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Evaluation of Thermal Conductivity from Temperature Profiles[1]

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A new dynamic technique for the measurement of thermal conductivity is being developed at IMGC. The experiment consists in bringing the specimen to high temperatures with a current pulse and in measuring the temperature profiles during the free cooling period. Different techniques can be used to extract the information on thermal conductivity from the profiles. The numerical computation of thermal conductivity from the experimental temperature profiles in absolute space is possible, but it is difficult and cumbersome because one must know and take into the account the exact position of the infinitesimal elements of the specimen in different profiles. Computations in tube-space (a fictitious space where no thermal expansion occurs) are simpler and lead to less complex numerical computations. Complementary techniques to evaluate thermal conductivity as a function of temperature or at constant temperature are presented with a discussion of advantages and disadvantages of each method. Computer simulations have tested the precision of the complex software. Numerically generated temperature profiles from known thermophysical properties have been obtained and thermal conductivity has been recomputed from the profiles. The relative difference using different computational approaches and different fitting functions is always less than 0.1%.

KEY WORDS: dynamic measurements; high temperature; scanning pyrometry; temperature profiles; thermal conductivity.

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1. INTRODUCTION

New dynamic measurement methods, based on applications of high-speed scanning pyrometry [1], are currently under development at the Istituto di Metrologia "G. Colonnetti" (IMGC). The experimental apparatus and the measurement techniques for thermal conductivity [2] and hemispherical total emittance [3] have been described in earlier publications; measurements on niobium are in progress. The dynamic experiment consists in bringing the specimen to high temperatures with a subsecond current pulse and in measuring during the free cooling (lasting 10–20 s) the evolving temperature profiles on the specimen via high-speed scanning pyrometry [4]. Figure 1 presents a schematic diagram of the specimen and of the optical instrumentation.

Dynamic experiments, like the one described before, must take into account the role played by thermal expansion, regarding both its effect on geometrical quantities and on thermophysical properties and its influence on the measurement technique. A microsecond time resolution scanning pyrometer will always measure temperatures in predefined positions in space, but in different profiles the measured temperature will be that of different points of the specimen, on account of thermal expansion effects.

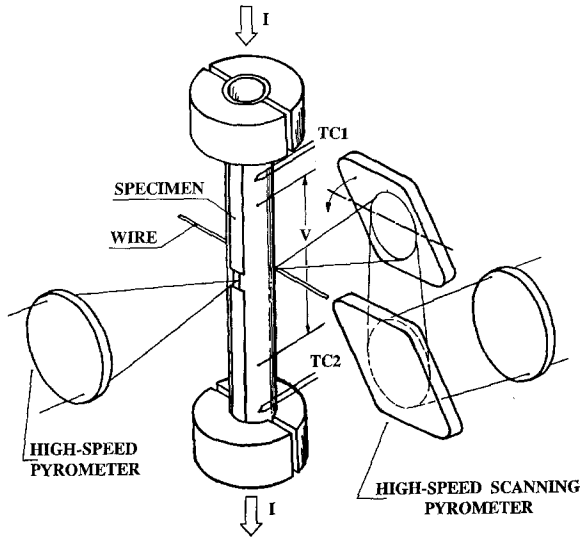

Fig. 1. Schematic representation (from Ref. 2) of the new dynamic technique used either for thermal conductivity or for hemispherical total emittance. *I*, current passing through the specimen; *V*, voltage drop across the central part of the specimen; TC1 and TC2, chromel–alumel thermocouples.

An earlier publication [5] considered the mathematical model of dynamic thermal conductivity experiments and presented different forms of the basic heat transfer equation, all of them taking fully into account thermal expansion effects. The present paper deals with different approaches that may be used to compute thermal conductivity from temperature profiles, assuming that the other necessary thermophysical properties are either accurately known or have been measured by other techniques. Thermal expansion effects are always considered and the different methods are analyzed both regarding their precision (with inevitable errors due to the estimation of derivatives and to the large amount of computer calculations) and their capability to extract the maximum amount of information from the measured temperature profiles.

