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TITLE: NUMERICAL DETERMINATION OF TEMPERATURE PROFILES IN FLOWING SYSTEMS FROM CONVERSIONS OF CHEMICALLY REACTING TRACERS

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NUMERICAL DETERMINATION OF TEMPERATURE PROFILES IN FLOWING
SYSTEMS FROM CONVERSIONS OF CHEMICALLY REACTING TRACERS

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ABSTRACT

This study presents the mathematical bases of the measurement of internal temperatures within flowing systems using chemically reacting tracers. It considers plug-flow (or piston-flow) systems. The differential equation for reactant conversion can be reformulated into a Fredholm integral equation of the first kind. In the Fredholm integral equation the unknown is the temperature distribution function, which characterizes the internal temperature profile of the flowing system. Due to nonlinearity of the kernel, the usual technique of regularization has been modified into an iterative approach. This new approach is employed to solve this Fredholm integral equation. The iterative approach successfully overcomes the usual difficulty of determining the optimal value of the regularization smoothing parameter. Advantages and disadvantages of this method are discussed, and the results are compared with those obtained by optimization of undetermined parameters in a postulated temperature distribution function. The insight acquired from this study can be used to determine temperature profiles for many existing systems, and can form a basis for analysis of the more complicated dispersed-flow systems.

The iterative Fredholm integral equation method is tested to see what is required to discriminate between two models of the temperature behavior of Hot Dry Rock geothermal reservoirs. It is found that using as few as two reacting tracers can distinguish between the models and provide a reasonable approximation of the temperature profile within a reservoir.

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INTRODUCTION

There are many flowing systems whose internal temperature characteristics affect their behavior significantly. Some important examples are continuous chemical reactors, aquifers, nuclear waste storage sites and geothermal reservoirs. For example, in Los Alamos National Laboratory's Hot Dry Rock geothermal energy program (Murphy et al., 1981), the measurement of temperature patterns in the regions between the wells will be a principal tool in predicting the life of the reservoir. The use of direct temperature probes within this system is impractical, and it would be beneficial if an indirect technique could be devised. It has been proposed to measure these temperatures using chemically reacting tracers (Brown et al., 1984; Robinson et al., 1984). A pulse of chemically reacting tracers, injected from one well, encounters different temperatures on its way to the other well(s). It is shown in this study that the temperature profile experienced by the pulse can be extracted from the extents of the conversions of different tracers.

THE PRINCIPAL EQUATIONS

For simplicity, in this paper it is assumed that the reacting tracers undergo first order reactions. The derivation of equations will need appropriate changes if the tracers follow a rate law different than the first order law. However, the general principles developed here can be used for other rate laws without any major modifications, as long as the expression for the reaction rate consists of two separate parts, a temperature-dependent part and a concentration-dependent part.

Consider a segment of fluid traveling along a particular flow path, and encountering different temperatures along its way. If chemically reacting tracers are added to the flow, the changes in the concentrations of the tracers are governed by

$$q \frac{dC_i}{dV} = -A_i e^{-E_i/RT} C_i, \quad (1)$$

for a constant density plug-flow system, where i denotes the i 'th tracer (all symbols are defined in the nomenclature). The integration of this differential equation with appropriate limits yields the following equation :

$$-\frac{q}{A_i V_s} \ln \left[\frac{C_{if}}{C_{io}} \right] = \int_{\xi=0}^1 e^{-E_i/RT} d\xi \quad (2)$$

where ξ is the dimensionless volume fraction (V/V_s), similar to the dimensionless reactor length in chemical reactor theory. The dimensionless group which composes the LHS of eqn(2) is equivalent to the ratio of the system average of the reaction rate constant to the

reaction rate constant which would exist if the temperature were infinitely high throughout the flowing system.

From the inlet and exit values of the concentrations, the LHS of eqn(2) can be computed for each tracer. Let us denote this quantity by $g(E_i)$. In order to determine the temperature profile, i.e., T as a function of ξ , from the observed values of $g(E_i)$, the integral equation (2) has to be inverted. In its current form, however, eqn(2) involves a nonlinear term, $\exp[-E_i / RT(\xi)]$, which makes its inversion difficult. The problem can be made amenable to standard numerical methods by reducing eqn(2) to a Fredholm integral equation of the first kind, i.e. $g(x) = \int K(x,y) f(y) dy$, using the following method.

An initial estimate of the temperature profile is assumed, $L_0(\xi)$, and a fractional deviation of $L_0(\xi)$ from $T(\xi)$ is denoted by $\epsilon(\xi)$, i.e., $\epsilon(\xi) = [T(\xi) - L_0(\xi)] / L_0(\xi)$. The nonlinear term $\exp[-E_i / RT(\xi)]$, can be expanded in terms of $L_0(\xi)$ and $\epsilon(\xi)$:

$$\exp\left(\frac{-E_i}{RT(\xi)}\right) = \left[\exp\left(\frac{-E_i}{RL_0(\xi)}\right) \right]^{\frac{1}{1+\epsilon(\xi)}} \approx \left[\exp\left(\frac{-E_i}{RL_0(\xi)}\right) \right]^{1-\epsilon(\xi)} \quad (3)$$

