NOTATION

A = cross-sectional area of annulus, m^2
C = tracer concentration at $t \geqq 0$
C_o = tracer concentration at $t \leqq 0$
C_1 = input tracer concentration, dimensionless
C_a = concentration of tracer in annulus, dimensionless
C_s = concentration of tracer in spout, dimensionless
D = dispersion coefficient, m^2/s
D_c = column diameter, m
D_i = gas inlet diameter, m
D_s = spout diameter, m
d_p = particle diameter, mm, taken as diameter of equivolume sphere
H = bed depth, m
H_{max} = maximum spoutable bed depth, m
I = horizontal grid lines in Figure 2
J = gas streamlines in Figure 2
L = length of flow path in annulus, m
M = number of divisions of H in Figure 2
N = number of streamlines in the annulus in Figure 2
$Q(J-1)$ = flow rate between streamlines $J-1$ and J in the annulus, m^3/s
R = radial distance from spout axis, m
R_c = column radius, m
t = time, s
U = superficial fluid velocity, m/s
U_a = superficial gas velocity in the annulus, m/s
U_{mf} = minimum fluidization velocity, m/s
U_{ms} = minimum spouting velocity, superficial, m/s
U_s = operating spouting velocity, superficial, m/s
u_s = interstitial gas velocity in the spout, m/s
u_z = interstitial gas velocity along the streamline in the annulus, m/s
Z = vertical distance from gas inlet orifice
z = linear distance along a streamline, starting from spout-annulus interface
z' = z/L
Z' = Z/H
ϵ_s = spout voidage
ϵ_a = annulus voidage
$\delta(t)$ = unit step function in Equation (16)
ρ_s = particle density, g/cm^3

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Multiple Minima in a Fluidized Reactor—Heater System

A minimum cost design problem for a single-reaction fluidized-bed reactor system is analyzed in this paper. The problem's mathematical interest stems from Wilde's statements (1974) that there can be only two types of design to this nonlinear, nonconvex, multimodal problem. It is shown by a direct search procedure that, in fact, there are at least four types of optimal design. Furthermore, the type 3, rather than the type 1 design, is the global solution to the numerical example considered in Wilde's work, if the required auxiliary cooler cost is excluded.

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SCOPE

This paper examines and discusses a procedure originally suggested by Wilde (1974) for achieving the minimum cost design of a single-reaction fluidized reactor system with feed and recycle heaters. The development of this procedure was based on an extension of Lagrange's method, supplemented by the ideas from geometric programming. It was shown that the globally minimum design necessarily belonged to one of two possible classes of solutions. In an illustrative example involving an exothermic reaction, the type 1 design was then found to be the optimum solution.

The main purpose of the present work is to point out that four types of designs can be found by means of a simple two-dimensional search and that the type 3 design, rather than the type 1 design, is the global solution to the numerical example in which the required cooler cost is excluded. The search procedure is simple to implement, and, unlike Wilde's, it is not necessary to distinguish the solution type in using this procedure. Although attention is focused on a particular second-order exothermic reaction, the procedure can be applied to a wide range of problems. In general, the reaction may be either exothermic or endothermic, of any order, and of any stoichiometric complexity.

CONCLUSIONS AND SIGNIFICANCE

The direct search design procedure is found to be computationally efficient and robust in achieving the true solution to the cost minimization problem. In addition to the third design, which is the global solution to the numerical example considered in this paper, a fourth type of design can be found if a design parameter (the maximum allowable reactor temperature) is permitted to take a higher value. Therefore, a multitude of feasible optimal design types is numerically shown to exist.

It should be reemphasized that the type 3 design as described in this work does not account for the required auxiliary cooler cost. Were the cooling cost to exceed 7.5% of the total, the cooler would not be worth adding to the reactor system, thus making the type 1 design the global solution to the problem. In a companion paper, Wilde (1976) will show, and we have confirmed by the direct search procedure, that this is indeed the case if the cooling cost is properly accounted for in the numerical example. In general, however, it may be advantageous to add an auxiliary cooler to an exothermic reactor-heater system, and this possibility should not be overlooked.