2. ABSOLUTE SPACE

We assume a set of coordinate axes fixed in the laboratory with the specimen constrained at $x=0$ and free to expand in the positive x-direction. The specimen is heated by an electrical current I and taken to high temperature, then the current is cutoff and the specimen cools freely to room temperature. Temperature profiles may be measured during heating and/or during cooling. Assuming the "long thin rod approximation" [6], in a previous paper [5] the basic heat transfer equation applicable to this dynamic heating experiment was given as

$$\frac{1}{S_c}\frac{\partial}{\partial x_c}\left(\lambda_c S_c \frac{\partial T}{\partial x_c}\right)+\frac{\rho_c I^2}{S_c^2}-\frac{\varepsilon_c p_c \sigma(T^4-T_a^4)}{S_c}-\frac{\mu_c I}{S_c}\frac{\partial T}{\partial x_c}=\delta_c(c_p)_c\frac{DT}{Dt} \tag{1}$$

The subscript c indicates that all quantities (both thermophysical properties and geometrical quantities) are corrected for thermal expansion effects. Equation (1) represents the general case; during cooling ($I=0$) two terms vanish. The quantities in Eq. (1), listed without the subscript c, are as follows: λ, thermal conductivity; ε, hemispherical total emittance; ρ, electrical resistivity; μ, Thomson coefficient; c_p heat capacity; δ, density; p, perimeter; S, cross-sectional area; σ, Stephan–Boltzmann constant; T, temperature; T_a, ambient temperature; and t, time. Temperature derivatives with respect to space $\partial T/\partial x$, $\partial^2 T/\partial x^2$, and time DT/Dt ("material" derivative [7]) are also present in Eq. (1).

Equation (1) has several different forms [5], depending on how the time-dependent heat capacity term is expressed. The following sections examine in detail various forms of the partial differential equation, showing their various advantages and disadvantages when used to compute thermal conductivity from temperature profiles in absolute space.

2.1. Material Derivative

Assuming a knowledge of all thermophysical properties except the unknown thermal conductivity and an accurate experimental measurement of temperature profiles (from which temperatures and all the derivatives with respect to time and space may be computed), Eq. (1) may be used to obtain the thermal conductivity. The computation of the various derivatives requires the following steps (see Fig. 2):

(a) take point P_i (in position x and time t in one profile) and identify the location P_0 (of the specimen), where point P_i was when the specimen was cold;

(b) identify where location P_0 has moved on each measured profile $(..., P_{i-1}, P_i, P_{i+1}, ...)$;

(c) the set of temperatures representing the temperature vs time history of location P_0 must be fitted and the derivative DT/Dt computed (derivation following the motion; see Ref. 5); and

(d) by selecting a window on the profile near P_i and by fitting the temperature $T=f(x)$, one may compute the derivatives $\partial T/\partial x_c$, $\partial^2 T/\partial x_c^2$.

Unfortunately, this procedure is extremely cumbersome and requires large amounts of computation because all the steps (a to d) must be repeated when another point on the profiles is selected. Considering that one

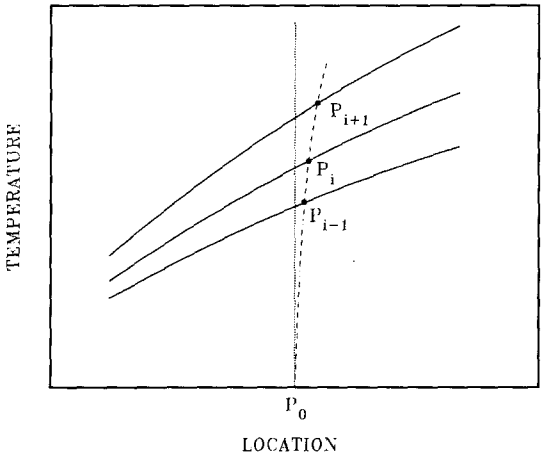

Fig. 2. Schematic representation of computations of the "material" derivative DT/Dt in absolute space according to Eq. (1).

dynamic experiment may produce a set of approximately 100 profiles (each defined by 200–500 temperature points), it is clear that even a partial analysis according to this method requires hours of interactive computer time. Interaction with the computer is necessary because the temperature vs time function is unknown a priori and noise and disturbances on the profiles make a computer-made selection unreliable.

