APPENDIX: CALCULATION OF V

The volume V given by Equation (18) was calculated by an analytical approximation and by numerical integrations.

Analytical Approximation

Equation (19) can be rewritten as

$$f_e(x,T) = c_1\left(\frac{1-x}{2-x}\right)^2 - c_2\left(\frac{x}{2-x}\right)$$

$$= \frac{(c_1+c_2)x^2 - 2(c_1+c_2)x + c_1}{(2-x)^2}$$

where

$$c_1 = 55\exp\left(-\frac{4\,770}{T}\right)$$

$$c_2 = 1.4\times 10^{-5}\exp\left(-\frac{19\,270}{T}\right)$$

Since $c_1 >> c_2$ for $485.44 \leqq T \leqq 826$

$$\int_0^\xi \frac{1}{f_e(x,T)}dx$$

$$= \frac{1}{c_1}\int_0^\xi \frac{(2-x)^2}{\left(1+\frac{c_2}{c_1}\right)x^2 - 2\left(1+\frac{c_2}{c_1}\right)x + 1}dx$$

$$\cong \frac{1}{c_1}\int_0^\xi \left(\frac{2-x}{1-x}\right)^2 dx$$

$$= \frac{1}{c_1}\left[\frac{1}{1-\xi} - (1-\xi) - 2\ln(1-\xi)\right]$$

Hence

$$V = \frac{0.0362}{\xi}\int_0^\xi \frac{1}{f_e(x,T)}dx$$

$$= \frac{0.0362}{55\xi}\exp\left(\frac{4\,770}{T}\right)\left[\frac{1}{1-\xi} - (1-\xi) - 2\ln(1-\xi)\right]$$

This expression for V was used in all calculations presented in this paper.

Numerical Integrations

The integral

$$\int_0^\xi \frac{1}{f_e(x,T)}dx$$

was also evaluated by Simpson's one third rule (eleven points) and by the four-point Tchebycheff quadrature. The first yielded the following optimal solution

$$F_0 = 146{,}435.8 \qquad T = 826.0000$$
$$\xi = 0.4498919 \qquad V = 1.160926$$

and the second

$$F_0 = 146{,}433.5 \qquad T = 826.0000$$
$$\xi = 0.4501003 \qquad V = 1.160481$$

Both sets of solutions, especially the first, are nearly equal to the solution obtained by the analytical approximation given in Table 2. This indicates that, in lieu of the previous analytical approximation, a numerical procedure can be used to carry out the integration if the reaction is of an arbitrary order or the stoichiometry is of a highly complex nature.

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Global Minimization of a Cooled Reactor by Using a Posynomial Lower Bounding Function

The cost of a reactor-heater system with an auxiliary cooler can have at least two local minima and a local maximum, with respect to the design variables: temperature and extent of reaction. This cost can be bounded below by a unimodal function which, being a posynomial (a sum of power functions), can be minimized efficiently by geometric programming. Construction of this lower bounding function is not obvious, since the cost involves both a definite integral and economies of scale.

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SCOPE

An earlier article by Wilde (1974) used a fluidized reactor-heater system as an example of how simple but rigorous design procedures can be applied to optimization problems appearing quite difficult from the standpoint of conventional mathematical programming. Subsequently, Chen and Fan (1976) showed that the exothermic thermokinetic design, in which fluid mechanics constraints are inactive at the optimum, might be improved by adding an auxiliary cooler. Here the original formulation is modified to include this auxiliary cooler, with a fixed cost, a credit for waste heat steam, and a heat exchanger variable cost. Although it is proven that the resulting objective function of two variables can have at least three extreme points (one maximum and two local minima), methods are developed which avoid an exhaustive search in the two dimensions. The optimum temperature can be determined before the optimum extent of reaction.

With the optimal temperature known, the objective function becomes a multimodal function of the extent, with a discontinuity at the locally minimal thermally balanced design, that is, the one with no auxiliary cooler. Economies of scale in the auxiliary cooler generate a local maximum near this local minimum, and the definite integral in the reactor cost is the wrong form for geometric programming. Yet, a posynomial function is constructed which is a rigorous lower bound on the total cost. This lower bounding function, being unimodal, lends itself to minimization by the Newton-Raphson method, which is not applicable to the original function. Moreover, its posynomial form permits it to be easily bounded below by a constant useful for terminating the search.

CONCLUSIONS AND SIGNIFICANCE

The system cost is discontinuous at one local minimum and has at least one local maximum if there is an interior minimum. Yet the global minimum can be found without exhaustive search in two variables.

Of principal interest to optimization theorists is the construction, for this multimodal cost, of a rigorous lower bounding function which can be minimized by the Newton-Raphson method and bounded below by geometric programming. The reactor cost, although containing a definite integral, is shown to have a positive and increasing second logarithmic derivative, making it boundable below by a positive power function. Economies of scale in the auxiliary cooler cost, which would generate a reversed inequality in a geometric programming model, permit bounding the cooler cost below by a linear function. The resulting lower bounding function is a unimodal posynomial which can be modified to bound the cost more closely as the search proceeds. Lower bounding constants obtained easily by geometric programming continually test the best cooled design against the best uncooled design, each of which is at a local minimum. In favorable cases, the global minimum is identified quickly. In no case will the procedure stop at a local minimum which is not also globally minimum.

