Numerical Solution of an Optimal Temperature Problem

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ABSTRACT

This paper presents a computational study of the problem of finding the optimal temperature profile for a chemical reactor. Fixed-step gradient, steepest ascent and conjugate gradient methods are compared and the relative merits of various numerical integration techniques discussed.

Finally the control function is represented by a number of parametric forms and the problem tackled directly by hill-climbing.

I INTRODUCTION

A major difficulty arising in problems of system optimisation is the choice of a suitable technique to be used for solution. Present experience indicates that no single optimisation technique is superior to all others in the solution of even a few types of problem and that the choice of method depends on many factors, including the characteristics of the problem and, not least, the computing facilities available.

Among many techniques proposed, probably the two most successfully applied in recent years have been dynamic programming developed by Bellman[1] and the maximum principle derived by Pontryagin and his associates.[2] Computationally the former is more complex and requires a substantial amount of programming and computer storage, whereas the latter suffers from the inherent difficulties of a two-point boundary-value problem. Of the methods available to solve the boundary-value problem the application of gradient techniques leads to direct methods in the form of particularly simple algorithms with light demands on computer storage. Computational experience using fixed-step gradient techniques[3, 4, 5, 6, 7, 8, 9] has shown that this method is effective although the rate of convergence slows as the optimum configuration is approached.

Recently, problems of system optimisation have been tackled using a conjugate gradient technique[10,11,12*] which has been shown to have improved convergence properties, although the numerical examples used were generally of simple type. Overall, the amount of computational experience yet available using Pontryagin's technique in these ways on realistic problems is not substantial.

In this paper the fairly complex problem of determining the temperature profile in a chemical reactor to give optimum yield is used to compare the computational merits of the maximum principle in conjunction with fixed-step gradient, steepest ascent and conjugate gradient techniques. To provide further comparison the temperature profile is parameterised and the problem solved using a suitable hill-climbing technique: several forms for the control are assumed in this relatively little used method.

II PROBLEM FORMULATION AND METHODS OF SOLUTION

(A) *The general problem*

The process to be controlled is described by a set of non-linear differential equations of the form

$$\frac{d\mathbf{x}}{dt} = \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}) \qquad (1)$$

$$t_0 \leq t \leq t_f$$

$$\mathbf{x}(t_0) = \mathbf{a} \qquad (2)$$

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where $\mathbf{x}(t)$ is an n-dimensional vector of state variables whose initial values $\mathbf{a}$ are given at time t_0, and $\mathbf{u}$ is an m-dimensional vector of control variables.

A particular optimisation problem related to such a process might be one of finding a piecewise continuous control vector $\mathbf{u}(t)$, subject to the constraints

$$G_i(\mathbf{u}) \leq 0 \qquad i = 1,2,\ldots,m \tag{3}$$

which makes some objective function of the final values of the state variables, for example:

$$F = \sum_{i=1}^{n} \mu_i x_i(t_f) \qquad \mu_i \text{ constant} \tag{4}$$

a maximum or minimum having regard to the differential constraints and initial conditions in the state variables given in eqns. (1) and (2). t_f here is the final time.

(*B*) *Methods of solution*

The procedure using Pontryagin's maximum principle is to introduce an n-dimensional vector $\mathbf{p}(t)$ of adjoint variables satisfying the adjoint differential equations

$$\dot{p}_i = -\sum_{j=1}^{n} p_j \frac{\partial f_j}{\partial x_i} \qquad i = 1, 2, \ldots, n \tag{5}$$

where

$$p_i(t_f) = \frac{\partial F}{\partial x_i(t_f)} = \mu_i \tag{6}$$

(when F is as specified earlier).

Also introduced is the Hamiltonian function H defined by the expression

$$H(\mathbf{p}, \mathbf{x}, \mathbf{u}) = \sum_{i=1}^{n} p_i f_i(\mathbf{x}, \mathbf{u}) \tag{7}$$

If the control vector $\mathbf{u}$ is subject to constraint, then according to Pontryagin the set of necessary conditions for a maximum (minimum) of the objective function F are the state and adjoint eqns. (1, 2) and (5, 6) together with the requirement

$$\max_{u \in R} \left\{ H = \sum_{i=1}^{n} p_i f_i \right\} \tag{8}$$

This last condition means that $\mathbf{u}$ must be chosen to maximise (minimise) H either directly from the equation

$$\frac{\partial H}{\partial u_j} = 0 \qquad j = 1, 2, \ldots, m \tag{9}$$

if $\mathbf{u}$ is within the region R of admissible control, or by inspection of its values on the boundaries of R. In either case the $\mathbf{u}$ selected is that which determines the greatest (least) H.