This paper discusses a procedure for achieving the global minimum cost design of a single-reaction fluidized reactor system with feed and recycle heaters. The present work is essentially based on the formulation and analysis of such a system by Wilde (1974); however, unlike Wilde's procedure, the simple search technique employed in this work does not require distinguishing the types of design. According to Wilde's analysis of the optimality conditions, there are two distinct design types for the reactor–heater system, and it is therefore only necessary to perform (at most) two sets of calculations: a straightforward substitution calculation for the type 1 design and a one-dimensional search over a limited range of temperature for the type 2 design. By direct comparison, the one with the lesser cost is then selected as the globally minimum cost design. Wilde applied this two-step procedure to a numerical example involving a catalytic aromatic exothermic hydrogenation reaction of the type

$$A + H_2 \rightleftarrows AH_2$$

and the type 1 design was found to be the optimal solution.

The purpose of this paper is to show, by using a two-dimensional direct search procedure, not only the existence of the third design (the type 3 design) but also the fact that, in this particular example, the third design is the globally optimal one.

THE MINIMUM-COST OPTIMIZATION PROBLEM

The example problem, as formulated by Wilde (1974) in the geometric programming format, is to globally minimize the objective cost function (representing the reactor, exchanger, and operating costs) given by

$$F_0 \equiv p_{01}V^{\alpha}T^{\beta} + p_{02}\xi^{-\gamma} + p_{03}\xi^{-1} \quad (1)$$

by choosing positive d (reactor diameter), V (reactor volume), ξ (extent of reaction), and T (absolute temperature) satisfying the following constraints dealing with either the fluid mechanics of the system or the thermokinetics of the reaction:

1. Minimum allowable gas velocity

$$F_1 \equiv p_{11}d^2\xi T^{-2} \leq 1 \quad (2)$$

2. Maximum allowable gas velocity

$$F_2 \equiv p_{21}d^{-2}\xi^{-1}T + p_{21}d^{-2}T \leq 1 \quad (3)$$

3. Maximum allowable bed height-to-diameter ratio

$$F_3 \equiv p_{31}Vd^{-3} \leq 1 \quad (4)$$

4. Maximum allowable temperature

$$F_4 \equiv p_{41}T \leq 1 \quad (5)$$

5. Thermal balance (exothermic case)

$$F_5 \equiv p_{51}\xi T + p_{52}T - p_{53}\xi \leq 1 \quad (6)$$

6. Mass balance

$$F_6 \equiv p_{61}V^{-1}\xi^{-1}\int_0^{\xi} f_e^{-1}(x, T)\,dx = 1 \quad (7)$$

where

$$f_e(\xi, T) = r_f(\xi, T) - r_r(\xi, T) = a_f\left(\frac{1-\xi}{2-\xi}\right)^2 \exp\left(-\frac{b_f}{T}\right) - a_r\left(\frac{\xi}{2-\xi}\right)\exp\left(-\frac{b_r}{T}\right) \quad (8)$$

The numerical constants p_{ij}, a_f, b_f, a_r, and b_r appearing in the objective and constraint functions are summarized in Table 1. It should be noted that the mass balance constraint 6 is a strict equality, and, hence, there are really at most three independent design variables. Moreover, the objective cost function F_0 is not directly dependent on the variable d, and it does not account for the cost of auxiliary coolers if they are ever needed.

WILDE'S DESIGN PROCEDURE

Based on a set of four optimality conditions which we shall discuss in more detail later, Wilde concluded that there are no more than two types of solutions to the minimization problem. The following is a brief outline of his design procedure.

In the type 1 design, thermokinetics constraints 4, 5, and 6 are active. Therefore, the three design variables T_1, ξ_1, and V_1 can be determined in seriatim from

$$T_1 = \frac{1}{p_{41}} \quad (9)$$

$$\xi_1 = \frac{1 - p_{52}T_1}{p_{51}T_1 - p_{53}} \quad (10)$$

$$V_1 = \frac{p_{61}}{\xi_1}\int_0^{\xi_1} \frac{1}{f_e(x, T_1)}\,dx \quad (11)$$

The corresponding objective cost function $F_0(T_1, \xi_1, V_1)$ is evaluated from Equation (1). As the rest of the constraints are inactive, the variable d_1 can be chosen at any suitable value satisfying the constraints 1, 2, and 3.