Reactor designers will find the method useful for bounding the reactor volume integral by a power function. They will also see how economies of scale, which produce annoying local maxima, can be handled by linear lower bounds. The interest of these results is, however, mainly theoretical, since in practice little more effort would be needed by the exhaustive search suggested by Chen and Fan (1976).

Chen and Fan showed that the cost of an exothermic reactor-heater system modeled by Wilde may be reduced by adding an auxiliary cooler. Here the cost of such a cooler is modeled and added to the cost of the uncooled system. As this is a sequel to the two earlier papers, the earlier nomenclature is used here without redefinition. After the cooler is modeled, the optimal reactor temperature is determined independently of the optimal extent of reaction. The remaining univariable, but multimodal, cost is minimized globally by constructing a unimodal lower bounding function minimizable by geometric programming (Duffin et al., 1967).

AUXILIARY COOLER COST

Suppose the total annual expense of an auxiliary cooler to be the sum of three costs: a positive fixed cost, independent of heat load, for controls, structure, piping, and accoutrements; a credit (negative cost) for the waste heat recovered; and a heat exchanger cost which increases with the heat transfer surface are needed. These three cost terms, being added to the three original cost terms, are labeled t_{04}, t_{05}, and t_{06}, respectively, making the auxiliary cooler cost $c \equiv t_{04} - t_{05} + t_{06}$. Here, t_{04} is the positive constant fixed cost, t_{05} is the positive steam credit, assumed proportional to $(\xi - \xi_t)$, the amount by which the design reaction extent exceeds that at thermal equilibrium (ξ_t)

$$t_{05} \equiv p_{05}(\xi - \xi_t)$$

and t_{06} is the variable heat exchanger cost assumed to have the form

$$t_{06} \equiv p_{06}g(T)(\xi - \xi_t)^\zeta$$

where ζ is a positive exponent usually not exceeding unity, and $g(T)$ is a nonincreasing function of temperature. The rationale for this form is that the heat exchanger area will be proportional to the heat generated, in turn proportional to $\xi - \xi_t$, and inversely proportional to the mean exchanger temperature gradient. The exchanger cost is then assumed to be a power function of the area, with the known exponent ζ being positive but only rarely exceeding unity. If y is the cost of the plant exclusive of the auxiliary cooler, then the total cost z is

$$z \equiv y + c = y + t_{04} - p_{05}(\xi - \xi_t) + p_{06}g(T)(\xi - \xi_t)^\zeta$$

with the fixed cost t_{04} applying only when cooling is required:

$$t_{04}\begin{cases} = 0 & \text{when } \xi = \xi_t \\ > 0 & \text{when } \xi > \xi_t \end{cases}$$

This creates a discontinuity at $\xi = \xi_t$, which guarantees that the cost of the uncooled design (Wilde's type 1) is always locally minimum with respect to ξ, since extents less than ξ_t are infeasible in this model, which excludes having an auxiliary heater.

The three design variables, V, T, and ξ must also satisfy the mass balance which can be arranged to give the volume V explicitly as an integral. Thus V may be eliminated from the objective, giving finally a cost function in only T and ξ:

$$z = p_{01}p_{61}{}^\alpha \xi^{-\alpha} \left[\int_0^\xi f_e{}^{-1}(x, T)\,dx \right]^\alpha + p_{02}\xi^{-\gamma} + p_{03}\xi^{-1} + c$$

where

$$f_e \equiv a_f p_f(\xi)\exp(-b_f/T) - a_r p_r(\xi)\exp(-b_r/T) > 0$$

is the net reaction rate. The first term is the reactor cost. The second, the primary cooler cost; the third, the operating cost. The problem then is to minimize this function z with the independent variables restricted only by $T \leqq T_m$ (the maximum temperature allowed) and $\xi_t \leqq \xi < \xi_e$ (the equilibrium extent). Chen and Fan (1976) showed, by exhaustive search of this two-dimensional region in Wilde's numerical example, that aside from the local minimum at the thermal equilibrium design, there can exist other local minima in the interior. What follows will show that the number of interior minima cannot exceed one, and that the optimal temperature can be found without searching on the extent. Thus the two-dimensional exhaustive search of Chen and Fan can be replaced by a unidimensional search on the extent. In favorable cases, the easily obtained thermal equilibrium design having no cooler can be proven globally optimal without iterative search.

OPTIMAL TEMPERATURE

This section proves that the optimal temperature can be determined in advance, without finding the optimal extent simultaneously. In most cases, it is the maximum temperature allowed. This optimal temperature will be the same whether or not there is auxiliary cooling.