In order to determine the optimal solution to the system by this method a two-point boundary value problem is encountered since the boundary conditions on the adjoint variables $\mathbf{p}$ are known at the end of the time interval in eqn. (6) while those for the state variables are known at the start (eqn. (2)). The major numerical difficulty in the subsequent solution arises here due to the instability of one or the other of the sets of state or adjoint differential equations when integrated in the required direction.

This is avoided by using gradient techniques which allow the integration of both sets in their respective stable directions of increasing time. This modified approach does not attempt to satisfy the coupling eqn. (9) or its equivalent directly but proceeds by solving a sequence of non-optimal problems with the property that each successive solution leads to an improved value of the objective function. More specifically, the technique performs iterations on the control function which is initially selected arbitrarily so that the condition for optimality is not satisfied.

For this type of method a direct search is made for the extreme value of the objective function. The computational scheme involving three types of gradient technique is described below.

(*C*) *Algorithm for modified methods*

In this scheme[10] a single control function $u(t)$ is assumed ($m = 1$); the algorithm is easily extended to the multicontrol case.

An arbitrary starting control $u = u_0$ is selected, then,

$$g_0 = \left\{ \frac{\partial H}{\partial u} \right\}_{u=u_0} = g(u_0) \tag{10}$$

and

$$s_0 = -g_0 \tag{11}$$

is the first direction for search. These equations hold at each time step and the discretisation involved is discussed (for a specific problem) in Section III.

In this, and subsequent directions s_k, a step θs_k is taken. The value of s_k may be

(i) fixed in value
or (ii) chosen to minimise $F(u_k + s_k s_k)$.

The $(k+1)$th approximation to the optimal control is then formed from

$$u_{k+1} = u_k + s_k s_k \tag{12}$$

So that

$$g_{k+1} = g(u_{k+1}) \tag{13}$$

with the next search direction from

$$s_{k+1} = -g_{k+1} + \beta_k s_k \tag{14}$$

where

$$\beta_k = \frac{(g_{k+1}, g_{k+1})}{(g_k, g_k)} \tag{15}$$

and

$$(g_k, g_j) = \int_{t_0}^{t_f} g_k(t) g_j(t)\, dt. \tag{16}$$

The search directions s_{k+1} computed via the gradient norms β_k constitute conjugate directions and represent the basis of a conjugate gradient method. Setting $\beta_k = 0$ recovers the method of steepest descent from the algorithm. Both techniques utilise steps ε_k as defined in (ii) of the stepping procedure whereas choice of ε_k as in (i) realises the fixed-step gradient scheme.

In the conjugate gradient/steepest descent techniques the choice of suitable linear search routine is an integral and important part of the overall computational scheme. In the fixed-step gradient approach choice of step-size is critical with respect to computing time. These points are discussed with the computational considerations of section IIIB.

(D) Parameterisation of control

The procedures necessary to deal with the two-point boundary value problem may also be avoided if, for example, sufficient knowledge is available concerning the form of the control variable. In particular, if the control can be represented by a suitable function then the performance index will in turn depend on the parameters involved in this function. The position then becomes one of optimisation of the performance index with respect to the parameters and may be tackled by a hill-climbing method.

An obvious drawback is the problem of providing a suitable form for the control—quite apart from the probable greater computation required especially when the number of parameters involved is large.

For the problem considered in Section III (Optimal temperature profile in a chemical reactor) the nature of the reaction scheme is such that a falling temperature profile from inlet to outlet would be expected for optimum yield; there will also be an optimal final or contact time.[3]

One significant feature of this method is the convenient manner in which variable final time may be considered by simply creating an additional parameter which is adjusted, with the other parameters involved, by the optimising routine. Several forms for the temperature profile were assumed (a selection of which are described in Appendix I) and the variable final time facility was incorporated in two of these.

