Minimum Cost Design of a Multimodal Fluidized Reactor-Heater System Involving an Exponential Function Inside an Integral Equation

A simple procedure for achieving the minimum cost design of a single reaction fluidized reactor system with feed and recycle heaters is presented and proven. The problem's mathematical interest stems from its multimodality, the handling of the exponential dependence of temperature, and the presence of an integral equation constraint. The proof technique is an extension of Lagrange's method, supplemented by ideas from geometric programming, extended to exponential and integral functions.

DOUGLASS J. WILDE

Engineering Design Division
Stanford University
Stanford, California 94305

SCOPE

This paper presents a simple procedure giving the minimum cost design for a wide range of fluidized bed recycled single reaction systems including feed and recycle heaters. The reaction may be of any order or stoichiometric complexity, and it may be either endothermic or exothermic. Auxiliary coolers or heaters may be required. The fluid dynamics are those of a plug flow isothermal reactor, but the major results still hold for more realistic models, provided reactor diameter does not influence the reaction rate integral.

The procedure merely requires checking two types of design and selecting the one with the lesser cost. One type operates at maximum temperature with no auxiliary heaters or coolers; the second, at fluidization velocity and maximum bed expansion, perhaps with auxiliary heat exchangers. The first requires only substituting into formulas and a single integration; the second, a single parameter search over a limited range of temperatures, each search requiring evaluation of a single integral. Although it can be computerized, the procedure is simple enough for manual calculation. No optimization theory or numerical methods are needed to carry out the procedure.

While the procedure should prove useful to chemical engineers new to reactor design, more experienced designers will find few if any surprises, although they might draw comfort from this rigorous theoretical justification of what they may have been doing for years. This article is directed more at the optimization theorists, who will be surprised that one can be assured of the global optimum to such an outrageously nonlinear, nonconvex, multimodal problem fitting none of the optimization theories now available. Not only do the posynomial and signomial functions of geometric programming appear; there are troublesome exponential and integral functions as well. Yet ideas from geometric programming manage to generate the procedure for the global optimum.

CONCLUSIONS AND SIGNIFICANCE

The conclusions to be drawn from this study are of three kinds. The first deals with what constitutes a solution to an optimization problem; the second, with technical implications for optimization theory; the third, with insight into the optimal design of fluidized bed reactors.

An academically respectable solution to an optimization problem has usually been either a single formula or an algorithm with associated proof of convergence to a single point, together with enough prior restrictions on the problem to ensure that only one stationary point exists. This approach, while producing elegant rigorous results, has too often discouraged the study of more realistic problems not satisfying such restrictions. The present work shows that such a realistic problem, even though it can have many stationary points, is solvable in the sense of having a rigorous procedure for locating the global optimum. Since the inelegance of the procedure is an unavoidable consequence of the difficulty of the problem, one need not apologize for it.

A second class of conclusions has technical implications for optimization theory. The principal one is the successful attempt to identify which inequality constraints must be tight at the optimum. This involved using not only the necessary conditions for optimality, but also the feasibility conditions for the original problem to screen out all but a few possibilities. This analysis went beyond the usual inspection of first derivatives of a Lagrangian function by employing the logarithmic derivative, followed by substitution of expressions for the terms of the original problem in order to clarify the signs or nullity of the multipliers. Although the original problem is written in a form suggested by geometric programming practice, one is concerned here not with the number of terms, but rather with the number of constraints. Thus, a problem such as this having too many degrees of difficulty in the eyes of the geometric programmer is seen as tractable from the Lagrange multiplier point of view. Not only can possibilities be eliminated for having a negative number of degrees of freedom, therefore being inconsistent with the original constraints. They can also be rejected for not having enough constraints tight to satisfy all the necessary conditions for optimality. The logarithmic derivative idea is shown to be valid, although not relevant in this case, even when there are exponential functions and integral equations. However, the elegant and useful duality theory of geometric programming does not hold in this nonconvex and multimodal situation. This is due not to a weakness in theory but rather to the difficulty of the problem.

The third set of conclusions has implications for the design of fluidized bed reactors. Diameter plays a peculiar role in determining the optimum design. Notice that it appears only in the first three constraints, all dealing with the fluid mechanics, and not in the last three, which involve the thermodynamics and kinetics of the reaction. Thus the type 1 reactor, in which the fluid mechanics constraints are loose, is determined entirely by the thermokinetics. For more general reaction systems, specifically those with multiple extents, the optimal reactors would fall into the same two classes as long as diameter did not appear in the mass balance integrals.

Past optimization theory, in its search for rigorous but elegant solutions, has tended to avoid some of the harder problems of engineering design, especially those involving nonconvex functions, or worse, multiple local stationary points. This article takes a different tack by showing how to generate all stationary points without iterative computation. Since they are all easy to find, and existence of a minimum is proven, one need only select that with the lowest value of the objective function. No second order computations are needed, for this point must be the global minimum. In many interesting cases, entire classes of stationary points will be infeasible and need not be computed at all.