TABLE 1. NUMERICAL CONSTANTS FOR THE EXAMPLE PROBLEM

Symbol	Value	Note (unit)	
p_{01}	1 750	Reactor cost coefficient	(\$/yr)
p_{02}	15 000	Exchanger cost coefficient	(\$/yr)
p_{03}	6 550	Operating cost coefficient	(\$/yr)
p_{11}	63.8	Minimum fluidization velocity coefficient	$\left(\frac{°K}{m}\right)^2$
p_{21}	3.6×10^{-4}	Terminal velocity coefficient	$\left(\frac{m^2}{°K}\right)$
p_{31}	0.85	Antislugging coefficient	(−)
p_{41}	$\frac{1}{826}$	Reciprocal maximum temperature	$\left(\frac{1}{°K}\right)$
p_{51}	0	Heat capacity ratio difference	(−)
p_{52}	$\frac{1}{485.4369}$	Reciprocal feed temperature	$\left(\frac{1}{°K}\right)$
p_{53}	2.76	Thermal reaction coefficient	(−)
p_{61}	0.0362	Reactor volume coefficient	$\left(\frac{m^3}{hr}\right)$
a_f	55	Forward reaction rate constant	$\left(\frac{gmole}{s}\right)$
a_r	1.4×10^{-5}	Reverse reaction rate constant	$\left(\frac{gmole}{s}\right)$
b_f	4 770	Forward reaction rate exponent	(°K)
b_r	19 270	Reverse reaction rate exponent	(°K)
α, β, γ	0.6	Cost function exponents	(−)

In the type 2 design, the constraints 1, 3, and 6 are active. If V and d are eliminated from these equations, we have the following equality constraint involving T and ξ:

$$\frac{p_{11}^{3/2} p_{31} p_{61} \xi^{1/2}}{T^3} \int_0^{\xi} \frac{1}{f_e(x, T)} dx = 1 \tag{12}$$

This equation, however, can be solved numerically for ξ if T is fixed at T_2. The design variables d_2 and V_2 can then be determined from Equations (2) and (7), and finally the cost function $F_0(T_2, \xi_2, V_2)$ from Equation (1). Since this type of design can have multiple solutions, in general a one-dimensional exhaustive search for the minimizing temperature T_2 must be carried out in a suitable temperature range. Wilde reasoned that higher temperatures cannot produce a type 2 design costing less than the type 1 system, and thus he gave an estimate of the upper bound on the temperature to be searched. Sometimes, the search need not be performed altogether, if this upper bound temperature turns out to be sufficiently low to preclude any possibility of generating the type 2 design with a lower cost. The example problem solved by Wilde (1974) was just such a case, and the type 1 design was taken as the globally minimizing solution to the problem.

Wilde's type 1 design is summarized in column 1 of Table 2. As his solution was apparently obtained by hand calculation, we recalculated the type 1 design as a mean of verification, and the results are shown in column 2 for comparison. The solution given in column 3 is the design obtained by a direct global search method to be described shortly. This solution, which is neither the type 1 nor the type 2, has a cost of $F_0 = 146\,435.6$ which is approximately 7.5% less than that of the type 1 design.

TABLE 2. COMPARISON OF SOLUTIONS

	Type 1 Wilde's solution	Type 1 recalculated solution	Type 3 direct search solution
F_0(\$/yr)	157 000	157 476.0	146 435.6
ξ(−)	0.256	0.2541884	0.4499112
T(°K)	826	826.0000	826.0000
V(m³)	0.99	0.9854218	1.160595
d_{max}	204	205.1124	154.1723
∫ (m)	∫	∫	∫
d_{min}	1.21	1.211279	0.9954815
λ_4	—*	—	—
λ_5	—	−50 989.05	+0.0031458
λ_6	—	+58 553.18	+64 593.03
F_4	—	1.000000	1.000000
F_5	—	1.000000	0.4598051
F_6	—	1.000000	1.000000

* The quantity is not given or calculated.