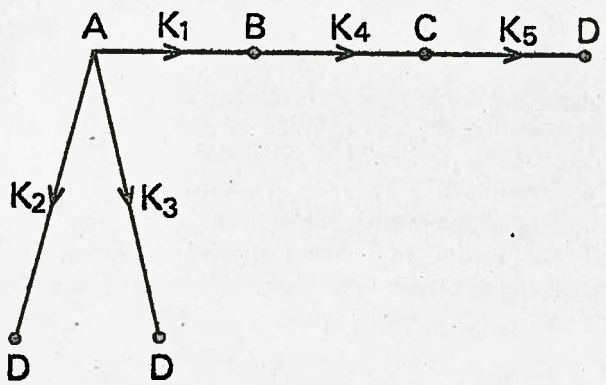
The optimising routine used was that due to Rosenbrock, which allows for constraints on the parameters involved—a necessary facility for the problem considered since, from physical considerations, the temperatures along the reactor were constrained to be $\leq 550°C$ at all times. The Rosenbrock scheme is described fully in Refs. 3 or 13.

III IMPLEMENTATION OF THE ALGORITHM

(A) Numerical example

The specific problem considered here was first investigated computationally by Rosenbrock and Storey.[3] Their work suggested the promising nature of the fixed-step gradient scheme and this is investigated further with, in addition, a comparison with the steepest ascent and conjugate gradient techniques and the method using parameterised control.

The reaction scheme is shown below



and is assumed to take place in a tubular reactor under plug flow conditions.

The concentrations of the feed material A, the required yield C and intermediate product B are denoted by x_1, x_3 and x_2 respectively; D is a waste product. With this notation, eqns. (1) and (2), which are the kinetic equations for this system become

$$\dot{x}_1 = -(k_1 + k_2 + k_3)x_1$$
$$\dot{x}_2 = k_1 x_1 - k_4 x_2$$
$$\dot{x}_3 = k_4 x_2 - k_5 x_3$$

with initial conditions at time $t = 0$,

$$x_1 = 1, \quad x_2 = 0, \quad x_3 = 0$$

The kinetic rate constants k_i, $i = 1, 2, \ldots, 5$ in these

equations are exponentially dependent on temperature and hence on time.

In this form, the problem is one of estimating a temperature profile $T(t)$ along the length of the reactor so as to provide maximum yield x_3 at final time t_f. From practical considerations of catalyst stability, the temperatures are constrained $\leq 550°C$.

The set of adjoint differential eqns. (5) and (6) for this example are

$$\begin{aligned} \dot{p}_1 &= (k_1 + k_2 + k_3)p_1 - k_1 p_2 \\ \dot{p}_2 &= k_4(p_2 - p_3) \\ \dot{p}_3 &= k_5 p_3 \end{aligned} \tag{19}$$

with end conditions

$$p_1(t_f) = 0, \qquad p_2(t_f) = 0, \qquad p_3(t_f) = 1 \tag{20}$$

From these, and the kinetic equations, the gradient trajectory g of eqn. (13) is

$$\begin{aligned} g = \frac{\partial H}{T} = \frac{1}{RT^2}\{&-(k_1E_1 + k_2E_2 + k_3E_3)x_1p_1 \\ &+ k_1E_1x_1p_2 - k_4E_4x_2(p_2 - p_3) \\ &- k_5E_5x_3p_3\} \end{aligned} \tag{21}$$

In the particular case of fixed-step gradient, ε_k has a fixed value, say ε, and eqn. (12) of Section IIC becomes

$$T_{k+1} = T_k + \varepsilon \frac{\partial H_k}{\partial T_k} \tag{22}$$

where the step is taken in the direction of the positive gradient.

For the steepest ascent and conjugate gradient schemes the step ε_k chosen at each new direction of search s_k is that which maximises $x_3(T)$

$$i.e. \qquad x_3\left(T_k + \varepsilon_k \frac{\partial H_k}{\partial T_k}\right) \tag{23}$$

The fundamental idea involved is that T_k, x and p and hence $\partial H/\partial T$ are all specified at the time previous to when T_{k+1} is required and thus the computation of the optimal temperature profile does not involve the solution of the necessary coupling eqn. (9) or its equivalent. Whenever the value of T at any point along the reactor, as computed from eqn. (22), exceeds 550°C it is set at that value. (In the case of conjugate gradient schemes this can, of course, destroy the conjugacy property.)