Past engineering design theory, in its search for simple formulas, has also tended to avoid some of the harder problems of engineering design, especially those where a single formula cannot cover all possibilities. This article goes beyond the notion of design formula to that of design procedure, which can be a set of simple formulas, all of which may have been used. A formula is seen as a simple special case of a procedure, and a procedure is regarded as preferable to any iterative numerical method, particularly if the latter carries no guarantee of convergence to the global optimum. To the designer this paper may therefore suggest a wider point of view toward more difficult engineering problems.

The article begins by stating the reactor design problem. Then it gives the design procedure without proof. Following this is an enumeration of the mathematical difficulties from the viewpoint of conventional optimization theory. Then the problem is solved, rigorous proofs of the procedure's optimality being given. Some extensions are noted, and then an example is worked. The concluding summary emphasizes the peculiar role of the reactor diameter, which, on the one hand, determines the form of the optimal design but, on the other, is not itself fixed by the design.

PROBLEM DESCRIPTION

A system is to be built for a single gas phase catalytic reaction having several reactants and several products. Both the exothermic and the endothermic cases will be treated. Unreacted materials are separated by condensation from the products and recycled. There are two heat exchangers, one for the make-up and one for the recycle. An auxiliary cooler may be needed in the exothermic case; a heater in the endothermic case. The reactor is a cylindrical fluidized bed, operating at a low fixed pressure, whose volume, diameter, and temperature are to be selected, as is the once through conversion, to minimize the operating plus discounted investment cost. To be feasible, a design must satisfy a mass balance equality constraint as well as five inequality constraints: a temperature upper bound, a thermal requirement also bounding the temperature, upper and lower bounds on gas velocity, and to avoid slugging, a height to diameter upper bound. A strict inequality must also be satisfied to guarantee that the reaction stays on the right side of equilibrium.

The constraints and objective function are given below with brief indications of their derivations, which are tedious but routine to a skilled process designer. The constraints are given in a form suggested by geometric programming, with the constraint function compared to unity, rather than in the nonnegative form conventional for general nonlinear programming. Attention is focused on the functional form of the equations rather than on the physical constants, which are grouped into coefficients p_{ij} identified by constraint i and term j. Derivations of these coefficients are omitted to save space. A later numerical example shows numerical values of these coefficients computed from physical constants. Plug flow isothermal operation and ideal gas laws are assumed.

The objective function has three terms: a discounted reactor investment cost, a discounted exchanger investment cost, and an operating cost. The first is assumed to be a power function of reactor volume V and absolute temperature T; the second, a power function of the conversion ξ, which determines the recycle rate and hence the heat loads; the third, an inverse proportion to the conversion to reflect energy costs. The objective does not depend on the reactor diameter d.

$$y = p_{01}\, V^{\alpha} T^{\beta} + p_{02}\, \xi^{-\gamma} + p_{03}\, \xi^{-1} \qquad (0)$$

The exponents α, β, and γ are usually around 0.6. The objective function equation is labeled zero to distinguish it from the constraints.

In summary, the problem is to minimize y by choosing positive d, V, ξ, and T satisfying constraint Equations (1) through (6) and the equilibrium inequality (e).

For a single reaction, the forward (reverse) reaction rate r_f (r_r) is proportional to the product of the reactant (product) concentrations, which is in general a ratio $p_f(\xi)/[p_r(\xi)]$ of polynomials in the extent of reaction ξ.

$$r_f = k_f(T)\ p_f(\xi); \quad r_r = k_r(T)\ p_r(\xi)$$

In a flow reactor, the forward rate must always exceed the reverse rate. If the rate constants $k_f(T)$ and $k_r(T)$ obey the exponential Arrhenius relation, then the reactor extent must satisfy the strict inequality

$$f_e(\xi, T) \equiv a_f p_f(\xi) \exp(-b_f/T) - a_r p_r(\xi) \exp(-b_r/T) > 0 \quad \text{(e)}$$

where a_f, a_r, b_f, and b_r are known positive constants. Since this inequality is strict, it cannot be tight or active (satisfied as an equality) at the optimum. Therefore it must be handled specially, as suggested by its appellation equation e (for equilibrium).

For the bed to fluidize, the gas velocity cannot fall below a certain minimum. Assuming that the Reynolds number is under 20 and that the gas viscosity is directly proportional to absolute temperature (Bird, Stewart, and Lightfoot, 1960) gives this inequality.

$$f_1(d, \xi, T) \equiv p_{11}\, d^2\, \xi\, T^{-2} \leqq 1 \quad (1)$$

The constraint function is a single term posynomial, in the parlance of geometric programming (Duffin et al., 1967), and it has been arranged to be less than or equal to unity, as required by the standard geometric programming form.

To avoid blowing the catalyst out of the reactor, the gas velocity cannot exceed the terminal velocity of the catalyst particles. Kunii and Levenspiel (1969) give a terminal velocity relation for the Reynolds number range 0.4 to 500 which is approximately independent of temperature, and the resulting constraint is

$$g_2(d, \xi, T) \equiv p_{21}\, d^{-2}\, \xi^{-1}\, T + p_{21}\, d^{-2}\, T \leqq 1 \quad (2)$$

Naturally, constraints (1) and (2) cannot both be tight simultaneously.