A DIRECT SEARCH DESIGN PROCEDURE

In order for the solution procedure to be sufficiently general and free from type restrictions, we first rearranged the original problem into a form suitable for a direct search. With all the numerical constants substituted, it can be stated as follows:

Globally minimize the objective cost function

$$F_0(\xi, T) \equiv 1\,750 V^{0.6} T^{0.6} + \frac{15\,000}{\xi^{0.6}} + \frac{6\,550}{\xi} \tag{13}$$

by choosing the two independent design variables ξ and T from the ranges

$$0 \leq \xi < 1 \tag{14}$$

$$485.4369 \leq T \leq 826 \tag{15}$$

and by satisfying the implicit inequality constraints

$$G_5(\xi, T) \equiv 1 + 2.76\xi - 0.00206T \geq 0 \tag{16}$$

$$G_{123}(\xi, T) \equiv \frac{T}{(63.8\xi)^{1/2}} - \max\left\{ \left[3.6 \times 10^{-4} T \left(1 + \frac{1}{\xi}\right) \right]^{1/2}, (0.85V)^{1/3} \right\} \geq 0 \tag{17}$$

where

$$V(\xi, T) = \frac{0.0362}{\xi} \int_0^{\xi} \frac{1}{f_e(x, T)} dx \tag{18}$$

$$f_e(x, T) = 55 \left(\frac{1 - x}{2 - x}\right)^2 \exp\left(-\frac{4\,770}{T}\right) - 1.4 \times 10^{-5} \left(\frac{x}{2 - x}\right) \exp\left(-\frac{19\,270}{T}\right) \tag{19}$$

In this reformulated problem, the constraint $G_5 \geq 0$ is equivalent to the thermal balance constraint $F_5 \leq 1$, while the constraint $G_{123} \geq 0$ amalgamates the three separate constraints $F_1 \leq 1$, $F_2 \leq 1$, and $F_3 \leq 1$ in the original formulation by eliminating d. The range (0, 1) for ξ follows from its definition. The lower bound for the temperature is the inlet feed temperature (485.44) obtainable by solving $G_5(0, T) = 0$; the upper bound (826) is equal to

$$T_u = \min[p_{41}^{-1}, T_m] = \min[826,\ 1\,825.24],$$

where T_m is the maximum adiabatic temperature satisfying

$$G_5(1, T_m) = 0$$

As the equilibrium extent of reaction ξ_e is nearly unity, it can be shown that $f_e(\xi, T) > 0$ for all possible combinations of ξ and T, and, therefore, it satisfies the requirement that the net reaction rate in a flow reactor must be strictly positive.

The variables V and d in the reformulated problem are strictly treated as dependent quantities. The volume V can be calculated from Equation (18) by using an approximate analytical expression or a numerical integration technique (see Appendix). The diameter d can always be recovered after a feasible optimal solution is found. Since the problem has only two independent variables ξ and T, any suitable global seeking method, even a simple grid search, should quickly find the true solution regardless of the type. All that is necessary is to repeatedly select a pair of (ξ, T) from the allowable ranges, calculate V, examine the solution in light of the constraints, and compare F_0 with the current best feasible solution. Actually, we used an efficient adaptive random search method which scanned the entire (ξ, T) plane in such a way that the thermal constraint (16) is always satisfied. The global solution was found in less than 2 s on an IBM 370/158 computer. We shall report the detailed workings of this adaptive random search method in another paper, as we are mainly concerned with the types of solutions here.

THE NECESSARY CONDITIONS FOR OPTIMALITY

As stated earlier, the solution obtained by the two-dimensional direct search is neither the type 1 nor the type 2 design, since both the thermal constraint (16) and the fluid mechanics constraint (17) are not tight. (Column 3 in Table 2 shows that the diameter d can be anywhere from 0.9955 to 154.17, and the function F_5 representing the thermal balance is not equal to 1.) This prompted us to reexamine the four optimality conditions derived by Wilde for the original problem.

