m = (t_2 - T_2) = (t_1 - T_1)$; nevertheless, identical conclusions result. Then it may be shown that

$$d_1 = q\,[(\alpha - 1)(rs - 1)^2 + p\,\{(rs)^2 - 1\}] \qquad (11)$$

$$d_2 = q\,[(\alpha - 1)(s - 1)^2 + p\,(s^2 - 1)] \qquad (12)$$

$$e = q\,[(\alpha - 1)(rs - 1)(s - 1) + p\,(rs^2 - 1)] \qquad (13)$$

where

$$s = \frac{\delta_2}{\delta_1} = \frac{C_D t_2 - Q - y_1}{C_D t_2 - rQ - y_1} > 1$$

$$p = \ln \frac{\delta_2}{\delta_1} > 0$$

$$q = K\,\alpha\,p^{\alpha - 2}/\delta_2{}^2 > 0$$

$$K = \gamma \left(\frac{C_D}{U(r-1)} \right)^{\alpha} > 0$$

It is the condition in Equation (10) that is telltale; substitution gives

$$\Delta \equiv (d_1 d_2 - e^2) = -\,q^2 p^2 s^2 (r - 1)^2 \qquad (14)$$

which implies that Δ is never positive and that regardless of the parameters of the problem the stationary point can never be a minimum. It is not necessary to add, therefore, that Condition (9) may sometimes be violated as well.

It is noticed that the curvature of the subobjective function l_i at the stationary point is determined solely by the subunit cost function c_2 in this case. For the design problem considered here, the subunit cost function c_2 is a nonseparable function of the two independent variables Q and y_1. Because cost functions of such general form may usually be expected to appear in the design problem, the Hessian will generally possess nonzero off-diagonal elements; the opportunity for the formation of a Hessian that is not positive definite is therefore considerable.

By contrast, in the *process operation* problem, one is more likely to find subunit cost functions that are separable functions of the independent variables. For example, the form

$$c_i = f_i\,(x) \cdot g_i\,(y) \qquad (15)$$

may represent the flow rate of a product stream times the concentration of a component in that stream. For an operations problem treated by Brosilow and Lasdon (*1*), the subunit cost function had this form. The Hessian is

$$\mathbf{H} = \begin{bmatrix} f''g & f'g' \\ f'g' & fg'' \end{bmatrix}$$

If, as is normally the case, f and g are positive, then the requirement that both f and g be strictly convex functions at the stationary point insures that the stationary point is a minimum.

While no blanket guarantee can be given that the separate elements of separable subunit cost functions will be convex, nevertheless this requirement is certainly less restrictive than that faced in the design problem and may account for the reported success of Brosilow and Nunez in finding the optimum operating conditions of a catalytic cracking plant (*2*). The success of the method in that application was not without qualification, however; difficulty was reported in locating the unconstrained optimum of the subobjective functions. Unfortunately, the source of the difficulty cannot be traced because the subunit cost functions were not reported.

LITERATURE CITED

1. Brosilow, C. and L. Lasdon, *Proc. AIChE-IChE Joint Meeting, London,* Section 4, 67 (1965).
2. Brosilow, C. and E. Nunez, *Can. J. Chem. Eng.* **46**, **205** (1968).