Expanding the exponential term in a Taylor series and neglecting all the terms higher than or equal to $\epsilon^2(\xi)$ leads to

$$\exp\left(\frac{-E_i}{RT(\xi)}\right) \approx \exp\left(\frac{-E_i}{RL_0(\xi)}\right) \left[1 + \frac{\epsilon(\xi) E_i}{RL_0(\xi)} \right]. \quad (4)$$

After substituting eqn(4) into RHS of eqn(2), integration of eqn(2) leads to

$$-\frac{q}{A_i V_s} \ln \left[\frac{C_{if}}{C_{id}} \right] - \int_{\xi=0}^1 \exp\left(\frac{-E_i}{RL_0(\xi)}\right) d\xi = \int_{\xi=0}^1 \frac{E_i}{RL_0(\xi)} \exp\left(\frac{-E_i}{RL_0(\xi)}\right) \epsilon(\xi) d\xi \quad (5)$$

Eqn(5) is in the form of a Fredholm integral equation of the first kind, and can be solved. Thus, for an assumed temperature profile $L_0(\xi)$, solution of eqn(5) yields $\epsilon(\xi)$. Since $\epsilon(\xi)$ is a fractional deviation of $T(\xi)$ from $L_0(\xi)$, the initial estimate of the temperature profile can be modified,

$$L_1(\xi) = L_0(\xi) [1 + \epsilon(\xi)],$$

to obtain a new estimate of the temperature profile. This iterative procedure can be continued until the norm of $\epsilon(\xi)$ becomes sufficiently small.

SOLUTION PROCEDURE

A Fredholm integral equation of the first kind has the form

$$g(x) = \int_{y=a}^b K(x,y) f(y) dy, \quad c \leq x \leq d, \quad (6)$$

where g is a function of the experimental variable x , the kernel K is a known representation of the experimental system and procedure, and f is a distribution function of an intrinsic system variable y . In our application, the experimental variable is the activation energy E_i . For an assumed temperature profile, $L_o(\xi)$, the LHS of eqn(5) depends only on E_i , whereas the kernel in that equation is a function of both E_i and the intrinsic system variable, ξ . The desired distribution function, $\epsilon(\xi)$, depends solely on the intrinsic variable.

The unknown in a Fredholm integral equation is usually the distribution function $f(y)$. The solution minimizes locally the integral

$$I = \int_{x=c}^d \left[g(x) - \int_{y=a}^b K(x,y) f(y) dy \right]^2 dx . \quad (7)$$

Unfortunately, when a Fredholm integral equation of the first kind is attacked directly to obtain $f(y)$, chaotic solutions are obtained (e.g., Allison, 1979). This is due to the ill-posedness of the problem (cf. Wing, 1984), which tends to cause $f(y)$ to change by a large margin when small variations occur in the experimentally observed $g(x)$. One way to resolve this difficulty, known as regularization (Tikhonov and Arsenin, 1977), has been the addition to eqn(7) of a stabilizing term $\alpha G(f)$, where $G(f)$ is a nonlinear differential operator on $f(y)$ with nonnegative coefficients. This term has the effect of smoothing the solution for $f(y)$. The value of α depends on the degree of smoothness desired. If the value of α chosen is too large, then the solution may be over-smoothed and valuable information may be lost. On the other hand, if the chosen α is too small, then spurious peaks may appear in the solution. In fact, choosing the proper value of α is critical to the success of the regularization approach (Miller, 1974). Unfortunately, no adequate criterion presently exists for choosing the optimal α (Brown and Travis, 1984).

The iterative approach used in this study avoids the difficulty of choosing an optimal value of α in the regularization process. In each iteration, a few values of α , significantly greater than the optimal value are used. This avoids spurious peaks in the solutions. Using this approach, the "best" solution is approached as a limit to the iteration process. This approach is computationally efficient; although it is an iterative process, at each iteration it solves the problem for only a few values of α .

In this study, a first order stabilizing term is employed, i.e., $G(f)$ is chosen to be

$$\int_{y=a}^b \left[q_0 f^2(y) + q_1 (df/dy)^2 \right] dy.$$

In the regularization approach, the sum of the residual I [given by eqn(8)] and the stabilizer $\alpha G(f)$ is minimized. The necessary condition for this minimization can be obtained by calculus of variations (see Britten et al., 1983 for details). It may be noted that the use of

the first order stabilizer emphasizes continuity of $f(y)$ as well as its first derivative in the final solution.

RESULTS AND DISCUSSION

All modeling reported in this study has been carried out in the following manner. A temperature profile $T(\xi)$ is first postulated. The three temperature profiles employed in this analysis are :

$$\text{Profile A : } T(\xi) = 500 + 150 [1 - \exp(-5\xi)]$$

$$\text{Profile B : } T(\xi) = 500 + 150 [1 - \exp\{-[0.5 / (1-\xi)]^4\}][1 - \exp(-5\xi)]$$

$$\text{Profile C : } T(\xi) = 500 + 150 [\beta_1 \xi \exp(-\beta_2\xi)].$$

Profile A has the characteristic shape exhibited by an adiabatic tubular reactor with an exothermic reaction. It also reflects one type of temperature profile exhibited by a Hot Dry Rock geothermal reservoir. Profile B has characteristics of another type of Hot Dry Rock reservoir, with about half its potential thermal energy extracted. Profile C has the temperature characteristics of a tubular reactor with an exothermic reaction which also has cooling at the wall. This profile exhibits a peak, and it is mainly used to test the applicability of the proposed iterative method to such profiles. The values of β_1 and β_2 were appropriately chosen to provide reasonable profiles, each with a maximum temperature of about 650 K.