The optimal conditions can be obtained by first defining a Lagrangian function

$$L \equiv F_0 - \sum_{i=1}^{6} \lambda_i(1 - F_i) \tag{20}$$

where λ_i are the multipliers. If we set

$$z\frac{\partial L}{\partial z} = 0 \tag{21}$$

where z represents V, d, ξ or T, we obtain the following four necessary conditions for optimality:

$(V)\quad \alpha t_{01} + \lambda_3 - \lambda_6 = 0$

$(d)\quad 2\lambda_1 - 2\lambda_2 - 3\lambda_3 = 0$

$(\xi)\quad -(\alpha t_{02} + t_{03}) + \lambda_1 - t_{21}\lambda_2 + (t_{51} - t_{53})\lambda_5 + [p_{61}V^{-1}f_e^{-1}(\xi, T) - 1]\lambda_6 = 0$

$(T)^*\quad \beta t_{01} - 2\lambda_1 + \lambda_2 + \lambda_4 + (t_{51} + t_{52})\lambda_5 - \lambda_6 p_{61} V^{-1}\xi^{-1}T^{-1}\int_0^{\xi} f_e^{-2}(x, T)\,[b_f r_f(x, T) - b_r r_r(x, T)]dx = 0$

* In Wilde's expression, the factor $p_{61}V^{-1}\xi^{-1}$ in the last term appears as a unity.

where t_{ij} is the abbreviation for the j^{th} term in the i^{th} F_i function [see Equations (1) through (7)]. It should be noted that a multiplier λ_i is nonzero if and only if the corresponding constraint is tight, that is, $F_i = 1$, and this observation has been utilized in simplifying the resultant expressions.

Applying the Kuhn-Tucker conditions ($\lambda_6 \neq 0$; $\lambda_i \geq 0$, $i = 1, 2, \ldots, 5$) in the subsequent analysis, Wilde (1974) correctly concluded that λ_6 must be strictly *positive* and that there are only two possible cases as far as λ_1, λ_2, and λ_3 are concerned: either they all vanish, or only λ_2 vanishes while λ_1 and λ_3 are strictly positive. The second case ($\lambda_1 > 0$, $\lambda_2 = 0$, and $\lambda_3 > 0$) thus gives rise to the type 2 design in which the constraints 1, 3, and 6 are active, since the corresponding multipliers λ_1, λ_3, and λ_6 are nonvanishing. However, the contention that the first case ($\lambda_1 = \lambda_2 = \lambda_3 = 0$) would automatically lead to the type 1 design in which, by definition, the constraints 4, 5, and 6 are active, that is, the corresponding multipliers λ_4, λ_5, and λ_6 do not vanish, appears to be invalid.

Wilde stated that "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." It is true that the condition (V) determines λ_6, that is

$$\lambda_6 = \alpha t_{01} > 0 \tag{22}$$

since the constraint 6 is an equality. It is also true that the conditions (ξ) and (V) determine λ_5 as

$$\lambda_5 = \frac{-[p_{61}V^{-1}f_e^{-1}(\xi, T) - 1]\alpha t_{01} + \alpha t_{02} + t_{03}}{t_{51} - t_{53}} \tag{23}$$

However, the first term in the numerator can be negative, and hence the right-hand side may vanish altogether. If λ_5 becomes zero, it will lead to a design which is neither of the type 1 nor of the type 2. This design, termed the type 3, is the solution which can be found by a direct search. By the same token, it can be shown that λ_4 may also become zero in some situations, even though it is "fixed by conditions (V), (ξ), and (T)." To verify these assertions, we calculated λ_5 and λ_6 for both the type 1 and type 3 designs by Equations (22) and (23). As can be seen in Table 2, $\lambda_5 = -50989.05$ for the type 1 design is negative, violating the Kuhn-Tucker condition that it be positive or zero. On the other hand, $\lambda_5 = +0.0031458$ for the type 3 solution is quite small. As it should be exactly zero, the small residual simply indicates that the convergence of the direct search was very slightly incomplete.