(B) Computational considerations

Several factors having considerable influence on the efficiency of the computational solution of the problem discussed in IIIA were considered and are discussed briefly here. (It is worth noting at this stage that had our only interest been in the solution of this particular problem, and not in comparison of the various techniques, the special nature of the state and adjoint equations could have been used to simplify computation.)

(i) Integration routine

The state and adjoint differential equations required a numerical method of solution, and of course the efficient solution of this part of the problem (performed many times) was highly important. The main factors influencing the choice of technique included accuracy, the absence of strongly unstable characteristics and reasonable simplicity leading to speed of computation. Three methods were used—trapezoidal, Runge-Kutta and a predictor-corrector scheme due to Hamming—all of which performed favourably. However, the Runge-Kutta fourth order method had the best overall qualities and in the problem considered reliable results were obtainable at a fairly coarse integration interval—thus saving computer time; typically, computation using this method was possible with an integration step some four times the size of that using the trapezoidal scheme to obtain similar accuracy. The method required no special starting procedure, it involved light demands on storage, and was ideally suited for automatic computation since a straightforward procedure was repeated several times. No problems of instability were encountered. (For details of acual step sizes, termination procedures, etc., see Ref. 18.)

(ii) Linear search

In the application of the steepest ascent and conjugate gradient techniques, the problem of maximising a function along a one-dimensional curve must be solved several times during the solution of the main problem. This linear search can, therefore, occupy a large proportion of the total time for the solution of the problem and should obviously be as efficient as possible. Some suitable balance should however be struck between the accuracy and required computation for a given scheme; the gain in accuracy implied by fitting a high order polynomial may be outweighed by excessive computation time due to complexity of form.

One scheme used in Ref. 10 is that proposed by Davidon and described by Fletcher and Powell.[14] This scheme involves a cubic fit but requires estimates of the first derivatives of the

function which were not available for the problem described in IIIA.

A common practice is the use of a quadratic fit to the function, and two variations of this idea were used here. In the first, the step was kept constant and when a reduction in the objective function was achieved the quadratic fit was taken through the last three points and the maximum located analytically. In the second method the technique adopted was one of starting with a nominally small step and doubling until a reduction in the objective function was achieved. At this stage a half-step back was taken and the maximum 'boxed in' with the three points much closer together. This method is as described by Swann[15] and increases the accuracy of the interpolation without increasing the number of function evaluations required. A disadvantage found was that the steps could become very large.

(iii) Choice of step size and starting configuration

The considerations involved here are discussed in some detail by Merriam[16] for example. For satisfactory behaviour of the gradient processes the step should be small enough to substantiate neglect of all but first order terms in the theory. However, with a small step there can be an intolerably slow rate of convergence which can seriously limit the efficiency of the method. Therefore, some compromise is seen to be necessary to satisfy both the condition that the objective function should show improvement and also that this improvement should be sustained at a substantial rate. It would appear that this compromise must be effected separately for each individual problem tackled by these methods. For the numerical problem considered in Section III the behaviour of the various methods under a comprehensive range of fixed-step sizes (starting step sizes when considering the step-doubling search technique) was noted. Although this procedure can be wasteful of computer time, experience from early results indicated trends which enabled certain definite reductions to be made in the later computations for all the methods considered. (See Ref. 18.)

For each method, using such a predetermined efficient step size, results were obtained from several different starting configurations including those remote from the apparent optimum. This not only served to give a check on the reliability of the optimum result but also tested the versatility of each method with regard to overall reliability of performance.

IV RESULTS AND DISCUSSION

(A) Solution of the problem

Consistent solutions to the numerical example were obtained by each of the four methods used. Typically, a yield of 43¾% was achieved at a contact time of 1 sec and an associated temperature profile constrained at 550°C c[illegible]ome 12–13% of the reactor's length at the inlet a[illegible] falling to 350° at the outlet. Typical growth of yield and temperature is