After selecting the temperature profile, the RHS of eqn (2) is evaluated for n different activation energies in a given range. The experimental data vector consisting of $g(E_i)$ is simulated by adding a specified degree of random error to each of these n data points. In all simulations in this study, a grid of 20 points of ξ is used to put the system equation into discrete form. Then the appropriate Fredholm integral equation is solved to obtain the desired temperature profile, which is compared with the originally assumed temperature profile.

The main focus of this study is distinguishing between Profiles A and B. The numerical strategy discussed so far will be judged by its ability to distinguish between these two temperature profiles.

Selection of Chemically Reacting Tracers

(a) Tracer Characteristics : Among the requirements for suitable tracer reactants and products are those common to all tracers. They must be soluble in the system medium, neither reactants nor products should adsorb appreciably on the system surfaces, and the capability must be present for analyzing the effluent for reactant and product concentrations easily, quickly, and accurately. For this problem, in addition to these general tracer requirements, the reactions must also satisfy following requirements. As has been mentioned earlier, the rate expressions must be separable into two parts, one depending on

temperature and the other on concentration. Also, the pre-exponential factors and the activation energies should be appropriate so that the tracers undergo significant, but not complete, conversions.

Fortunately, such reactions do exist, e.g., the hydrolysis of organic esters to yield organic acids and alcohols (cf. Kirby, 1972). At any particular temperature, there usually can be found a number of such reactions with similar reaction rates but different activation energies compensated by different pre-exponential factors. Even though there might be many reactions which would be candidates for use as tracers for a particular situation, it is always desirable to reduce the number of reacting tracers to as few as possible. In this study this possibility is investigated. Also, since the reaction activation energy E_i is the only possible experimental variable for multiple-tracer tests, another important consideration is the determination of the range of activation energies that is best suited for chemical tracer experiments.

(b) Activation Energies : In general, the required range of activation energies depends mainly on two factors, the kernel and the possible temperature profiles. In this particular case, it was found that $g(E_i)$ decreases exponentially with E_i as the latter is changed from 20 kJ/mol to 200 kJ for all three temperature profiles. It follows that the sensitivity of the tracer data to the activation energy, i.e. $\partial g(E_i)/\partial E_i$, also decreases exponentially with the activation energy. Thus it is prudent to use the tracers undergoing chemical reactions of lower activation energies. However, once the range of activation energies is selected, the increase in the number of tracers within that range does not seem to be very important. These two observations are substantiated by simulations shown in Figs. 1 and 2. Fig. 1 depicts the results obtained with a grid of 20 points from $\xi = 0$ to 1, using five different ranges of activation energies, each consisting of seven data points. The solid curve represents the true temperature profile (Profile B), the dashed line denotes the initial estimate of the temperature profile (a straight line between known inlet and exit temperatures). The two ranges covering relatively lower activation energies (viz., 20-80 kJ/mol and 40-100 kJ/mol) give better results than the two ranges of higher activation energies (viz., 80-140 kJ/mol and 140-200 kJ/mol). Also, it can be seen that when lower activation energies in a narrow range (e.g., 40-46 kJ/mol) are used, the results suffer. The results obtained for Profile A, using the lowest range of activation energies (20-80 kJ/mol), but varying the number of data points from as high as 13 to as low as 2, are shown in Fig. 2. The figure clearly shows that the number of reacting tracers used does not affect the final results. When only 2 reacting tracers are used, however, the number of iterations required increases significantly. Hence, in order to save computational efforts, throughout this study about 4 or 5 data points are used while studying the effects of other variables.

Effect of Error Level in the Experimental Data

In any experiment, a certain amount of error is inherent. The inversion of a Fredholm integral equation of the first kind is an ill-posed problem. Thus a small level of error in the LHS can cause large changes in the solution if proper precautions are not undertaken. The success of the regularization method used in this study largely depends on how robust is the solution for different levels of error in the data values $g(E_i)$. It is apparent from Fig.3a that the iterative method passes this test. Out of four different error levels used (0%, 1%, 5% and 10%), the first three give about the same results. More importantly, as can be seen from Fig. 3b, even at 10% error the proposed method succeeds in distinguishing between profiles A and B (the two alternative models for a Hot Dry Rock geothermal reservoir). Both temperature profiles have the same inlet and exit temperatures, so the same initial temperature profile has been assumed in both cases. Thus, using the same initial conditions and with up to 10% statistical error in observations, this method is able to discriminate between competing models for geothermal reservoirs.