All of this follows from the fact that for an exothermic reaction, the extent ξ_t at thermal equilibrium strictly increases with temperature, and so

$$\partial \xi_t / \partial T > 0$$

Differentiation of the auxiliary cooler cost with respect to temperature gives

$$\frac{\partial c}{\partial T} + \frac{\partial c}{\partial \xi_t}\frac{\partial \xi_t}{\partial T} = p_{06}(\xi - \xi_t)^{\zeta}\frac{\partial g(T)}{\partial T} + [p_{05} - p_{06} g(T)\zeta(\xi - \xi_t)^{\zeta - 1}]\frac{\partial \xi_t}{\partial T}$$

$$= p_{06}(\xi - \xi_t)^{\zeta}\frac{\partial g}{\partial T} + (\xi - \xi_t)^{-1}[t_{05} - \zeta t_{06}]\frac{\partial \xi_t}{\partial T}$$

The first term is negative by the hypothesis that $g(T)$ decreases in T. Since $\partial \xi_t/\partial T > 0$, the second is also negative whenever the cost of the cooler t_{06} exceeds the steam credit t_{05} divided by ζ. In practice, the cooler cost will far exceed the steam credit, and ζ will usually be near unity, so it is reasonable to assume that

$$\zeta t_{06} > t_{05}$$

in which case the cooler cost c strictly decreases with T. Therefore, the derivative of the total cost is bounded above by the derivative of the cost exclusive of the cooler:

$$\frac{\partial z}{\partial T} + \frac{\partial z}{\partial \xi_t}\frac{\partial \xi_t}{\partial T} = \left(\frac{\partial y}{\partial T} + \frac{\partial y}{\partial \xi_t}\frac{\partial \xi_t}{\partial T}\right) + \left(\frac{\partial c}{\partial T} + \frac{\partial c}{\partial \xi_t}\frac{\partial \xi_t}{\partial T}\right) < \frac{\partial y}{\partial T} + \frac{\partial y}{\partial \xi_t}\frac{\partial \xi_t}{\partial T}$$

Hence, if $\frac{\partial y}{\partial T} + \frac{\partial y}{\partial \xi_t}\frac{\partial \xi_t}{\partial T} < 0$ when T is at its maximum value T_m, then T_m must be the optimal temperature, whether or not there is an auxiliary cooler.

The reactor cost t_{01} is such a complicated expression that in practice the derivative $\partial y/\partial T + (\partial y/\partial \xi_t)(\partial \xi_t/\partial T)$ would be determined by direct perturbation in the neighborhood of T_m rather than by rigorous differentiation. But in the interesting case where the reverse reaction rate at thermal equilibrium is negligible compared to the forward rate, a closed form expression is obtainable. Suppose, then, that

$$f_e(\xi, T) \approx a_f p_f(\xi) \exp(-b_f/T)$$

Then

$$\partial f_e/\partial T = b_f f_e/T^2$$

and

$$\frac{\partial}{\partial T}\int_0^{\xi_t} f_e^{-1}\,dx = -\int_0^{\xi_t} f_e^{-2}\frac{\partial f_e}{\partial T}\,dx = -\frac{b_2}{T^2}\int_0^{\xi_t} f_e^{-1}\,dx$$

Consequently, at thermal equilibrium

$$(\partial y/\partial T)_t = t_{01}T^{-2}(\beta T - \alpha b_f)$$

Other derivatives needed are

$$\partial \xi/\partial T = (p_{52}p_{53} - p_{51})/(p_{53} - p_{51}T)^2$$

and

$$\left(\frac{\partial y}{\partial \xi}\right) = \alpha t_{01}\left\{\left[f_e(\xi_t, T)\int_0^{\xi_t} f_e^{-1}(x, T)\,dx\right]^{-1} - \xi_t^{-1}\right\} - (\gamma t_{02} + t_{03})$$

Although the last expression appears complicated, the integral must be calculated anyway to design the uncooled system (type 1). Thus it is straightforward to evaluate $[(\partial y/\partial T) + (\partial y/\partial \xi)(\partial \xi/\partial T)] \equiv (\partial \bar{y}/\partial T)_t$ at the maximum allowable temperature T_m. Since $T \leqq T_m$, the maximum temperature is locally optimal if and only if $(\partial \bar{y}/\partial T)_t \leqq 0$. The reader can verify that the Chen and Fan type 4 design has this derivative equal to zero, and at higher temperatures the derivative is positive, indicating nonoptimality. Notice also that when $\partial \bar{y}/\partial T$ strictly increases with T, there can only be one temperature where the derivative vanishes. At lower allowable temperatures, the maximum temperature is therefore locally optimal.

GLOBALLY OPTIMAL EXTENT

The optimal temperature known, the optimal extent of reaction remains to be found. As a last but practical resort, one can always find the global optimum by exhaustive search of the objective function. This section will show how one can accelerate this search, or even avoid it entirely, by detecting immediately when the thermal equilibrium design is globally optimal. Although the saving in effort is not great for this problem, the novel methods used are interesting because of their applicability to other problems having multiple optima.