2.2. Separate Variables

An alternative possibility for computations in absolute space is to use the second form of the differential equation presented in Ref. 5, where variables x, t are completely separate. In this equation, the time-dependent heat capacity term is

$$\delta_c(c_p)_c \frac{\partial T}{\partial t} + \delta_c(c_p)_c \int_0^x \frac{d\omega_c}{dT} \frac{\partial T}{\partial t} dx \tag{2}$$

where $\omega_c = \delta_c S_c$ is the linear density of the specimen. In this case, $\partial T/\partial t$ is computed for $x = \text{constant}$ (taking a vertical line at the chosen x-position in absolute space) and the amount of computation needed for the time derivatives is drastically reduced. Unfortunately, a major problem is the numerical calculation of the integral in Eq. (2), that requires the computation of $\partial T/\partial t$ at all the integration points from the constraint ($x = 0$) to the chosen x-position for each profile. The initial and final part of each profile cannot be measured experimentally because temperatures in these regions are too low for high-speed pyrometry. The ends of each profile are known only by interpolation between the pyrometer readings and the temperatures measured by thermocouples spot-welded on the specimen as close as possible to the clamps (see Fig. 1). This interpolated part of the profile is adequate for thermal expansion corrections, but it cannot be used for evaluating the temperature derivatives and consequently any computation of the integral of Eq. (2) is inaccurate.

In conclusion, computation of thermal conductivity from experimental temperature profiles in absolute space is possible, but it has severe disadvantages. Computations according to Eq. (1) require large amounts of interactive time and computations according to Eq. (2) are inaccurate.

3. TUBE-SPACE

Tube-space does not exist: it is an imaginary space where no thermal expansion occurs and it is so named because in tube-space the molecules of the material always remain fixed in a location. The name is chosen in

relation to our tubular specimens, but the concept is clearly usable for any specimen shape. Imagining that the dynamic experiment occurs in tube-space leads to considerable simplifications in mathematics and computation, so this approach is a valid alternative on account of the mentioned difficulties for computations in absolute space.

In tube-space all quantities will be identified by the subscript u (meaning uncorrected for thermal expansion). Thermophysical properties in tube-space maintain their temperature dependence, but are uncorrected for thermal expansion effects and a careful analysis of how properties have been measured is necessary to use the correct numerical expression [8]. Some useful relations for corrected and uncorrected geometrical quantities and for space derivatives are

$$\begin{aligned} p_c &= p_u(1+f) \\ S_c &= S_u(1+f)^2 \\ \delta_c &= \delta_u(1+f)^{-3} \\ \frac{\partial T}{\partial x_c} &= \frac{\partial T}{\partial x_u}(1+f)^{-1} \\ \frac{\partial^2 T}{\partial x_c^2} &= \frac{\partial^2 T}{\partial x_u^2}(1+f)^{-2} \end{aligned} \tag{3}$$

where $f(T) = \Delta L(T)/L_{293}$ is the thermal expansion function of the material under consideration (relative expansion of a small element at constant temperature T with respect to its length at ambient temperature).