Comparison With the Traditional Method

In many modeling studies, a parametric functional form of the desired distribution function is assumed and the parameters are adjusted to best fit the experimental data. If the correct functional form is assumed, this traditional method gives excellent results. However, it can give misleading results when the assumed functional form is incorrect. This pitfall is illustrated in Fig.4. The actual temperature profile is assumed to be of the form of Profile B (with 1% error), as shown with the solid line in Fig.4a. However, if a temperature profile similar to Profile A, viz. $T(\xi) = 500 + 150 [1 - \exp(-\beta\xi)]$, is used to model the experimental data by the traditional method, then the value of β that fits the experimental data best is found to be 2.680. The resulting temperature profile is shown in Fig.4a by the dashed line. However, when the method of regularization developed in this study is used, where no assumption is made regarding the functional form of the temperature profile, superior results are obtained (shown in Fig.4a by squares). A similar analysis is shown in Fig.4b, where the actual profile is of the form of Profile A and the traditional method wrongly assumes a functional form of Profile B.

Temperature Profiles Exhibiting a Maximum

In order to test the solution procedure for temperature profiles exhibiting a maximum, Profile C is used for three sets of values for β_1 and β_2 , which are reported in Table 1.

Table 1

Profile number	β_1	β_2	T_{max}	ξ at which $T = T_{max}$	T at $\xi = 1$
C1	3.398	1.25	650	0.8000	646.0
C2	5.437	2.00	650	0.5000	610.4
C3	16.31	6.00	650	0.1667	506.1

Fig.5 reports the results obtained for these three temperature profiles. For profiles C1 and C2, the method yields reasonably good results, which are depicted in Fig.5 by empty squares and partially filled squares, respectively. For Profile C3, the results from the regularization (shown by filled squares) do not agree with the actual profile, although the tolerance of 1 % is satisfied. The numerical details of the final results for this latter case are shown in Table 2.

Table 2

Activation energy, E_i (J / mol)	$g(E_i)$, without error	$g(E_i)$, with error	data simulated from the computed temperature profile
40000	2.51422E-4	2.43014E-4	2.49610E-4
50000	3.40946E-5	3.42493E-5	3.38032E-5
60000	4.73006E-6	4.68331E-6	4.68022E-6
70000	6.68764E-7	6.77676E-7	6.59878E-7
80000	9.60264E-8	9.78366E-8	9.44147E-8

By observing the computed data values in Table 2, it is obvious that in this situation there are several temperature profiles that can be obtained from the same experimental data. Thus in the cases where multiple solutions are possible, the solution obtained by the regularization will largely depend on the initial temperature profile assumed for the first iteration. In fact, it was numerically observed that by varying the initial estimate, many significantly different solutions can be obtained.

It can be analytically shown that infinitely many temperature profiles can be constructed that yield the same experimental observations [i.e., the vector $g(E)$ or LHS of eqn(2)]. However, most of these profiles would not be valid solutions to the problem, because either the boundary conditions would not be satisfied or the temperature profile would not be continuous. Apparently, multiple solutions exist which are both continuous and match the boundary conditions if the actual temperature profile (a) exhibits a sharp profile and, (b) the values of temperature at both boundaries are not far apart. Under these conditions, it is possible to reassemble segments of the profile and still satisfy the boundary conditions and continuity. While multiple solutions are possible when the profiles are

monotonic, such as Profiles A and B, the different solutions may not be widely different. Thus an approximation to the true profile is achieved.

It must be noted that in this study a plug flow model has been assumed for the fluid flow. A more complex model including additional information of the flow process might be able to resolve this issue of multiple solutions. However, there are many systems for which the plug flow model is sufficient. The developments presented here form a basis for the more complicated dispersed-flow situation.

CONCLUSIONS

It is possible to determine the temperature profile in a flowing system with the use of chemically reacting tracers. An iterative form of regularization method can be successfully employed to solve the resulting Fredholm integral equation of the first kind. This iterative method eliminates the need of determination of the optimal value for the regularization parameter.

Using reactions with lower activation energies enables more sensitive determination of temperature profiles. Also, the wider range of activation energies in the tracer reactions, the more sensitive the profile determination.

For geothermal reservoirs, it is possible that as few as two reacting tracers can give an adequate measurement of the temperature profile within the reservoir.

The method can successfully discriminate between two rival models for a Hot Dry Rock type geothermal reservoir with as large as 10% error in data.

The method presented in this paper gives excellent results for monotonic temperature profiles. The method does not give a unique solution for a temperature profile exhibiting a sharp maximum, however; in this case, the solution is dependent upon the initially assumed profile.