The values of λ_6, which represent the sensitivity of the objective cost function to the change in the reactor volume V, are also given in Table 2. We did not calculate λ_4, however, since the constraint 4 is active in both the type 1 and type 3 designs.

DISCUSSION

For further clarification, F_0 vs. ξ is plotted in Figures 1 and 2, in which the upper bound temperature T_u is treated as the parameter. At a relatively low value of T_u (Figure 1), the type 3 design is clearly the global solution; however, the difference between the value of the objective cost function of the type 1 design and that of the type 3 design becomes less as the upper bound temperature is allowed to increase. Figure 2 shows that at approximately $T_u = 1{,}285$, the loci of these two designs merge into one. At a higher temperature, the type 1 design becomes the global solution in which both the constraints 4 and 5 are active. However, when T_u becomes higher than 1522.7,

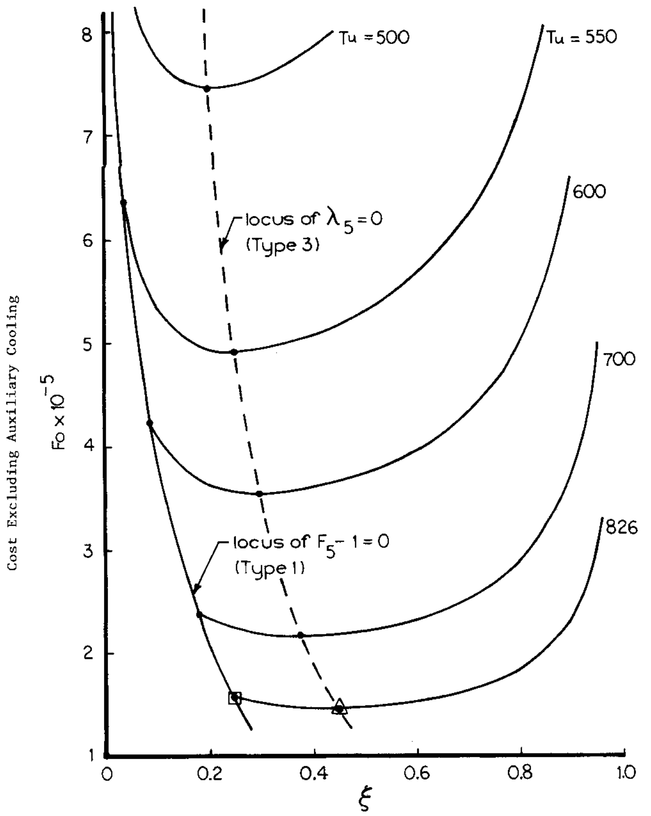

Fig. 1. A plot of F_0 vs. ξ (parameter T_u is the maximum allowable temperature).
At $T_u = 826$, F_0 for the type 1 design (⊡) is \$157 476.0 and F_0 for the type 3 design (△) is \$146 435.6.