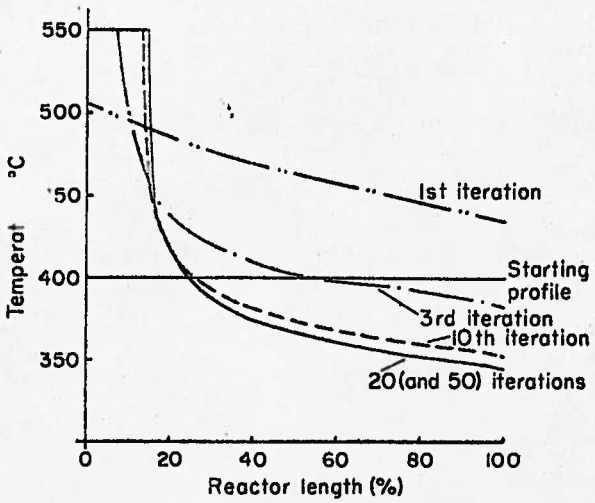


Fig. 1. Progressive changes in temperature profile.

shown in Figs. 1 and 2. Increases of the order of 1% in yield were obtained by substantial increase in contact time and associated changes in temperature profile—whether such increases would be worthwhile in practice would depend on many factors. Among the results were those which were the best achievable consistent with restrictions implied by the method used. In particular (see next section) the

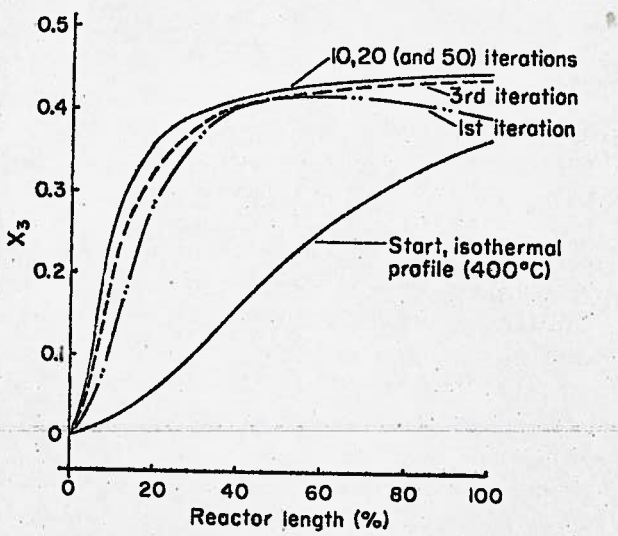


Fig. 2. Progressive growth of yield.

method of parametric representation of the temperature profile gave best temperature profiles of given assumed form (*e.g.* linear) and the yields associated with these.

(B) Performance of the methods

(i) Gradient method

The method was relatively easy to program and required the least storage compared with the other gradient techniques. The best yield using this method was consistently 43·7%, and the associated temperature profile is shown in Fig. 1. In attaining this yield the proportion of inlet temperatures under constraint was critical. The characteristics of the problem solved by this method made increases in search step-sizes tolerable with associated reductions in computing time (see Fig. 3). With large steps the same

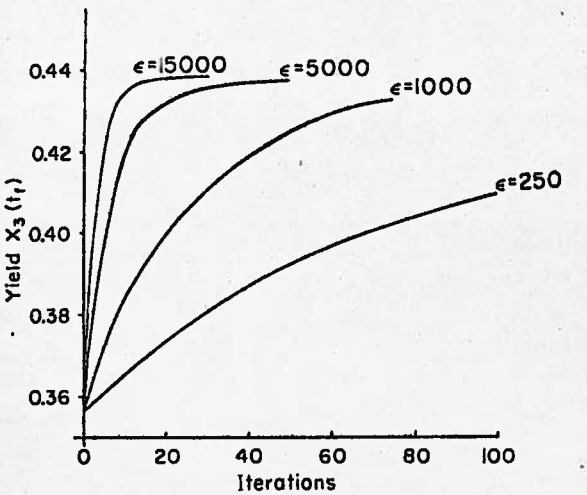


Fig. 3. Effect of ϵ on yield.

yield and profile were recoverable in as few as ten iterations, and under these extreme conditions the method produced the fastest solution of all. Predictably, for this problem, the method was not a good one when used from starting conditions remote from the optimum, nor was it convenient to incorporate variable contact time although interesting trends were established by varying this quantity separately.

(ii) Steepest ascent

This involved substantially more programming mainly because of the linear search technique required. Two types of linear search were used, one at constant step throughout, the other using step-doubling from a nominal starting value, although both used a quadratic fit to the local maximum. The search with step-doubling was faster for the problem considered here.

Results using the gradient method were confirmed, not only from identical starting conditions, but also from a wide range of other starting configurations, including those remote from the optimum—the steepest ascent technique was particularly versatile in this respect (see Table 1).