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REFERENCES

- Allison, H., "Inverse Unstable Problems and Some of Their Applications," *Math. Scientist*, 4, 9-30 (1979).
- Britten, J. A., B. J. Travis, and L. F. Brown, "Calculation of Surface Site-Energy Distributions from Adsorption Isotherms and Temperature-Programmed Desorption Data," *AIChE Symp. Ser. No. 230*, 79, 7 (1963).
- Brown, L. F., and B. J. Travis, "Optimal Smoothing of Site-Energy Distributions from Adsorption Isotherms," in *Fundamentals of Adsorption* (A. L. Myers and G. Belfort, eds.), pp. 125-134. Engineering Foundation, New York, 1984.
- Brown, L. F., B. A. Robinson, and J. W. Tester, "Determination of Temperature Characteristics of Flowing Systems Using Chemically Reacting Tracers, paper 67c presented at 1984 Summer AIChE Meeting, Philadelphia, PA. August 19-22, 1984.
- Kirby, A. J., "Hydrolysis and Formation of Esters of Organic Acids," in *Comprehensive Chemical Kinetics* (C.H. Bamford and C.F.H. Tipper, eds), pp. 57-207. Elsevier, New York, 1972.
- Miller, G. F., "Fredholm Equations of the First Kind," in *Numerical Solution of Integral Equations* (L. M. Delves and J. Walsh, eds.), pp. 175-187. Clarendon Press, Oxford, 1974.
- Murphy, H. D., J. W. Tester, C. O. Grigsby, and R. M. Potter, "Energy Extraction from Fractured Geothermal Reservoirs in Low Permeability Crystalline Granite," *J. Geophysical Res.*, 86(B8), 7145-7158 (1981).
- Robinson, B. A., J. W. Tester, and L. F. Brown, "Using Chemically Reactive Tracers to Determine Temperature Characteristics of Geothermal Reservoirs," *Trans. Geothermal Resources Council*, 8, 337-341 (1984).
- Tikhonov A. N. and V. Y. Arsenin, *Solutions of Ill-Posed Problems*. Halsted Press, 1977.
- Wing, M., "A Primer on Integral Equations of the First Kind," Report LA-UR-84-1234, Los Alamos National Laboratory, Los Alamos, NM (1984).

NOMENCLATURE

Roman

a	=	lower limit for the system variable
A	=	pre-exponential term, used in eqn(1)
b	=	upper limit for the system variable
c	=	lower limit for the experimental variable
C	=	concentration
d	=	upper limit for the experimental variable
E	=	activation energy of a chemical reaction
f	=	distribution function of the system variable
g	=	function representing the experimental observations
G	=	a nonlinear differential operator on f(y)
I	=	objective function defined by eqn(7)
K	=	kernel of the integral equation
L_0	=	initial estimate of the function $T(\xi)$
L_1	=	new estimate of the function $T(\xi)$, derived from L_0
m	=	dimension of the grid used to discretize the range of system variable, y
n	=	number of experimental observations
q	=	volumetric flow rate
q_0	=	coefficient of $f^2(y)$ in the stabilizer
q_1	=	coefficient of $(df/dy)^2$ in the stabilizer
R	=	Universal gas constant
T	=	temperature
V	=	volume
x	=	generic experimental variable
y	=	generic intrinsic system variable

Greek

α	=	regularization parameter
β	=	a parameter used to define a temperature profile
β_1	=	a parameter used to define profile C
β_2	=	a parameter used to define profile C
ϵ	=	fractional deviation of $L_0(\xi)$ from $T(\xi)$
ξ	=	dimensionless volume fraction, V/V_s

Subscripts

i	=	pertaining to i'th chemical tracer
f	=	pertaining to exit conditions
max	=	pertaining to the maximum value
o	=	pertaining to inlet conditions
s	=	pertaining to system, as a whole

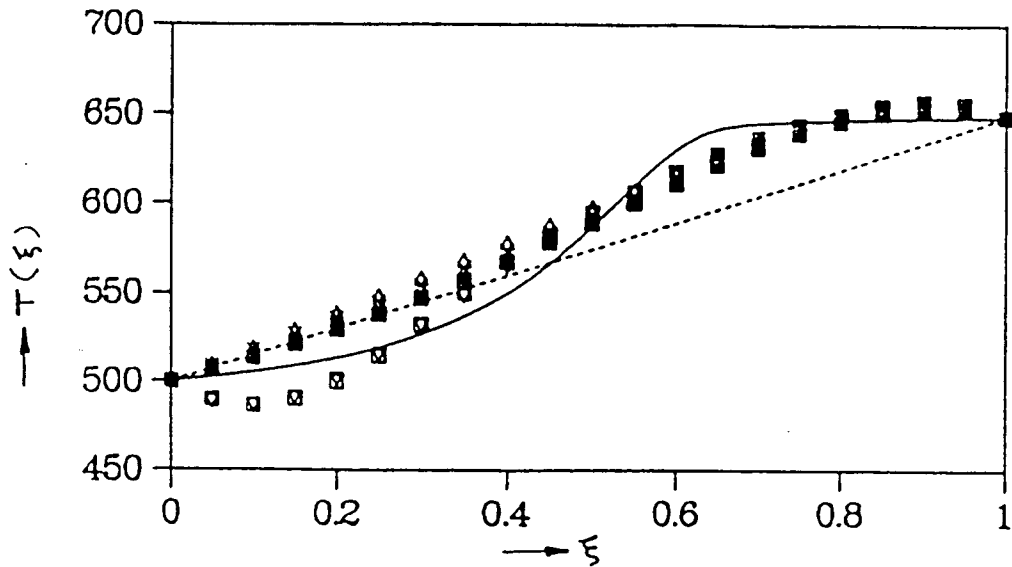


Fig. 1 Effect of the Range of Activation Energies on the Results for Profile B. The solid curve shows actual temperature distribution, whereas various symbols depict the results obtained. Legend for range of E (in kJ/mole) : square (20-80), triangle (80-140), x (140-200), inverted triangle (40-100), solid square (40-46). $n = 7$, $q_0 = q_1 = 1$, error = 1 %, tolerance = 0.01.