The objective function for this problem is particularly challenging. Not only is it discontinuous at the locally optimal thermal equilibrium design, but also, as will be shown, it increases with extent whenever the cooler exhibits economies of scale. Thus it must pass through a maximum before achieving any minimum, precluding any search procedure employing derivatives, such as the Newton-Raphson method, or even requiring unimodality, such as the Fibonacci method.

These obstacles are overcome by constructing a function bounding the objective from below at every feasible value of extent. This lower bounding function is a posynomial, that is, a sum of positive power functions, to which the powerful theorems of geometric programming apply. Posynomials have no stationary points other than the global minimum, lend themselves readily to the Newton-Raphson method, and can themselves be easily bounded below by constants. Thus, if the bounding function increases at the thermal equilibrium design, there is no need to explore further, since this design must be globally minimal. Otherwise, a Newton-Raphson step approximates the interior minimum, in the neighborhood of which a good lower bounding constant can be computed. This may terminate the search by showing either that the thermal equilibrium design cannot be bettered, or that the approximate design cost is sufficiently low that further improvement is not worth pursuing. Even when this procedure is inconclusive, it narrows the range of extents known to contain the minimum. The method can be iterated, or else the cost function can be explored directly within this smaller range. A lower bounding constant can be computed at any time to terminate the process.

The lower bounding function is remarkable in two regards. First, the reactor cost, which involves an integral, can be bounded below rigorously and with small error by an easily computed power function. Second, the auxiliary cooler cost, which does not lend itself to the posynomial form, can be bounded below by a linear function with accuracy sufficient for this procedure.

Consider first the variable cost t_{06} of the auxiliary cooler, which is proportional to $(\xi - \xi_t)^\zeta$. If there are economies of scale, then $\zeta < 1$, and the first derivative increases without limit as ξ approaches ξ_t from above. Since the derivatives of all other cost terms are finite at ξ_t, this implies that the total cost must increase with ξ in the neighborhood of ξ_t and, if there is a local minimum for any $\xi > \xi_t$, must pass through a maximum. Thus there would be a local minimum at ξ_t even if the fixed cost t_{04} were zero. This prevents the use of the Newton-Raphson method near ξ_t, since it would move toward the maximum rather than the minimum.

When $\zeta = 1$, t_{06} is linear in ξ, permitting it to be combined with t_{05} which is also linear. The first derivative being a positive constant, the derivative of the total cost would be finite at ξ_t, and the Newton-Raphson method could be employed. This linear case will in fact be used as a bound on the nonlinear case where $\zeta < 1$. Suppose the locally minimizing value ξ_* of ξ is known to lie in the range $\xi_t < \xi_* < \hat{\xi} \leqq 1$. The function $(\xi - \xi_t)^\zeta$ has a negative second derivative over this range, so it is bounded below by the straight line connecting the end points on its graph as a function of $\xi - \xi_t$. This gives the inequality

$$(\xi - \xi_t)^\zeta > (\hat{\xi} - \xi_t)^\zeta (\hat{\xi} - \xi_t)^{-1} (\xi - \xi_t) = (\hat{\xi} - \xi_t)^{\zeta-1} (\xi - \xi_t)$$

The linear right member can be combined with the linear steam credit to give the following linear lower bound on the auxiliary cooler cost:

$$c(\xi) \geqq \{t_{04} - [p_{06} g(T_*) (\hat{\xi} - \xi_t)^{\zeta-1} - p_{05}]\} + [p_{06} g(T_*) (\hat{\xi} - \xi_t)^{\zeta-1} - p_{05}]\,\xi$$
$$\equiv q + q_{04}\xi \qquad (\xi_t \leqq \xi \leqq \xi_t)$$

Initially, the upper bound $\hat{\xi}$ can be taken as the equilibrium extent if it is known or, more simply, as unity. Once a smaller upper bound $\hat{\xi}$ on the minimizing extent has been established, it can be inserted in the formula. Later it will be shown how to generate such a bound by the Newton-Raphson method.

To complete construction of a posynomial lower bounding function, a power function lower bound on the reactor cost term t_{01} is needed. It is convenient to work with the reactor volume V as an intermediate variable, for which the exponent of a power function of $(1 - \xi)$ would be

$$\frac{\partial \ln V}{\partial \ln(1-\xi)} = \left(\frac{\xi}{V}\right)\left(\frac{\partial V}{\partial \xi}\right)\left[\frac{\partial \ln \xi}{\partial \ln(1-\xi)}\right]$$
$$= \left[-1 + \frac{p_{61}}{V f_e(\xi, T_*)}\right](-\xi^{-1} + 1)$$
$$= (1-\xi)\xi^{-1}[1 - p_{61} V^{-1} f_e^{-1}(\xi, T_*)] < 0$$

The product $\xi V f_e(\xi, T_*)$ increases linearly with ξ, for

$$\frac{\partial \xi V f_e(\xi, T_*)}{\partial \xi} = \frac{\partial}{\partial \xi}\int_0^\xi \frac{f_e(\xi, T_*)}{f_e(x, T_*)}\,dx = \frac{f_e(\xi, T_*)}{f_e(\xi, T_*)} = 1$$