One form of the heat transfer equation applicable to the dynamic thermal conductivity experiment in tube-space is

$$\frac{\partial}{\partial x_u}\left(\lambda_u \frac{\partial T}{\partial x_u}\right) + \frac{\rho_u I^2}{S_u^2} - \frac{\varepsilon_u p_u \sigma(T^4 - T_a^4)}{S_u} - \frac{\mu_u I}{S_u}\frac{\partial T}{\partial x_u} = \delta_u (c_p)_u \frac{\partial T}{\partial t} \tag{4}$$

Equation (4) is immediately derived from Eq. (1) taking into account that in tube-space $DT/Dt = \partial T/\partial t$. Each term in Eqs. (1) and (4) has a defined physical meaning: it is the power per unit volume due to the particular physical process taking place in the control volume at time t (heat conduction, Joule heating, radiation loss, Thomson heating, heat storage). The two equations refer to the same experiment, so they must be related by a common factor, which is easily identified taking into account that in Eq. (1) the specimen expands, so the power is distributed over larger volumes with the expansion of the specimen, while this does not happen in the imaginary tube-space. The mathematical relation between each power density term is

$$(\textit{power density in tube-space}) = (\textit{power density in absolute space})\ (1+f)^3$$

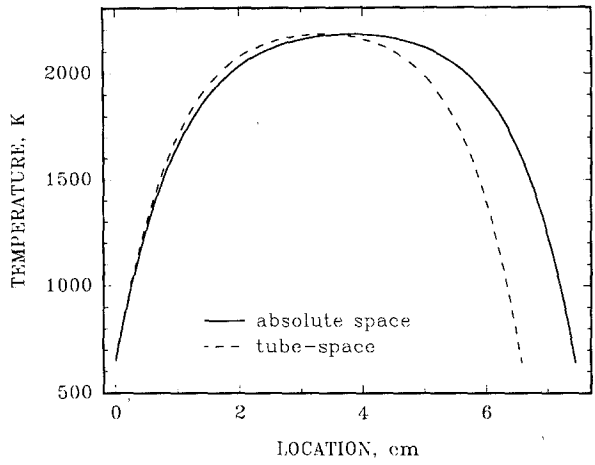

Fig. 3. Typical transformation of a temperature profile from absolute space to tube-space. For viewing purposes the thermal expansion correction is exaggerated (a correction 10 times bigger than in reality has been used).

Taking into account the relation between power density terms, the evaluation of thermophysical properties leads to the following relations:

$$\left.\begin{aligned} (c_p)_c &= (c_p)_u \\ \mu_c &= \mu_u \\ \lambda_c &= \lambda_u(1+f)^{-1} \\ \rho_c &= \rho_u(1+f) \\ \varepsilon_c &= \varepsilon_u(1+f)^{-2} \end{aligned}\right\} \tag{5}$$

The computation of thermophysical properties in tube-space requires a set of temperature profiles as if they were measured in a space where no thermal expansion occurs. Experimental profiles are measured in absolute space: they are transformed to tube-space by "shrinking them backward" as if the specimen did not expand (see Fig. 3). For this operation a knowledge of another thermal expansion function $g(T) = \Delta L(T)/L(T)$ is necessary to perform the transformation [$g(T)$ is the relative expansion of a small element at constant temperature with respect to its length at temperature T, with $\Delta L = L(T) - L_{293}$]. Numerical values for the thermal expansion functions $f(T)$ and $g(T)$ for niobium, the material for which measurements are in progress, may be found in Ref. 9.

3.1. Thermal Conductivity as a Function of Temperature

The technique to evaluate thermal conductivity as a function of temperature from profiles in tube-space has already been described [2]. This is done by opening a vertical window on the profiles (see Fig. 4), and writing and solving a set of linear equations of the unknown thermal conductivity (as a function of temperature) for the middle point of each profile in the window. The space derivatives are computed by fitting the portion of each profile in the window, and the evaluation of temperature vs time of each point is simple because in tube-space each infinitesimal portion of the specimen remains at a fixed x-position during the entire experiment. The overdetermined set of linear equations is solved by least-squares techniques. Details of the mathematical procedure and of the various computer programs are described in an earlier publication [2].