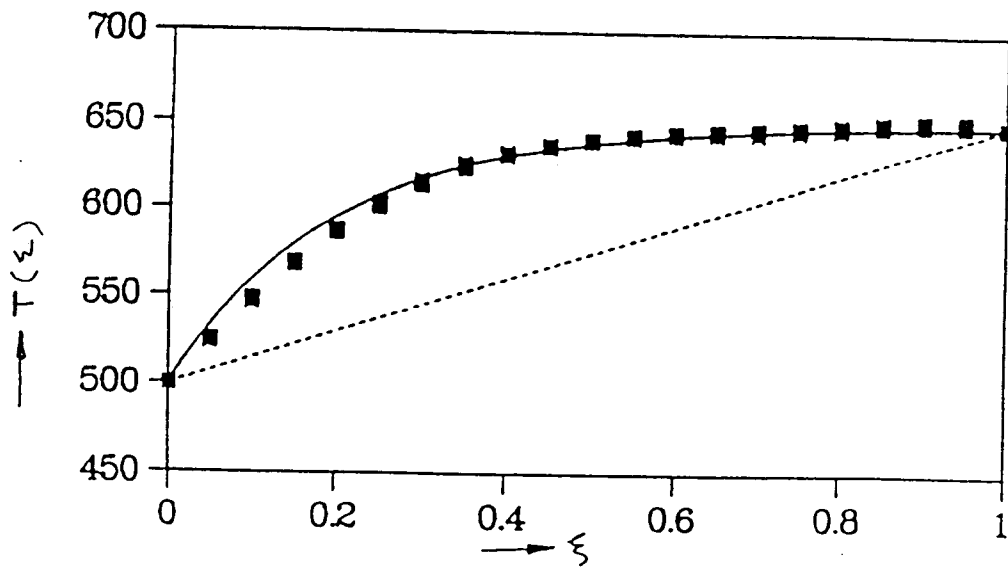


Fig. 2 Effect of the Number of Data Points (n) on the Results for Profile A. Legend : square ($n=2$), triangle (3), x (5), inverted triangle (7), star (13). $q_0 = q_1 = 1$, error = 1 %, range of $E = 20-80$ kJ/mole.

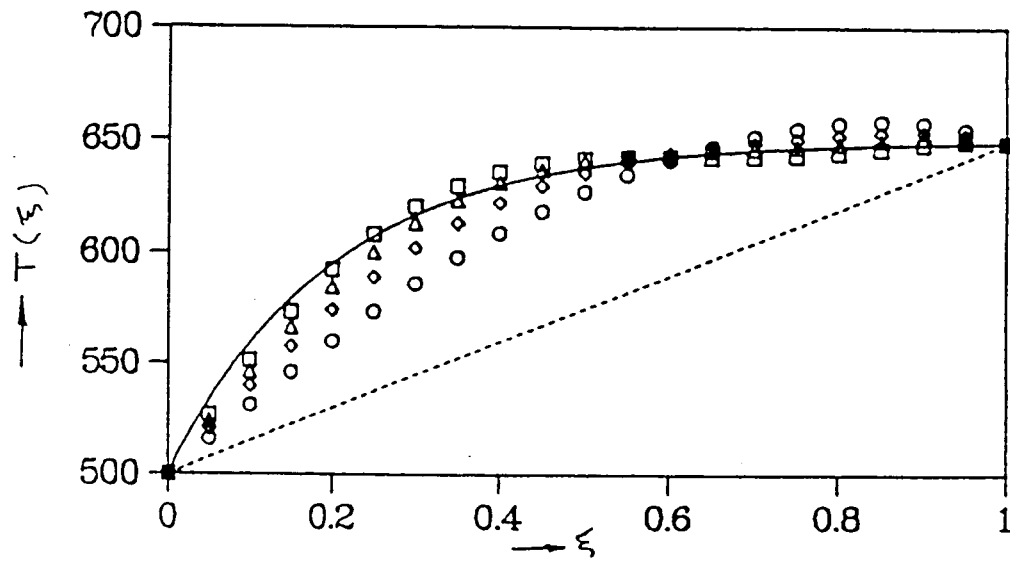


Fig. 3a Effect of the Error on the Results for Profile A.
 $q_0 = q_1 = 1$, range of $E = 40-80$ kJ/mole, $n = 5$, tolerance = 0.01.
 Legend : square (no error), triangle (1 % error), x (5 % error), circle (10 % error).