To prevent slug formation, the bed height-to-diameter ratio should not exceed a certain predetermined constant. In terms of volume, this leads to the following constraint:

$$g_3(V, d) \equiv p_{31}\, V d^{-3} \leqq 1 \quad (3)$$

The materials and method of construction of the reactor determine a maximum allowable absolute temperature, whose reciprocal is the coefficient of the next constraint.

$$g_4(T) \equiv p_{41}\, T \leqq 1 \quad (4)$$

In the exothermic case, the temperature is bounded above by the thermal balance, which is simplified by assuming the heat capacities are independent of temperature. It is not assumed, however, that the heat capacity of the products is the same as that of the reactants. This refinement leads to an unavoidable negative term, qualifying the function as a *signomial*, in the terminology of Duffin, or a *generalized polynomial* in that of Wilde and Beightler (1967), although the inequality is still in the proper sense.

$$g_5(\xi, T) \equiv p_{51}\, \xi\, T + p_{52}\, T - p_{53}\, \xi \leqq 1 \quad (5a)$$

The inequality assumes that a reactor cooler could be installed economically but that a reactor heater would be impractical. Looseness of this thermal balance inequality would imply a need for cooling.

For an endothermic reaction, the temperature is bounded below by the thermal balance, and the constraint (5a) must be replaced with that below, in which the inequality is reversed.

$$p_{51}\, \xi\, T + p_{52}\, T + p_{53}\, \xi \geqq 1 \quad (5b)$$

The switch from exothermic to endothermic reaction produces the difference in signs in the third terms of Equations (5a) and (5b). Even though this makes the left member a posynomial in Equation (5b), the reversal of the inequality departs from the standard geometric programming form.

The following mass balance equality relates extent of reaction, reactor volume, and temperature for isothermal operation of a plug flow reactor. It is obtained by integrating the reaction rate equation and dividing one side by the other to normalize.

$$f_6(V, \xi, T) \equiv p_{61}\, V^{-1}\, \xi^{-1} \int_0^{\xi} f_0^{-1}(x, T)\, dx = 1 \quad (6)$$

By equilibrium inequality (e), the denominator of the integrand is strictly positive since x is the variable of integration over the range of feasible extents from 0 to ξ. This equation is especially troublesome from the standpoint of geometric programming, not only because the equality is strict, but because ξ appears in an integral. Moreover, T occurs in a transcendental rather than a power function. It will be shown, however, that these difficulties do not prevent solution of the design problem.

SOLUTION

The design procedure given here will be proven rigorously in a later section. It involves testing at most two types of design for feasibility and then directly comparing the objective function values for any feasible design.

Both types of design have corresponded to having exactly three constraints tight. The first type has maximum temperature [Equation (4)] and thermal balance [Equation (5)] constraints tight in addition to mass balance constraint (6). This type of design has unique volume, extent, and temperature, but a range of diameters, all of which give the same value of the objective function. The second type has minimum velocity [Equation (1)] and maximum bed height [Equation (3)] constraints tight in addition to mass balance constraint (6). This type can have multiple solutions, all of which must be determined by an exhaustive search on a single variable. Some of these solutions may correspond to thermally unstable operations, in which case the cost of a stabilizing control system must be added to the objective function. Unless thermal balance constraint (5) happens to be tight by coincidence, the cost of a cooler (for an exothermic reaction) or a heater (for an endothermic reaction) must be added to the objective function.

Consider now the first type of design, in which the temperature t_1 is the maximum allowed.

$$t_1 \equiv T_m \equiv p_{41}^{-1} \quad (8)$$

A type 1 reactor cannot exist when the reaction is endothermic because the reactor temperature cannot exceed that of the feed, which must be below the maximum allowed. The corresponding extent ξ_1 is the solution of Equation (5) at maximum temperature. For an exothermic reaction,

$$\xi_1 \equiv (1 - p_{52}T_m)/(p_{51}T_m - p_{53}) \quad (9a)$$

This extent must be tested for feasibility relative to chemical equilibrium; that is, it must satisfy Equation (e).

$$a_f p_f(\xi_1) \exp(-b_f/T_m) - a_r p_r(\xi_1) \exp(-b_r/T_m) > 0 \quad (10)$$

If it does not, this design must be discarded; otherwise the reactor volume V_1 is obtained by specializing Equation (6).

$$V_1 = p_{61}\, \xi_1^{-1} \int_0^{\xi_1} f_e^{-1}(x, T_m)\, dx \quad (11)$$

The total optimized cost is therefore

$$y_1 = p_{01} V_1^{\alpha} T_m^{\beta} + p_{02} \xi_1^{-\gamma} + p_{03} \xi_1^{-1} \quad (12)$$

The diameter need not be selected until this design has been proven optimal.

The second type of design must be generated in principle by an exhaustive search of the temperature over its entire range. The computations for each temperature examined are straightforward but considerable so it is fortunate that in practice much (or all) of the temperature range may be infeasible or not as economically attractive as the type 1 design, calculated with relative ease. An upper bound on the temperature to be searched is given by

$$T < [(y_1 - p_{02} - p_{03})/p_{01} (p_{11}^{-3/2} p_{31}^{-1})^{\alpha}]^{1/(3\alpha+\beta)} \equiv \hat{T} \quad (13)$$

It is proven later that higher temperatures cannot produce a type 2 system costing less than the type 1 system. In the example this bound is so low that no type 2 design need be evaluated.