TABLE 1

PERFORMANCE OF STEEPEST ASCENT METHOD FROM DIFFERENT STARTING PROFILES USING A LINEAR SEARCH WITH STEP-DOUBLING

Starting Temperature °C	*Starting Yield*	*Final Yield*	*Number of Steps*	*Final Yield*	*Number of Steps*
10	0	0·437	77	0·438	82
100	0	0·437	53	0·438	65
200	0·001	0·437	52	0·438	76
300	0·054	0·437	47	0·438	70
400	0·357	0·437	34	0·438	60
500	0·331	0·437	47	0·438	78

Again, as in the case of the fixed-step gradient method, a considerable reduction in computing time was achieved by increase of step size in both types of linear search, although this reduction was greater when the linear search with step-doubling was being used. The computing time to the optimum configuration using either of the linear searches was less than in the fixed step gradient method under almost all conditions considered. A typical comparison under fixed-step conditions for a 400°C isothermal starting profile is given in Table 2.

TABLE 2

ITERATIONS TO 0·437 YIELD; 400°C ISOTHERMAL STARTING PROFILE

Time per Iteration (sec)	2·4	2·0	2·1
$\epsilon(\times 10^{-3})$	*Gradient*	*Steepest Ascent*	*Conjugate Gradient*
2·5	76	77	52
5·0	38	39	27
10·0	19	22	—

(iii) Conjugate gradient

A further numerical technique was necessary here to estimate the norm of each gradient trajectory. Both Simpson's rule and a high accuracy Newton-Cotes formula were used, the former being generally sufficiently accurate provided an appropriate integration step was used. (For full details see Ref. 18.)

The additional programming required over that for the method of steepest ascent was small and there was a corresponding increase in

computing time per iteration and computer storage requirement.

The method worked well in conjunction with the linear search at constant step so long as a relatively small step was used; results at this stage were produced more quickly than any other method under comparable conditions. This is illustrated in Fig. 4 and Table 2. With

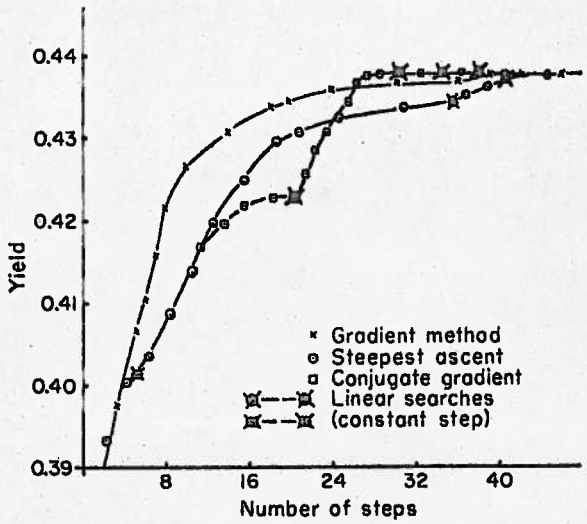


Fig. 4. Progress to final yield (Isothermal starting profile 400°C).

longer search steps and also when using the search with step-doubling from a nominal starting size the method brought a greater proportion of the temperatures at the reactor inlet under constraint early in the computations with correspondingly lower yield; recovery from this state was generally not possible and at best extremely slow (see Table 3

TABLE 3

PERFORMANCE OF CONJUGATE GRADIENT METHOD FROM DIFFERENT STARTING PROFILES USING A LINEAR SEARCH WITH STEP-DOUBLING

Starting Temperature °C	*Starting Yield*	*Yield after*		
		25 steps	*50 steps*	*100 steps*
100	0	0·005	0·373	0·373
200	0·001	0·408	0·410*	—
300	0·054	0·437	0·437	0·437
400	0·357	0·423	0·432	0·432
500	0·331	0·430	0·433	0·435

* Constraint not reached.

compared with Table 1). This again emphasises the delicate relationship between the proportion of inlet region under constraint and the yield, in the optimum state. A factor detracting rather from the overall performance of this method was the rather approximate nature of the method for determining directions of search except when in the vicinity of the optimum. Away from this vicinity, directions generated were often inferior to those of steepest ascent and, at positions remote from the optimum, perhaps not even directions of ascent. Starting from these latter regions the method was often quite unworkable (again see Table 3)—this diminished effectiveness is perhaps the penalty to be paid for the computational simplicity. Any more accurate determination of directions in this method would appear to result in very substantial increases in complexity and computation,[11,12] particularly when adapted to complex problems. (Poor directions can also arise through the imposition of constraints.)