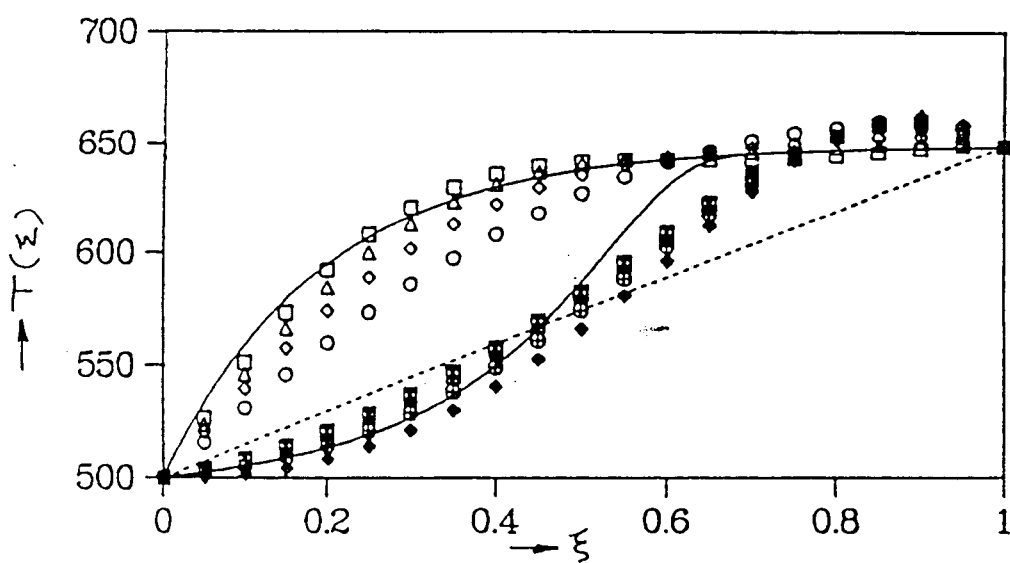


Fig. 3b Effect of the Error on the Results for Profile A and B. The dash curve denotes the initial estimate for the temperature distribution.
 $q_0 = q_1 = 1$, range of $E = 40-80$ kJ/mole, $n = 5$, tolerance = 0.01.
 Errors used : 0 %, 1 %, 5 % and 10 %.