For any temperature T_2, the extent ξ_2 for a type 2 design is the root of the following integral equation.

$$p_{11}^{3/2} p_{31} p_{61} \xi_2^{1/2} T_2^{-3} \int_0^{\xi_2} f_e^{-1} (x, T_2) \, dx = 1 \quad (14)$$

Since the integrand is strictly positive, the right member is strictly increasing in ξ_2 for fixed T_2, so the root ξ_2 is unique if it exists. The reactor volume V_2 is then determined by

$$V_2 = p_{11}^{-3/2} p_{31}^{-1} \xi_2^{-3/2} T_2^3 \quad (15)$$

This in turn gives enough information to fix the objective function, to which a term y_a must be added to allow for the cost of an auxiliary cooler (for an exothermic reaction) or a heater (for an endothermic reactor) required by the fact that the thermal balance is not satisfied for type 2 designs. Thus the extent $\xi_2(T_2)$, the volume $V_2(T_2)$ and cost $y(T_2)$ all depend on the given temperature T_2.

$$y(T_2) = y(T_2, \xi_2(T_2), V_2(T_2)) + y_a(T_2) \quad (16)$$

Only designs for which $y(T_2) < y_1$ need be considered; if there are none, then the type 1 design is optimal.

At any temperature T_2, the design extent $\xi_2(T_2)$ is bounded by the equilibrium extent $\xi_e(T_2)$, the solution to equilibrium constraint (e) treated as a strict equality. That is, $\xi_e(T_2)$ satisfies

$$\frac{a_r p_r [\xi_e(T_2)]}{a_f p_f [\xi_e(T_2)]} = \exp [(b_r - b_f)/T_2] \quad (18)$$

and

$$\xi_2(T_2) < \xi_e(T_2) \quad (19)$$

Thermal balance constraint (5a) gives a lower bound on $\xi_2(T_2)$ for exothermic reactions.

$$\xi_2(T_2) > (1 - p_{52} T_2)/(p_{51} T_2 + p_{53}) \equiv \xi_t(T_2) \quad (20a)$$

For endothermic reactions, thermal balance constraint (5b) gives an upper bound.

$$\xi_2(T_2) < (1 - p_{52} T_2)/(p_{51} T_2 - p_{53}) \equiv \xi_t(T_2) \quad (20b)$$

If $\xi_e(T_2) < \xi_t(T_2)$ in the exothermic case, then of course there is no optimal feasible design at T_2. Otherwise, the left member of Equation (14) can be evaluated for $\xi_2 = \xi_t$. If the result exceeds 1, then there is no optimal feasible extent at T_2. Otherwise, the right member can be evaluated for $\xi_2 = \xi_e$. If the result is less than 1, there is no optimal feasible design at T_2. Otherwise, there exists a root $\xi_2(T_2)$ within the interval $\xi_t(T_2) \leq \xi_2(T_2) < \xi_e(T_2)$ which can be found by any one dimensional root-finding method (Wilde, 1964). In the endothermic case both $\xi_t(T_2)$ and $\xi_e(T_2)$ are upper bounds, and the interval to be searched is $0 \leq \xi_2(T_2) \leq \min \{\xi_t(T_2), \xi_e(T_2)\}$.

A systematic search on T would begin at the $(T_m, \hat{T})$. If this temperature is infeasible, lower temperatures must be attempted until either feasibility is achieved or it is proven that no feasible type 2 design exists. Suppose that a feasible design does exist at some temperature. Then the corresponding extent, volume, and objective function can be evaluated. If this value is lower than y_1, then the type 1 design is eliminated from consideration, and the temperature is searched carefully to find the minimum cost type 2 design. Otherwise, the temperature may be lowered drastically in the search for a design costing less than y_1. If one is found, then a more careful search is in order. On the other hand, a few cases may suffice to show that no type 2 design can cost less than y_1. In practice, this procedure should rapidly identify the globally optimal design since in the search there is really only one degree of freedom over a limited range.

An important special case arises if, at one of the feasible temperatures, the thermal balance constraint (5) is satisfied as a strict equality. When this happens, no auxiliary cooler or heater is needed, and $y_a = 0$, so such a design is certainly a good candidate for the optimum. This temperature will be the highest feasible, and if by coincidence this is also the maximum allowable T_m, then this type 2 design will be identical with the type 1 design already obtained.

If the type 1 design turns out to be the best, the diameter d_1 can be chosen to be any satisfying minimum and maximum velocity constraints (1) and (2), as well as height ratio constraint (3). Thus

$$\max \{(p_{31}V)^{1/3}, [p_{21} T_1 (1 + \xi_1^{-1})]^{1/2}\} \leq d_1 \leq p_{11}^{-1/2} \xi_1^{-1/2} T_1 \quad (21)$$

In the coincidental case where the two types of design are identical, the upper bound, which corresponds to minimum velocity, would be achieved.