Therefore, $\partial \ln V/\partial \ln(1-\xi)$ decreases with $\ln(1-\xi)$ and can be bounded above for $\xi \geqq \xi_t$:

$$\partial \ln V/\partial \ln(1-\xi) \leqq (1-\xi_t)\xi_t^{-1}[1 - p_{61} V_t^{-1} f_e^{-1}(\xi_t, T_*)] \equiv -\mu\alpha^{-1} < 0$$

Hence the following inequality is valid for $\xi \geqq \xi_t$:

$$V \geqq V_t[(1-\xi)/(1-\xi_t)]^{-\mu/\alpha}$$

From this follows

$$t_{01} \geqq [p_{01}(1-\xi_t)^\mu](1-\xi)^{-\mu} \equiv q_{01}(1-\xi)^{-\mu}$$

This lower bounding function has very little error in the example, being within 1% of the true cost over twice the range of ξ encompassing the interior optimum. Designers therefore may find this power function lower bound useful in any problem involving well-stirred reactors.

In order to use posynomial geometric programming theory, the bound must be expressed as a power function of a single variable

$$\eta \equiv 1 - \xi$$

This inequality constraint can be replaced by the inequality

$$\eta + \xi \leqq 1$$

since in minimizing $q_{01}\eta^{-\mu}$, which decreases in η, the argument η will increase until the upper bound is achieved.

The full lower bounding function $l(\xi)$ which bounds $z(\xi)$ from below for all feasible ξ, is therefore obtained by combining the bounds on $c(\xi)$ and t_{01} with the other cost terms

$$z(\xi) \geqq l(\xi) \equiv q_{01}\eta^{-\mu} + p_{02}\xi^{-\gamma} + p_{03}\xi^{-1} + q_{04}\xi + q$$

subject to $\xi_t \leqq \xi \leqq \xi_e$, $\quad \eta \geqq 0$, $\quad$ and $\quad \eta + \xi \leqq 1$.
Although $z(\xi)$ may have several stationary points, $l(\xi)$, being the objective function for a posynomial geometric program, can only have one, a global minimum (Duffin et al., 1967).

It has not been recognized that a principal advantage of the geometric programming form is that both first and second derivatives with respect to the logarithms of the variables are quite easy to obtain. This makes practical the application of the Newton-Raphson method, as will now be demonstrated. Let λ be a positive Lagrange multiplier for the constraint, defining a Lagrangian function

$$L(\eta, \xi, \lambda) \equiv l(\eta, \xi) - \lambda[1 - (\eta + \xi)]$$

Then

$$\partial L/\partial \ln \eta\xi = \eta \partial L/\partial \eta = -\mu t'_{01} + \eta\lambda$$
$$\partial L/\partial \ln \xi = -\gamma t_{02} - t_{03} + t'_{04} + \xi\lambda$$

where the primes emphasize that the corresponding terms are in l, not z. These will be called semilog derivatives. In this case the undetermined multiplier λ can be expressed as a function of the reactor cost bound t'_{01} by invoking the necessary condition that $\partial L/\partial \ln \eta = 0$ at a stationary point. Then

$$\lambda = \mu\eta^{-1}t'_{01} = \mu(1-\xi)^{-1}t'_{01}$$

Substitution of this into $\partial L/\partial \ln \xi$ gives $\partial L/\partial \ln \xi = \mu\xi(1-\xi)^{-1}t'_{01} - \gamma t_{02} - t_{03} + t'_{04}$, an expression that involves only ξ. A second differentiation gives

$$\partial^2 L/\partial(\ln \xi)^2 = \mu\left\{\xi(1-\xi)^{-1}(-\mu t'_{01}) + t'_{01}\frac{\partial[\xi(1-\xi)^{-1}]}{\partial \ln \xi}\right\} + \gamma^2 t_{02} + t_{03} + t'_{04}$$

$$= \frac{\mu\xi[1-\mu(1-\xi)]}{(1-\xi)^2} t'_{01} + \gamma^2 t_{02} + t_{03} + t'_{04}$$

The Newton-Raphson method would involve evaluating first and second semilog derivatives at ξ_t and computing a change in $\ln\xi$ driving $\partial L/\partial \ln\xi$ to zero:

$$\Delta\ln\xi = \{-(\partial L/\partial\ln\xi)[\partial^2 L/\partial(\ln\xi)^2]^{-1}\}_t$$

The predicted minimum for $l(\xi)$ is

$$\hat{\xi} = \xi_t \exp\{-(\partial L/\partial\ln\xi)[\partial^2 L/\partial(\ln\xi)^2]^{-1}\}$$

This estimate $\hat{\xi}$ is actually too great, since a more accurate bound on the auxiliary cooler cost would give a considerably larger coefficient for t'_{04} This would increase the first semilog derivative, that is, decrease its absolute value, and increase the second semilog derivative, shortening the Newton-Raphson step. Hence it is proper to construct such a closer bound for the range $\xi_t \leq \xi \leq \hat{\xi}$, since the minimum for the new function will be inside it.