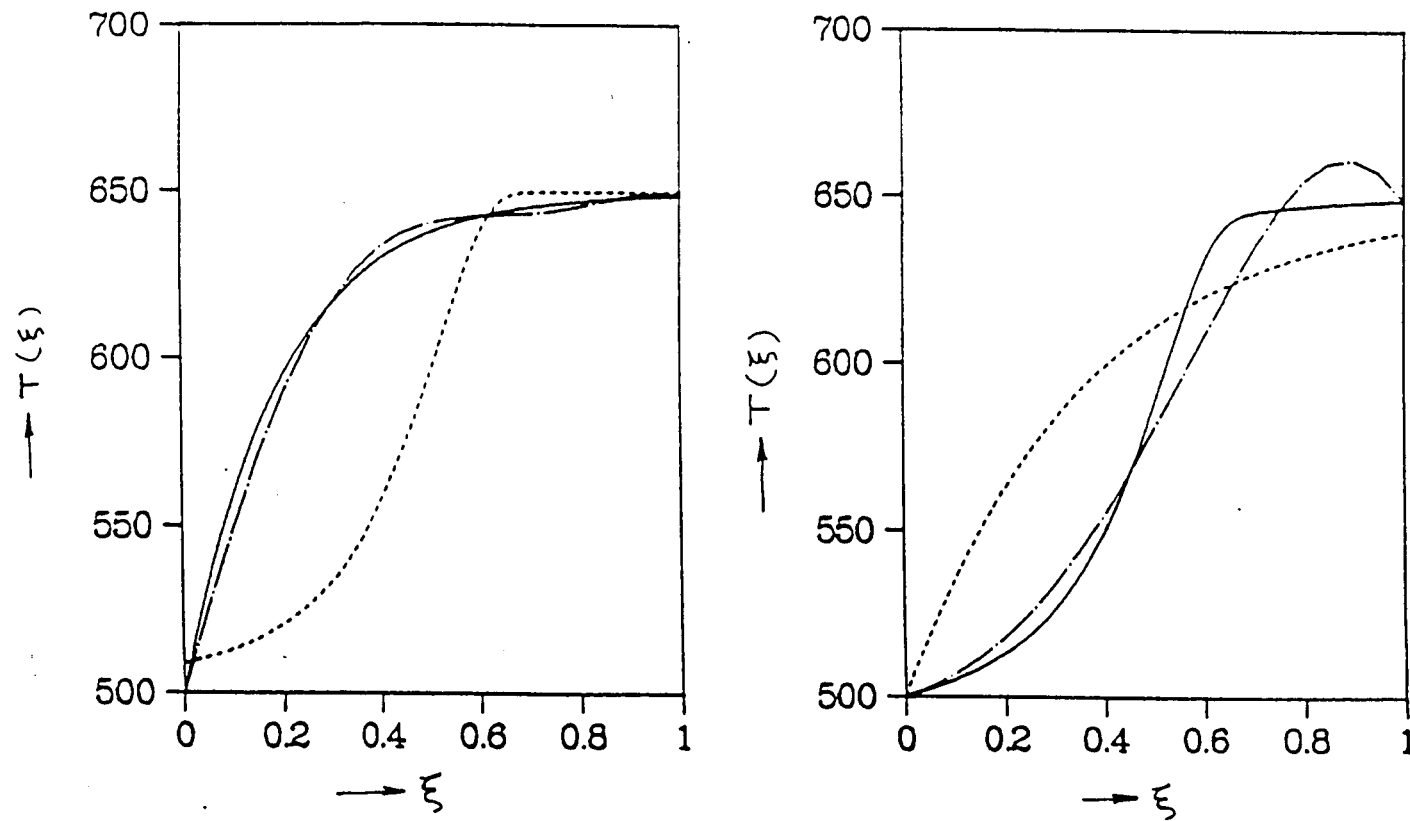


Fig. 4 Comparison with the Optimization Method. (a) Results for Profile A, (b) Results for Profile B. Solid curve : actual temperature distribution, chain-dot curve : results from inversion of Fredholm equation, dash curve : results from optimization, if wrong functional form is used.

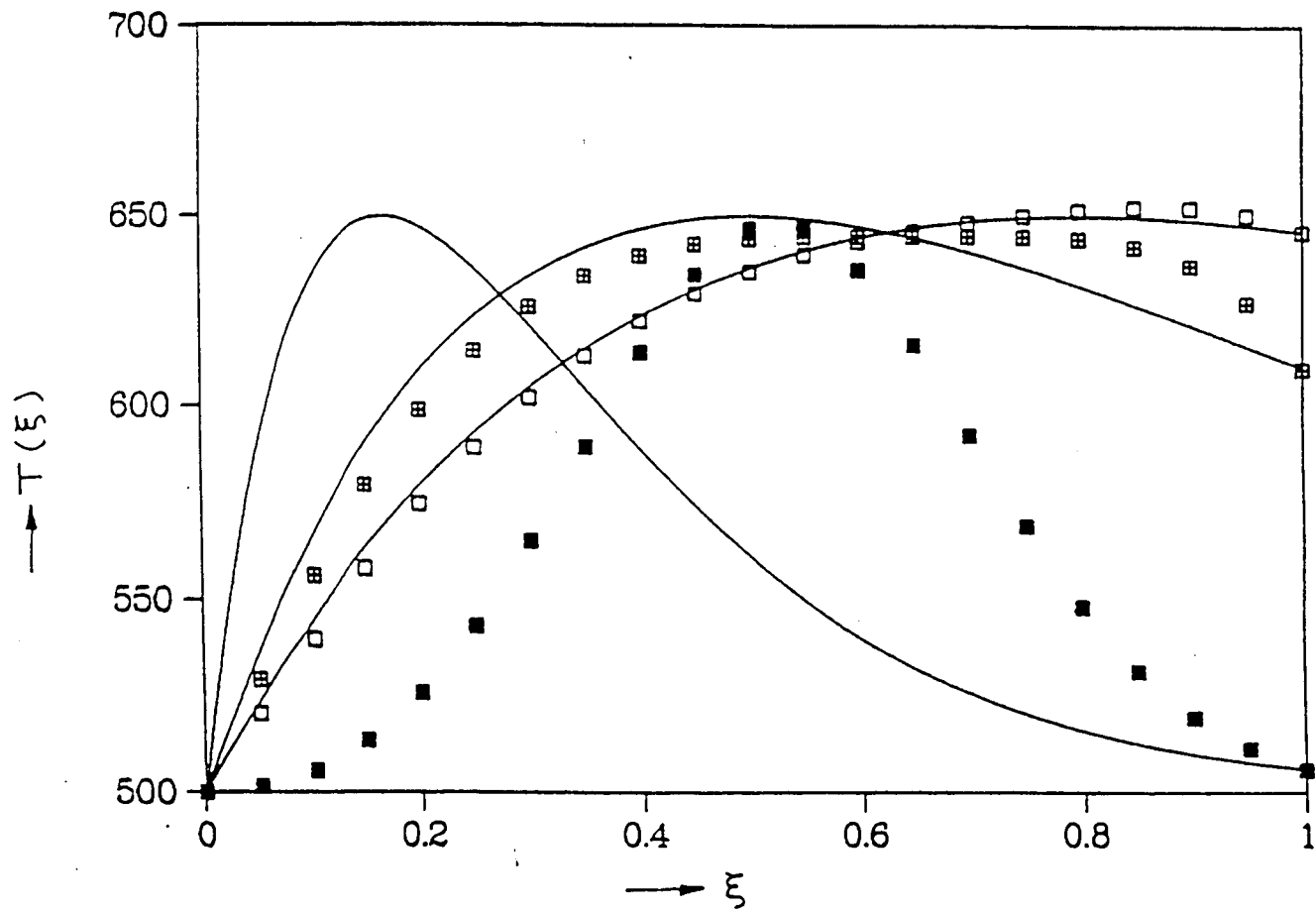


Fig. 5 Results obtained for temperature distributions exhibiting maximum. The solid curves are the actual distributions and various symbols depict the results (for details, please refer to the text)