(iv) Non-gradient method

In this method, with parameterised temperature profile, the optimum configuration was approached by direct search. Computation under various conditions confirmed that computer time was greater than that required in the implementation of Pontryagin's maximum principle in conjunction with the several gradient techniques.

Several distinct assumptions as to the form to be taken by the temperature profile led to different final temperature profiles with associated differing yields lower in value than those achieved by the other methods—see, for example, Figs. 5 and 6. However, previous consistent results were again confirmed when other initial assumptions as to the profile form,

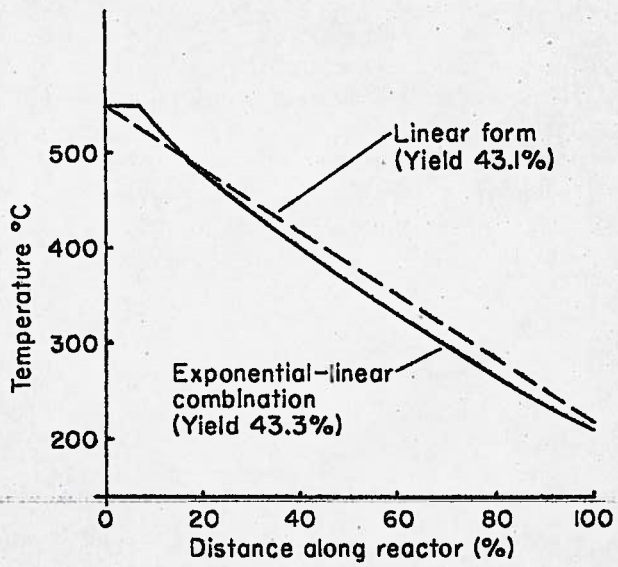


Fig. 5. Comparison of final profiles (400°C isothermal starting profile).

for example the discrete temperature profile, gave a final temperature profile and reactor yield approximating to those realised by the various gradient techniques (see Fig. 7).

The method worked reasonably well from several different starting profiles but some difficulty was experienced starting from profiles

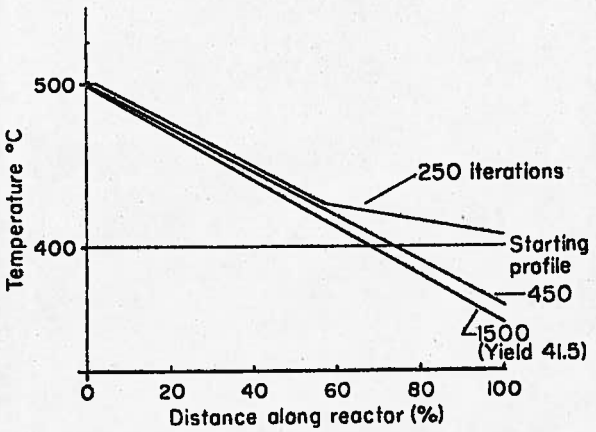


Fig. 6. Progressive changes in profile—three straight line assumption.

remote from the optimum configuration. A useful feature of this method is the ease with which variable final (or contact) time may be incorporated as just another parameter even though considerable additional computation may be necessary to produce results. These results suggested that different temperature profiles determined different contact times. This

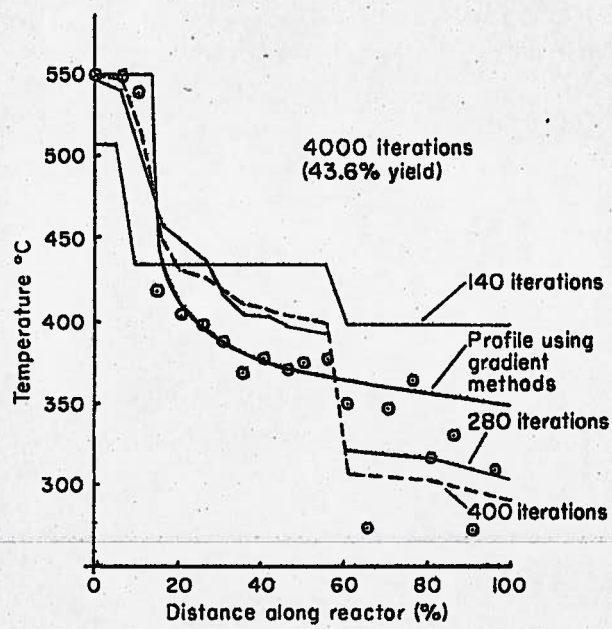


Fig. 7. Progressive changes in profile—discrete temperatures assumption. Starting profile 400°C isothermal.