At the new point $\hat{\xi}$ it is simple to evaluate the terms of l and compare $l(\hat{\xi})$ to z_t. If $l(\hat{\xi}) < z_t$, then there is promise that the interior local minimum is globally minimal, and one can continue to search for it, say by another Newton-Raphson iteration or by exhaustive search over the smaller range. If one suspects that $l(\hat{z})$ is already nearly minimal, a lower bounding constant can be constructed to see if significant improvement is possible. And when $l(\hat{z}) > z_t$, construction of a bounding constant may allow immediate termination of the search by proving that the global optimum is at ξ_t.

Geometric programming permits construction of such a lower bounding constant [D, P, Z]. Let δ_{01}, δ_{02}, δ_{03}, and δ_{04} be positive variables associated with the first four variable terms of $l(\xi)$. At the optimum, they would be the fractions of the total variable cost associated with the four terms, respectively, and so they satisfy a normality condition.

$$\delta_{01} + \delta_{02} + \delta_{03} + \delta_{04} = 1$$

Let δ_{11} and δ_{12} be dual variables associated with the terms η and ξ, respectively, in the constraint function $\eta + \xi$. At the optimum they are proportional to the terms and sum to the Lagrange multiplier λ, and so

$$\delta_{11} = \eta\lambda \quad \text{and} \quad \delta_{12} = \xi\lambda$$

These six dual variables and λ must satisfy the necessary conditions for optimality, namely, that the first logarithmic derivatives must vanish:

$$(\partial \ln l/\partial \ln\mu)_* = l_*^{-1}(\partial l/\partial\ln\mu)_* = -\mu\delta_{01} + \mu_*\lambda = 0$$

$$(\partial\ln l/\partial\ln\xi)_* = -\gamma\delta_{02} - \delta_{03} + \delta_{04} + \xi_*\lambda = 0$$

For any value of ξ (and η), there are five variables in these three equations, so any three of the variables can be expressed as functions of the other two. It is convenient to let δ_{03} and δ_{04} be the two degrees of freedom, for the solutions can be written in closed form with the abbreviation

$$k \equiv \mu\xi(1-\xi)^{-1}$$

The solutions are obtained serially:

$$\delta_{02} = [k - (1+k)\delta_{03} + (1-k)\delta_{04}](\alpha + k)^{-1}$$

$$\delta_{01} = 1 - \delta_{02} - \delta_{03} - \delta_{04}; \; \lambda = \mu\xi(1-\xi)^{-1};$$

$$\delta_{11} = (1-\xi)\lambda; \quad \delta_{12} = \xi\lambda$$

For any choice of dual variables satisfying all these conditions, the following dual function is a constant bounding l below:

$$l(\xi) \geq (q_{01}/\delta_{01})^{\delta_{01}}(p_{02}/\delta_{02})^{\delta_{02}}(p_{03}/\delta_{03})^{\delta_{03}} (q_{04}/\delta_{04})^{\delta_{04}}\eta^{-\delta_{11}}\xi^{-\delta_{12}} + q \equiv d$$

To get a good bound, one needs a decent estimate of δ_{03} and δ_{04}. These are taken here to be, respectively, the fractions of the total variable cost associated with the operating cost and the auxiliary variable cost; that is

$$\delta_{03} = [l(\hat{\xi}) - q]^{-1} t_{03}(\hat{\xi}); \quad \delta_{04} = [l(\hat{\xi}) - q]^{-1} t_{04}(\hat{\xi})$$

These values generate all the others, from which the lower bound constant d is computed. Since $z(\xi) \geq l(\xi) \geq d$ for all feasible ξ, the search can be terminated if $d > z_t$, in which case the global optimum must be at ξ_t. When $d < l(\hat{\xi}) \leq z_t$, the global minimum z_* is bounded by

$$z(\hat{\xi}) \geq z_* \geq d$$

If this interval is suitably small, the search for the global minimum can be terminated.

EXAMPLES

Consider the same example as in [W] and [C, F]. The thermal equilibrium design has $T_t = T_m = 826°K$ and $\xi_t = 0.254$. To check this temperature for local optimality, compute

$$(\partial y/\partial T)_t = 97\,590(826)^{-2}[0.6(826) - 0.6(4\,770)] = -338$$

$$(\partial y/\partial\xi)_t = 0.6(97\,590)[(0.0312)^{-1}(6.92)^{-1} - (0.254)^{-1}] - [0.6(34\,120) + 25\,770] = -5570$$

$$(\partial\xi/\partial T) = p_{52}/p_{53} > 0$$

and so $\partial y/\partial T < 0$, proving that $T_* = T_m$. Thus the cost of the system, excluding an auxiliary cooler is, at 826°K

$$y(10^{-3}) = 98.4V^{0.6} + 15.0\xi^{-0.6} + 6.55\xi^{-1}$$

The exponent in the reactor volume lower bound is

$$\mu = \frac{(1-\xi_t)}{\xi_t}\left(1 - \frac{p_{61}}{V_t f_e(\xi_t)}\right) = -0.522, \quad \alpha\mu = -0.313$$