If no feasible optimum solution exists for either type of design, then the constraints are inconsistent, meaning the design specifications were too stringent to permit any feasible design.

If a type 2 design is optimal, the diameter d_2 is obtained from constraint (3).

$$d_2 = (p_{31}V_2)^{1/3} \quad (22)$$

MATHEMATICAL DIFFICULTIES

Viewed as a computation problem in mathematical programming, model Equations (e), and (1) through (7) present many difficulties. First, everything is nonlinear. Second, the power function forms of Equations (1) to (4) are not even convex, although geometric programming theory shows that they can be made so under a logarithmic transformation. Third, the nonlinear equality (6) excludes convexity of the constraint set, even under transformation, so that many local stationary points can in principle occur. Fourth, the transcendental functions and the integral in Equation (6) exclude geometric programming so useful in other nonlinear design problems. Fifth, even if the transcendentals of Equation (6) were approximated by power functions so that geometric programming could be applied, the result would still have 7 degrees of difficulty (one less than the number of terms minus the number of variables), making the substitute dual optimization problem of geometric programming possibly more difficult than the original one. Sixth, Equation (6) turns out (as will be shown in the next section) to be replaceable by an inequality having the wrong sense for geometric programming, forcing the use of the less powerful signomial theory, which not only cannot generate lower bounds on the minimum as can geometric programming, but also raises the possibility of computing false optima. Seventh, the inevitable presence of loose inequalities (strictly < 1) at the optimum can lead to computational annoyances, and the number of possible combinations of tight constraints (no more than 4 out of 6–57 varieties) is too many to enumerate. Eighth, the problem has more than one stationary point, and not only might several starts be necessary to find them all, but also second-order computations would be needed to guard against false optima. Ninth, the constraints might be inconsistent, leading to wasteful attempts to find a feasible starting point. And tenth, the strict inequality (0) can produce computational difficulties because it makes the constraint set open, raising the possibility of having an infimum rather than a minimum.

True, there are only four design variables, and even the most simple-minded differential algorithm (Wilde and Beightler, 1967) had no trouble finding one of the stationary points in the numerical example given at the end of the article. Unfortunately, it found the wrong one. Yet even this amount of computation is not really needed since the simpler design procedure finds the optimum without iteration, approximation, or verification of second-order sufficient conditions for local optimality. Without the proofs following, the designer perhaps would feel confident in the simple design procedure only after many needless confirmatory computations had been performed.

EXAMPLE

The example is a coded version of a catalytic aromatic exothermic hydrogenation reaction with a symbolic chemical reaction

$$A + H_2 \rightleftharpoons AH_2$$

The objective function, reflecting the high cost of heating steam in a European location, is:

$$y = 1750\, V^{0.6}\, T^{0.6} + 15{,}000\, \xi^{-0.6} + 6550\, \xi^{-1} \quad (0')$$

For 1 atmosphere total pressure the forward and backward reaction rates (coded) are given in the equilibrium inequality.

$$f_e(\xi, T) \equiv 55\,(1-\xi)^2\,(2-\xi)^2 \exp(-4770/T)$$
$$- 1.4 \times 10^{-5}\, \xi (2-\xi)^{-1} \exp(-19270/T) > 0 \quad (e')$$

The six constraints are, for this system, constructed using styrene C_6H_5-C_2H_3 as the reactant A, and 826°K as the maximum temperature allowed. The heat capacity of products is assumed to equal that of the reactant, which simplifies thermal balance constraint (5a).

$$63.8\, d^2\, \xi\, T^{-2} \leq 1 \quad (1')$$

$$3.60 \times 10^{-4}\, d^{-2}\, \xi^{-1}\, T + 3.60 \times 10^{-4}\, d^{-2}\, T \leq 1 \quad (2')$$

$$0.850\, V\, d^{-3} \leq 1 \quad (3')$$

$$0.00121\, T \leq 1 \quad (4')$$

$$0.00206\, T - 2.76\xi \leq 1 \quad (5a')$$

$$0.0362\, V^{-1}\, \xi^{-1} \int_0^{\xi} f_e^{-1}(x, T)\, dx = 1 \quad (6')$$

The type 1 design has $T_1 = 826$°K, the maximum allowable, and an extent determined by the heat balance Equation (9a) as

$$\xi_1 = [0.00206\,(826) - 1]/2.76 = 0.256$$

Since this extent satisfies the equilibrium constraint (e'), the equilibrium extent being close to unity at 826°K, the reactor volume is found by Equation (11).

$$V_1 = 0.0362\,(0.256)^{-1} \int_0^{0.256} f_e^{-1}\,(x, 826°\mathrm{K})\, dx$$

where

$$f_e(x, 826) = 0.171\,(1-x)^2\,(2-x)^{-2} - 10^{-17}\, x\,(2-x)^{-1}$$

The volume V_1 is 0.99 m^3, whence the cost is

$$y_1 = 1750\,[(0.99)\,(826)]^{0.6} + 15{,}000\,(0.256)^{-0.6} + 6550\,(0.256)^{-1} = \$157{,}000$$

Before carrying out the computations for a type 2 design, inequality (13) is checked to place an upper bound on the temperature.