may perhaps be explained by the fact that the hill-climbing technique is forced to act within the framework set up by the assumed control form, and therefore theoretically should give the best control of a type. If the form assumed is substantially flexible then one evidently has more opportunity of attaining the best overall control form—this was shown to be the case in the results obtained here.

V CONCLUSION

In this work, all of the methods used produced consistent results, and each had certain advantages to offer, but none exhibited overall superiority to the others on the problem considered.

Taking into account ease of programming, numerical techniques required, convergence rate and overall versatility the maximum principle in conjunction with the method of steepest ascent was slightly better on average for the problem considered than any other method. However, it is obviously unwise to generalise on this conclusion with respect to other problems.

The characteristics of the numerical example considered here made it possible, by various means, to considerably reduce computing times. One likely generalisation, whatever the characteristics of other problems, is that computing times can be reduced by appropriate choice of optimisation and numerical techniques; the uncertainties involved in these choices will lessen as computational experience grows.

The possibility of a multi-purpose computer program to deal with the problem of system optimisation has already been explored[17] but the writers have no evidence to hand on the success or otherwise of this project.

APPENDIX I

Parameterised form of temperature profile

Several assumptions were made concerning the form of the temperature profile $T(t)$ along the reactor. To summarise, these were:

(i) a simple profile in which the temperature varied linearly from inlet to outlet. In this form the temperature variation with time t along the length of the reactor was given by

$$T = a_2 - a_1 t$$

a_1 and a_2 being the two parameters involved.

(ii) a profile in which the temperature was constant over a variable region at the inlet followed by exponential reduction to the outlet. This combination was possible in terms of three parameters a_1, a_2 and a_3 where,

$$T = a_1, \qquad t \leq a_2$$
$$T = a_1 e^{a_3(t-a_2)}, \quad t \geq a_2$$

Here a_2 was the variable point of intersection of the two forms.

(iii) a profile consisting of the combination of three straight lines, two having variable slope. Now

$$T = a_1, \quad t \leq a_2$$
$$T = a_1 + a_2 a_3 - a_3 t, \quad a_2 < t \leq a_4$$
$$T = a_1 + a_2 a_3 + a_4(a_5 - a_3) - a_5 t, \quad t > a_4$$

where a_1 is the intercept, a_2 and a_4 variable points of intersection, and a_3 and a_5 the variable slopes. The number of parameters was now five.

(iv) a form was then considered in which the discrete temperatures at selected points along the reactor were themselves chosen to be the parameters involved,

$$i.e. \qquad T = a_i \qquad (i = 1,2, \ldots, n).$$

One difficulty here was the compromise necessary between burdening the optimising routine with too many parameters and having an inadequate description of the profile with too few.

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RÉSUMÉ

Le présent article étudie par voie numérique le problème de la recherche du profil optimal de température dans un réacteur chimique.

Diverses méthodes d'optimisation (méthode du gradient à pas fixé, méthode de la plus grande pente, méthode des gradients conjugués) sont comparées entre-elles et on discute les avantages relatifs de plusieurs techniques d'intégration.

Enfin, les auteurs donnent une représentation paramétrique de la fonction de contrôle et résolvent le problème par la méthode directe.

ZUSAMMENFASSUNG

In einer Untersuchung mittels eines Elektronenrechners wird die Frage nach dem optimalen Temperaturverlauf in einem chemischen Reaktor behandelt. Es werden die Verfahren mit stufenweisem Gradienten, steilstem Anstieg und konjugierten Gradienten miteinander verglichen und die Vorteile verschiedener numerischer Integrationsverfahren erörtert. Schließlich wird die Kontrollfunktion durch eine Anzahl parametischer Formen dargestellt und die Frage direkt durch Bergsteigen angegangen.