The bound gives

$$t_{01} \geq 97\,590\,[1 - 0.254)^{+0.522}(1-\xi)^{-0.522}]^{0.6}$$

$$= 89.0(10^3)(1-\xi)^{-0.313} \quad \text{for} \quad \xi \geq \xi_t$$

Consequently

$$y(10^{-3}) \geq 89.0(1-\xi)^{-0.313} + 15.0\xi^{-0.6} + 6.55\xi^{-1}$$

Suppose the auxiliary cooler cost is

$$c(10^{-3}) = 3.00 - 3.40(\xi - \xi_t) + 33.0(\xi - \xi_t)^{0.6}$$

$$= 3.86 - 3.40 + 33.0(\xi - 0.254)^{0.6}$$

In the range $0.254 \leq \xi \leq 1$

$$33.0(\xi - 0.254)^{0.6} \geq (1 - 0.254)^{-0.4}(\xi - 0.254) = 37.1\xi - 9.42$$

and so

$$c(10^{-3}) \geq 33.7\xi - 5.56$$

The first semilog derivative of L at ξ_t is

$$10^{-3}(\partial L/\partial \ln \xi)_t = (0.313)(0.254)(1-0.254)^{-1}(97.6) - 0.6(34.1) - 25.8 + 33.7(0.254) = -27.3 < 0$$

Since this is negative, the lower bounding function has a minimum value less than z_t, so the search begins. The second semilog derivative is

$$10^3[0.313(0.254)(0.746)]^{-2}[1-0.313(0.746)]\,97.6 + (0.6)^2(34.1) + 25.8 + 8.56 = 57.3(10^3)$$

The Newton-Raphson method gives

$$\hat{\xi} = 0.254 \exp[-(-27.3)(57.3)^{-1}] = 0.409$$

A sharper lower bound can now be applied in the range of $0.254 \leqq \xi \leqq 0.409$, within which the minimum of l is now known to be:

$$33.0(\xi-\xi_t)^{0.6} \geqq 33.0(0.409-0.254)^{-0.4}(\xi-0.254) = 69.6\xi - 17.7$$

whence the new bound on c is $c(10^{-3}) \geqq 66.2\xi - 13.8$.

The new lower bounding function, designated $l'(\xi)$, is now evaluated at $\hat{\xi}$:

$$z(\xi) \geqq l'(\xi) = 10^3[(104.9 + 25.7 + 16.0 + 27.1) - 13.8] = (173.7 - 13.8)10^3 = 159.9(10^3) > z_t = 157.5(10^3)$$

Since this exceeds z_t, there is hope of terminating the search by constructing a good lower bounding constant by using

$$\delta_{03} = 16.0(173.7)^{-1} = 0.092$$

and

$$\delta_{04} = 27.1(173.7)^{-1} = 0.156.$$

From these is computed

$$(0.313)(0.409)(0.591)^{-1} = 0.217,$$

whence

$$\delta_{02} = [0.217 - 1.217(0.092) + (1-0.217)(0.156)][0.6 + 0.217]^{-1} = 0.278;$$

$$\delta_{01} = 0.474$$

$$\lambda = 0.313(0.474)(0.591)^{-1} = 0.251;$$

$$\delta_{11} = 0.149; \quad \delta_{12} = 0.103$$

Then

$$l'(10^{-3}) \geqq \left(\frac{89.0}{0.474}\right)^{0.474}\left(\frac{15.0}{0.278}\right)^{0.278} \times \left(\frac{6.55}{0.092}\right)^{0.092}\left(\frac{66.2}{0.156}\right)^{0.156}\left(\frac{1}{0.591}\right)^{0.149} \times \left(\frac{1}{0.409}\right)^{0.103} - 13.8$$

$$= 163.5 - 13.8 = 149.7$$

Since this is less than $z_t(10^{-3}) = 157.5$, the search must continue.

A Newton-Raphson step is taken from $\hat{\xi}$, by using the new bounding function, and gives the new point

$$\hat{\xi}_1 = (0.409)\exp[-18.4(84.38)^{-1}] = 0.329$$

Here

$$l'(\hat{\xi}_1) = 10^3[(100.8 + 29.2 + 19.9 + 21.8) - 13.8] = (171.8 - 13.8)10^3 = 158.0(10^3) > z_t = 157.5(10^3)$$

A new lower bounding constant is constructed by using

$$\delta_{03} = 19.9(171.8)^{-1} = 0.116,$$

and

$$\delta_{04} = 21.8(171.8)^{-1} = 0.127.$$

Then

$$\delta_{02} = 0.168; \quad \delta_{01} = 0.589; \quad \lambda = 0.276;$$

$$\delta_{11} = 0.184; \quad \delta_{12} = 0.090$$

$$10^{-3}(l') \geqq \left(\frac{89.0}{0.589}\right)^{0.589}\left(\frac{15.0}{0.168}\right)^{0.168} \times \left(\frac{6.55}{0.116}\right)^{0.116}\left(\frac{66.2}{0.127}\right)^{0.127}\left(\frac{1}{0.671}\right)^{0.184} \times \left(\frac{1}{0.329}\right)^{0.090} - 13.8$$

$$= 171.8 - 13.8 = 158.0 > z_t(10^{-3})$$

This proves that the global minimum is at ξ_t and terminates the search. An exhaustive search on z would have located a local minimum of $159.4(10^3)$ at $\xi = 0.36$, as well as a local maximum of $161.2(10^3)$ at $\xi = 0.26$.