The main advantages of this technique are that

(a) a simple transformation (from absolute space to tube-space) computed only once for each set of profiles is necessary;

(b) the thermal conductivity may be evaluated over a large temperature range; and

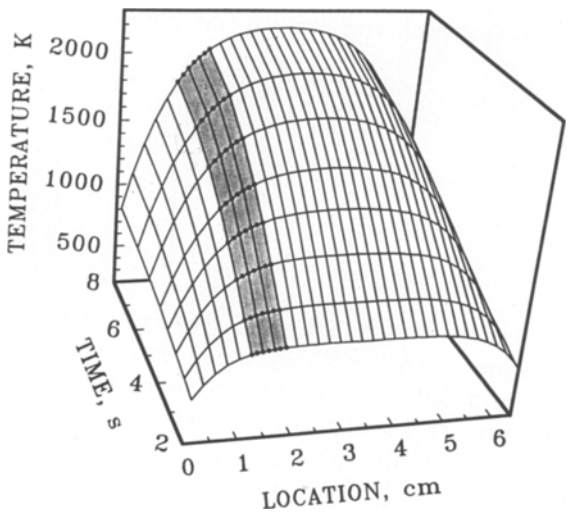

Fig. 4. Three-dimensional view of the evolving temperature profiles in a simulated heating experiment in tube-space. The shaded area shows a typical vertical window used for computations of thermal conductivity and of its temperature dependence.

(c) the evaluation may be performed in different parts of the profiles, avoiding regions where disturbances on the surface of the specimen might create problems in the computation of derivatives.

The main disadvantage of this computational procedure is that the best regions of the profiles for the evaluation of thermal conductivity cannot be used. Thermal conduction is higher at both ends of high-temperature profiles, in the regions characterized by steep gradients. Unfortunately in cooling experiments (the best ones to evaluate thermal conductivity), the ends cool rapidly and a vertical window cannot be opened in those regions, because only a few profiles are available and hence the temperature vs time history of these locations cannot be obtained accurately. An alternative technique was developed to extract the information available in regions with steep temperature gradients at the ends of the profiles.

3.2. Thermal Conductivity at a Fixed Temperature

A different form of Eq. (4) in tube-space must be considered to evaluate thermal conductivity at a fixed temperature. We may assume that an identical experiment occurs, but in this case the specimen moves and we observe what happens in the fixed control volume. An identical experiment will produce identical temperature profiles on the specimen and we are interested, among all possible motions that the specimen may have, in the particular speed that will always maintain the same temperature in the control volume. When temperature is constant with time in the control volume, then $\partial T/\partial t = 0$, but we observe mass flow through the control volume due to the motion of the specimen. The expression for mass flow (convection term) has already been considered [5] and the new form of the heat transfer equation is

$$\frac{\partial}{\partial x_u}\left(\lambda_u \frac{\partial T}{\partial x_u}\right) + \frac{\rho_u I^2}{S_u^2} - \frac{\varepsilon_u p_u \sigma (T^4 - T_a^4)}{S_u} - \frac{\mu_u I}{S_u}\frac{\partial T}{\partial x_u} = \delta_u (c_p)_u v_u \frac{\partial T}{\partial x_u} \tag{6}$$

where $v_u(t)$ is the speed of the specimen in tube-space when we observe no temperature change in the control volume. In tube-space, the hypothetical heating experiment just described is equivalent to moving all profiles until they cross each other at a fixed temperature and this can be done at either side of the profiles (on the left-hand side with a positive speed and on the right-hand side with a negative speed). The separate consideration of each side is necessary because the temperature gradient $\partial T/\partial x_u$ changes sign in the two regions.