$$T < [(157{,}000 - 15{,}000 - 6550)/ 1750\,[(0.00196)\,(1.18)]^{0.6}]^{0.526} = 78°\mathrm{K} \equiv \hat{T}$$

This temperature is, of course, so low that the type 1 design is clearly optimum so the more complicated type 2 calculations need not be carried out. The optimal diameter is bounded by inequality (21).

$$\max\{[(0.850)\,(0.99)]^{1/3}, [(3.60 \times 10^{-4})\,(826)\,(1 + (0.256)^{-1})]^{1/2}\} \leq d_1 \leq [(63.8)\,(0.256)]^{-1/2}\,(826)$$

or

$$1.21 = \max\{0.944, \quad 1.21\} \leq d_1 \leq 204.$$

All in all, the design procedure is strikingly simple, considering the mathematical complexity of the original problem. Nowhere are iterative computations required.

PROOFS

The proof strategy is to combine the feasibility conditions, represented by the constraints, with the necessary conditions for optimality obtained by setting derivatives of a Lagrangian to zero. The optimality expressions are simplified by a nonlinear transformation suggested by geometric programming. Then Kuhn-Tucker conditions restricting signs or nullity of the multipliers are applied to deduce that only the two cases generated by the design procedure can be stationary points.

While in principle the strict inequality (e) may mean that no minimum exists, this could only happen when design conditions attain equilibrium. Hence if Equation (e) holds, a minimum must exist because the objective is bounded below, provided that Equations (1) through (6) are consistent. Therefore, the global minimum is found by comparing the objective function values for all feasible designs. Overly stringent requirements could also lead to a situation in which all designs violate some constraints and leave no feasible stationary points. Since a minimum must exist if there are any feasible designs at all, this circumstance would imply inconsistency of the original constraints.

Necessary conditions for a local minimum are obtained by differentiating a Lagrangian function L defined below

$$L \equiv y - \sum_{m=1}^{6} \lambda_m\,(1 - f_m) \quad (23)$$

where y and the f_m ($m = 1, \ldots, 6$) are the functions of Equations (0) through (6), and the λ_m are Lagrange multipliers. At a feasible stationary point of L, it is necessary that the first partial derivatives of L with respect to the design variables vanish. Moreover, the Kuhn-Tucker necessary conditions for optimality require that λ_6, the multiplier for the strict equality, not be zero

$$\lambda_6 \neq 0 \tag{24}$$

and that the other multipliers must all be nonnegative.

$$\lambda_1 \geqq 0, \quad \lambda_2 \geqq 0, \quad \lambda_3 \geqq 0, \quad \lambda_4 \geqq 0, \quad \lambda_5 \geqq 0 \tag{25}$$

The necessary conditions are clarified for analysis if they are presented as the product of the derivative with the variable of differentiation. Then the terms of the original objective and constraint functions reappear, abbreviated t_{mi} for the ith term of the mth constraint, with $m = 0$ used for the objective. Often an entire constraint function f_m will occur as a coefficient, in which case it can be replaced by unity. This follows from the complementary slackness conditions which require, in this context, that a multiplier λ_m be positive if and only if the corresponding constraint is tight, that is, $f_m = 1$. The optimality condition for V immediately shows that λ_6 must be positive.

$$\alpha t_{01} + \lambda_3 - \lambda_6 = 0 \tag{V}$$

This is because λ_6 is the only variable having a negative coefficient in a sum which must add to zero.

$$\lambda_6 > 0 \tag{26}$$

The optimality condition for (d) is simply

$$2\lambda_1 - 2\lambda_2 - 3\lambda_3 = 0 \tag{d}$$

This immediately eliminates the possibility that the optimal design will operate at maximum velocity [Equation (2)]. For to satisfy Equation (d), either all $\lambda_1 = \lambda_2 = \lambda_3 = 0$, or else $\lambda_1 > 0$, since it is the only variable with a positive coefficient in a vanishing sum. But by complementary slackness, this would imply $f_1 = 1$, that is, operation at minimum velocity, which of course precludes maximum velocity. Since

$$\lambda_2 = 0 \ (f_2 < 1) \tag{27}$$

it follows that $\lambda_3 > 0$ $(f_3 = 1)$ if $\lambda_1 > 0$; that is, minimum velocity implies maximum height to diameter ratio. Since there are only four design variables, no more than one more equation can be tight; it can be either f_4 (maximum temperature) or f_5 (heat balance). Such a design is of type 2.

If $\lambda_1 = \lambda_2 = \lambda_3 = 0$, then the remaining multipliers λ_4, λ_5, and λ_6 cannot vanish identically because the three necessary conditions (V), (ξ), and (T) involve all these three multipliers. These conditions are nonsingular, since Equation (6) is the only active constraint in which V appears, and so condition (V) determines λ_6. Similarly, ξ appears only in potentially active constraints (5) and (6), so conditions (ξ) and (V) would determine λ_5. Finally, T appears in all potentially active constraints (4), (5), and (6), so it is fixed by conditions (T), (ξ), and (V), completing the proof that none of the λ_4, λ_5, and λ_6 can vanish identically. Equivalently, all three constraints (4), (5), and (6) must be active whenever (1), (2), and (3) are all loose. Such a design is of type 1.