As a second example to illustrate the linear case, let the exponent on the surface cost be made unity, so that

$$c = 3.00 - 3.40(\xi-\xi_t) + 33.0(\xi-\xi_t) = 29.6\xi - 4.5$$

The Newton-Raphson step of the first example is readily modified, since only one term in each derivative is changed, namely, the difference (-1.04) between $29.6\xi_t$ and $33.7\xi_t$. Consequently

$$\hat{\xi} = \xi_t \exp(-(-27.3 - 1.04)/(57.3 - 1.04)) = 0.421$$

$$(10^{-3})l(\hat{z}) = (105.6 + 25.2 + 15.6 + 12.5) - 4.5 = 158.8 - 4.5 = 154.3 < z_t(10^{-3}) = 157.5$$

Since this is considerably less than the value at ξ_t, the thermal equilibrium design is probably not optimal, making it worthwhile to find the interior minimum. To see if further searching is required, compute a lower bound on $l(\xi)$ by taking

$$\delta_{03} = 15.6/158.8 = 0.098; \quad \delta_{04} = 12.5/158.8 = 0.078$$

whence the other dual variables give

$$(10^{-3})z(\xi) \geqq 10^{-3}l(\xi) \geqq \left(\frac{89}{0.621}\right)^{0.621}\left(\frac{15.0}{0.203}\right)^{0.203} \times \left(\frac{6.55}{0.098}\right)^{0.098}\left(\frac{29.6}{0.078}\right)^{0.078} \times \left(\frac{1}{0.579}\right)^{0.194}\left(\frac{1}{0.421}\right)^{0.141} - 4.5$$

$$= 157.7 - 4.5 = 153.2$$

Thus, further search cannot improve the lower bounding function more than $1 100. Given the data, this difference is only barely significant. In fact, exhaustive search shows that the minimum value of z is $154.1(10^3)$ anywhere in the range $0.38 \leqq \xi \leqq 0.40$.

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Dialysis Study of Diffusion in a Flowing Suspension

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Comparison of solute concentrations at the outlet of a model dialyzer with values calculated from the appropriate convective diffusion equation yielded effective diffusion coefficients for mass transfer of sodium chloride in sheared suspensions of 37 to 74 μ spheres of a copolymer of styrene-divinylbenzene. Significant mass transfer augmentation was observed over that attributable to molecular diffusion, and the effective diffusivity increased with increasing concentration of suspension but remained relatively constant with respect to shear rate over the experimental range.

SCOPE

The augmentation of heat or mass transfer in a sheared suspension has been well established (Singh, 1968; Collingham, 1968; Keller, 1971; Turitto et al., 1972). The secondary fluid motion associated with the rotation of the suspension particles may result in a greater transfer of solute transverse to the direction of bulk flow than would be produced by simple diffusion. These considerations are essential to an optimal design of artificial kidneys.

The present work studied the mass transfer of sodium chloride through a neutrally buoyant suspension of spheres of a copolymer of styrene-divinyl-benzene in a model dialyzer. The fluid was treated as being homogeneous, and the situation was formulated as a convective diffusion problem involving an effective diffusion coefficient. In a more elaborate formulation this effective diffusivity would vary with position as a function of local shear rate and concentration of suspension. In this work the effective diffusivity was regarded as a constant dependent upon shear rate at the wall and average particle concentration. This relationship was evaluated by comparing the value of the concentration of solute measured at the dialyzer outlet with the value predicted from the mathematical formulation involving the effective diffusivity.

CONCLUSIONS AND SIGNIFICANCE

The dialyzer studies showed that the presence of 50 μ particles served to augment the diffusion of a solute in laminar flow. The effective diffusivity increased with increasing particle concentration but remained relatively constant with increasing shear rate at the wall. These results are in the direction indicated by a model in which the particles do not interact (Leal, 1973) but differ in the nature of the dependence. From Figure 5 the effective diffusivity is seen to be almost constant with shear rate as opposed to the result expected on the basis of an independent particle model. The value of $D/D_o - 1$ is seen from Figure 6 to be negligible at particle concentrations of 5%; it increases rapidly with increasing particle concentration over the concentration range of 5 to 10% and approaches a limit at a concentration of about 30%. At the particle concentrations studied, particle interactions undoubtedly have a strong effect on mass transfer augmentation, and particle migration as well as particle rotation is expected to be important. These movements seemed to depend mainly on the particle concentration and were not significantly affected by the shear rate within the range of shear rates at the wall employed in the experiment.

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