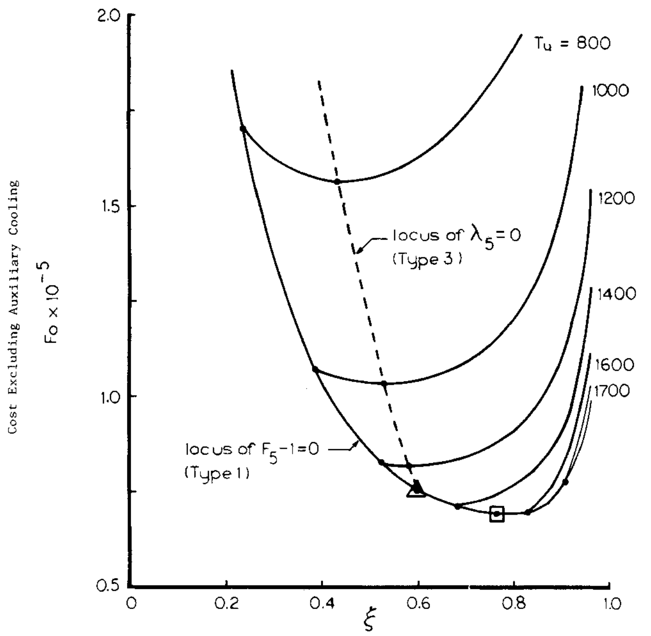

Fig. 2. A plot of F_0 vs. ξ (parameter T_u is the maximum allowable temperature).
△ Type 1 and type 3 designs merge at $T_u = 1285$.
⊡ Type 4 T = 1 522.7 and $\xi = 0.7741$.

another new type of design, which may be termed the type 4 design, emerges. In this design, the maximum allowable temperature constraint 4 is inactive ($\lambda_4 = 0$); the optimum reactor temperature is equal to 1522.7 for any value of T_u in the range between 1 522.7 and 1 825.24. The corresponding optimum value of the extent of reac-

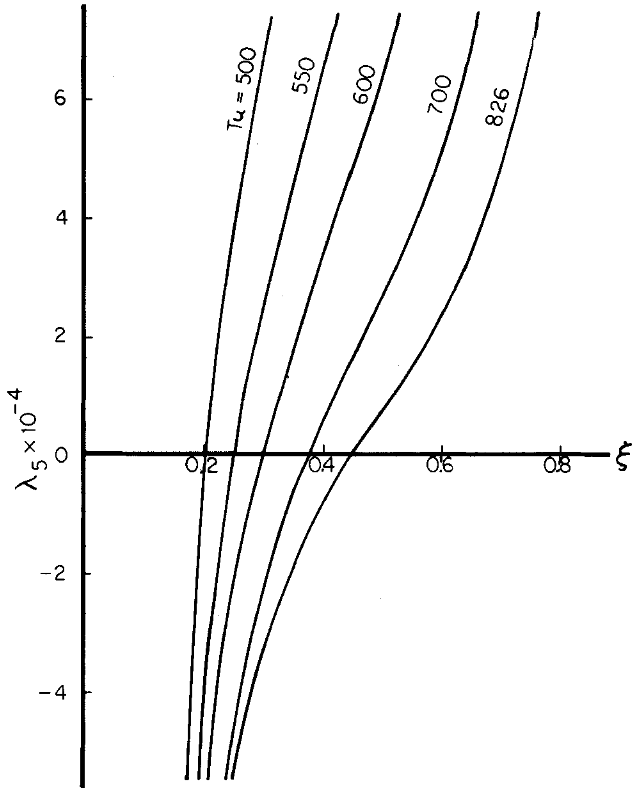

Fig. 3. A plot of λ_5 vs. ξ (parameter T_u is the maximum allowable temperature).

tion also remains constant at $\xi = 0.77411$ since the thermal balance constraint 5 is still active. Since the value of its objective cost function 69 623.50 is the lowest, the type 4 design is the overall optimum solution if the maximum allowable temperature can be set higher than the critical value of 1 522.7.

Figure 3 is a plot of λ_5 against ξ in the lower range of the parameter T_u. It can be seen that the variation of λ_5 to ξ is very large, and it vanishes at a unique value of ξ. Thus, for a given value of T_u, the corresponding type 3 design can alternatively be determined by setting the right-hand side of Equation (23) to zero and by solving the resultant equation by an iterative scheme, rather than by direct minimziation of the objective cost function F_0.

Although the type 3 design is seen to be the global solution at a relatively low upper bound temperature, actually a direct comparison with the type 1 solution in terms of the cost is somewhat meaningless. Since the thermal balance is not tight in the type 3 design, there is a need for cooling in the reactor system. As in the type 2 design of Wilde, which also requires cooling if the reaction is exothermic, the objective function for the type 3 design must be modified to account for the cost of an auxiliary cooler. A meaningful comparison can then be carried out; however, this is not specifically done here because the primary objective of this paper is to show that there can be a multitude of feasible design types to the minimization problem under consideration, and that the correct global solution can be readily obtained by a direct search procedure.

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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