In an endothermic reactor, maximum temperature constraint (4) cannot be satisfied, implying that $\lambda_4 = 0$, in which case a type 1 design does not exist. Therefore optimal endothermic reactors must be of type 2.

There are therefore no more than two classes of stationary points, type 1 when constraints (4), (5), and (6) are active, and type 2 when (1), (3), and (6) are active. In either case other constraints may be tight coincidentally. Optimality conditions (ξ) and (T) will show that none of these cases can be eliminated.

The type 1 design Equations (8) to (12) follow immediately from the defining requirement that constraints (4), (5), and (6) all be tight. The bounds (21) on diameter simply express the range imposed by bounds on velocity.

Since in a type 2 design constraints (1), (3), and (6) are tight, two variables d and V can be eliminated by using Equations (1) and (3). The resulting optimization problem can be written as minimize the objective function subject to the single equality constraint (14). The procedure described examines all feasible solutions of this constraint which are better than the type 1 design, picking out the minimum.

Following is the derivation of the upper bound $\hat{T}$ on the temperature to be searched in a type 2 design, given the type 1 cost y_1. The type 2 cost y_2 must be at least that of the reactor, obtained by combining objective cost Equation (0) with volume Equation (15), and only designs where this cost y_2 is less than y_1 are of interest. Hence

$$\begin{aligned} y_1 > y_2 &\geqq p_{01}\, V_1{}^{\alpha} T^{\beta} + p_{02}\, \xi^{-\gamma} + p_{03}\, \xi^{-1} \\ &= p_{01}\, p_{11}{}^{-3\alpha/2}\, p_{31}{}^{-1}\, T^{3\alpha+\beta}\, \xi^{-3\alpha/2} + p_{02}\, \xi^{-\gamma} + p_{03}\ {}^{-1} \\ &> p_{01}\, p_{11}{}^{-3\alpha/2}\, p_{31}{}^{-1}\, T^{3\alpha+\beta} + p_{02} + p_{03} \end{aligned}$$

The last inequality follows from the fact that extent ξ cannot exceed unity, and all exponents of ξ are negative. Inequality (13) is obtained by solving for T in the inequality between the first and last members above.

OTHER TWO OPTIMALITY CONDITIONS

Conditions (V) and (d) previously derived are the familiar linear orthogonality conditions of geometric programming, which do not contain any design variables. They were easily obtained because V and d appear only as the power functions required by geometric programming. Since, however, ξ appears in an integral and T in a transcendental function, the optimality conditions not only will be nonlinear but also will contain the design variables. Still, the conditions are linear in the multipliers and since, as will be shown, the signs of the nonlinear coefficients can be established, it is sometimes possible to eliminate one of the stationary points from consideration.

Even though such elimination of a stationary point will only rarely be practical in reactor design problems, the steps are carried out to show that integral constraints do not present insurmountable obstacles to this style of optimization.

Since the preceding variables of differentiation appeared in positive power function terms, the coefficients in the optimality conditions were merely the corresponding exponents. Here ξ appears in a negative term in f_5, but the only change is in the sign of the optimality condition coefficient. What is new is the handling of the integral of f_6, which is detailed in the manipulations following:

$$\begin{aligned} &\xi(\partial f_6/\partial \xi) \\ &= p_{61}\, V^{-1} \xi \left[\xi^{-1} f_e{}^{-1}(\xi, T) - \xi^{-2} \int_0^{\xi} f_e{}^{-1}(x, T)\, dx \right] \\ &= p_{61}\, V^{-1} f_e{}^{-1}(\xi, T) - p_{61}\, V^{-1} \xi^{-1} \int_0^{\xi} f_e{}^{-1}(x, T)\, dx \\ &= p_{61}\, V^{-1} f_e{}^{-1}(\xi, T) - 1 \end{aligned} \tag{33}$$

The optimality condition for (ξ) is therefore

$$\begin{aligned} -(\gamma t_{02} + t_{03}) + \lambda_1 - t_{21}\lambda_2 + (t_{51} - t_{53})\lambda_5 \\ + [p_{61}\, V^{-1} f_e{}^{-1}(\xi, T) - 1]\lambda_6 = 0 \end{aligned} \tag{ξ}$$

The minus sign of t_{53} must be changed to plus for endothermic reactions.

It can be shown that $(t_{51} - t_{53})\ \lambda_5$ is negative in physically interesting examples. If the coefficient of λ_6 could also be proven negative, then the only positive term in condition (ξ) would be λ_1, proving that f_1 cannot be loose. Although this would reduce the number of possible stationary points to 1, the extra effort is not justified in this case for two reasons: First, the coefficient is usually positive; second, its computation requires the evaluation of the integral in Equation (6), which is more work than calculating the value of the objective function anyway.

For completeness, the optimality condition (T) will also be given because the handling of a transcendental function inside an integral is of interest, even though no elimination of stationary points is possible.

$$\beta t_{01} - 2\lambda_1 + \lambda_2 + \lambda_4 + (t_{51} + t_{52})\lambda_5 - \left[T^{-1} \int_0^{\xi} f_e^{-2}(x, T)\ [b_f r_f(x, T) - b_r r_r(x, T)]\ dx \right] \lambda_6 = 0 \quad \text{(T)}$$

Whenever $b_f \geqq b_r$ the integrand in the bracketed quantity, and hence the quantity itself, is positive, which, however, is inconclusive as far as proving $\lambda_1 > 0$ is concerned. This quantity was obtained by interchanging the order of partial differentiation with respect to T and integration with respect to x.

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NOTATION

Expressions or numbers in brackets are those used in the example. Formulas not in brackets are general, their symbols being defined alphabetically at the end of the table.

p_{01} [= \$1750/yr.] = reactor cost coefficient
p_{02} [= \$15,000/yr.] = exchanger cost coefficient
p_{03} [= \$6550/yr.] = operating cost coefficient
$p_{11}\left[= \left(\frac{\Pi}{4}\right)\left(\frac{3600\ \text{s}}{\text{hr.}}\right)\frac{(273°\text{K})\ Mv_0}{RF} = 68.3\ (°\text{K/m})^2\right]$ = minimum fluidization velocity coefficient
$p_{21}\left[= \left(\frac{\Pi}{4}\right)\left(\frac{3600\ \text{s}}{\text{hr.}}\right)\frac{Mv_t}{RF} = 3.60 \times 10^{-4}\ \text{m}^2/°\text{K}\right]$ = terminal velocity coefficient
$p_{31} = \frac{4}{\Pi r}$ [= 0.850] = antislugging coefficient
$p_{41} = (T_m, °\text{K})^{-1}$ [= 0.00121 $°\text{K}^{-1}$] = reciprocal maximum temperature
$p_{51} = \frac{c_p}{c_r} - 1$ [= 0] = heat capacity ratio difference
$p_{52} = T_f^{-1}$ [= 0.00206 $°\text{K}^{-1}$] = reciprocal feed temperature
$p_{53} = p_{51} - \frac{M\Delta H}{T_f F c_r}$ [= 2.76] = thermal reaction coefficient
$p_{61} = F\ (1 - \epsilon)^{-1}\ \rho_c^{-1}$ [= 0.0362 m³/hr] = reactor volume coefficient
a_f [= 55 gmol/s] = forward reaction rate constant
a_r [= 1.4×10^{-5} gmol/s] = reverse reaction rate constant
b_f [= E_f/R = 4770°K] = forward reaction rate exponent
b_r [= E_r/R = 19270°K] = reverse reaction rate exponent
c_p [= 50 cal/mol °K] = mean heat capacity of products
c_r [= 50 cal/mol °K] = mean heat capacity of reactants
d = reactor diameter, meters
d_p [= 0.02 cm] catalyst particle diameter
d_1 (d_2) = case 1 (2) reactor diameter
f_e = [Equation (e)] difference in reaction rates
F [= 125 kg/hr] = reactant make-up feed rate
g [= 9.80 cm/s²] = acceleration of gravity
h = height of fluidized bed, m
L = [Equation (23)] Lagrangian function
M [= 104] = molecular weight of reactant
p_f [= $(1 - \xi)^2/(2 - \xi)^2$] = forward reaction rate function
p_r [= $\xi/(2 - \xi)^2$] = reverse reaction rate function
r [= 1.50] = maximum bed height/diameter ratio
r_f = forward reaction rate, gmol/s
r_r = reverse reaction rate, gmol/s
R = gas constant
T = reactor absolute temperature, °K
T_f = feed absolute temperature, °K
T_m = maximum allowable abs. temperature, °K
$\hat{T}$ = [Equation (13)] upper bound on temperature to be searched, °K
T_1 (T_2) = case 1 (2) optimal reactor temperature, °K
v_0 [= $d_p^2\ (\rho_c - \rho)/1650\mu_0$, m/s] = minimum fluidization velocity at 273°K
$v_t\left[= \left(\frac{4(\rho_c - \rho)^2 g^2}{\rho\mu}\right)^{1/3} d_p,\ \text{m/s}\right]$ = terminal velocity, m/s
V = reactor volume, m³
V_1 (V_2) = case 1 (2) reactor volume, m³
x = variable of integration
y = [Equation (0)] total cost objective function, \$
y_a = [Equation (16)] auxiliary cooler cost, \$
y_1 (y_2) = case 1 (2) = total cost, \$

Greek Letters

α, β, γ [0.6, 0.6, 0.6] = Equation (0) cost components
ΔH [= − 14500 cal/g-mol] = heat of reaction
ϵ [= 0.7] = void fraction in fluidized bed
ξ = extent of reaction
ξ_e = equilibrium extent of reaction
ξ_t = thermally balanced extent of reaction
ξ_1 (ξ_2) = case 1 (2) extent of reaction
λ = Lagrange multiplier
μ = gas viscosity, g/cm s
μ_0 [= 68.5×10^{-6} g/cm s] = gas viscosity at 273°K (extrapolated)
ρ [= 4.71×10^{-3} g/cm³] = gas density at 273°K (extrapolated)
ρ_c [5.0 g/cm³] = catalyst particle density

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