If we now return from the imaginary experiment to a classical set of profiles in tube-space, all the information necessary to perform computations according to Eq. (6) is available. By opening a horizontal window on the profiles (see Fig. 5), the crossing of line $T=$ constant with the profiles provides a set of locations in tube-space with constant temperature. The distances between these locations provide the space that each profile (identified by a certain time) should travel so that all profiles cross together at the same point and from these data (space, time) the speed of each side may be computed. The concept may be clarified with the help of Fig. 6, which shows the left-hand side of the profiles (a similar reasoning holds for the right-hand side).

When we want to write Eq. (6) for point P_i on the ith profile, we need to imagine that all profiles would cross each other at P_i with the same temperature. This would require a motion of the specimen such that point P_1 reaches P_i (distance traveled $x_i - x_1$) in the time $t_1 - t_i$. A similar reasoning holds for all other points $P_2,..., P_n$. From the distance that the specimen should move and the relative time, a relation space = function(time) may be obtained and by derivation the speed v_u may be computed. It should be remembered that in the imaginary experiment in tube-space (no expansion), all the points of the specimen move with the same speed v_u, but this

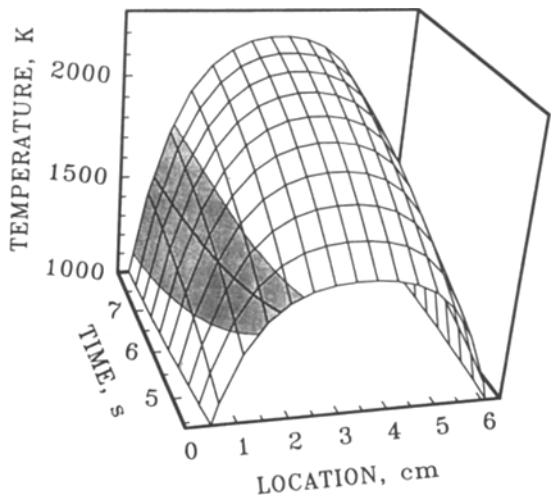

Fig. 5. Three-dimensional view of the evolving temperature profiles in a simulated heating experiment in tube-space. The shaded area shows the horizontal window (centered at $T=1500$ K) used for computations of thermal conductivity at a constant temperature.

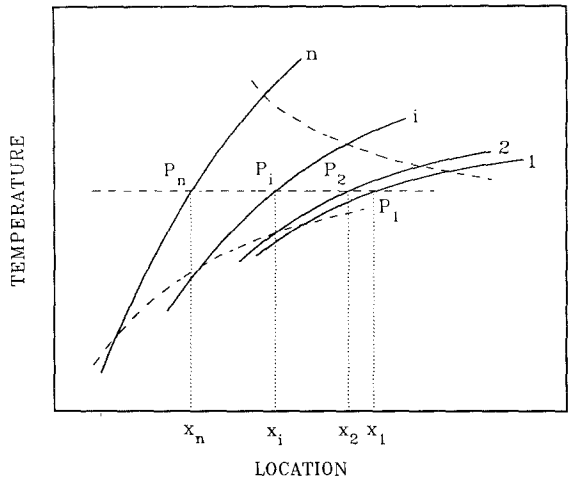

Fig. 6. Two-dimensional view of the left-hand side of the evolving temperature profiles in a simulated heating experiment. Equations (6) are written and solved for points P_1, P_2,..., P_n at a constant temperature; these points are at the center of the horizontal window used for computations.

speed may arbitrarily change with time. So the computation of speed v_u for all points P_1, P_2,..., P_n requires one fitting of positions x_1, x_2,..., x_n versus time t_1, t_2,..., t_n and the derivation of the fitted function to obtain $v_u(t_1)$, $v_u(t_2)$,..., $v_u(t_n)$ for all the P points.

The horizontal window opened on the profiles provides the same environment as described for a vertical window. Temperature derivatives with space may be computed by fitting the portion of each profile in the window. This leads to an overdetermined set of linear equations in the unknown parameters (the value of λ and of its temperature derivative $d\lambda/dT$ at $T=$ constant) that may be solved by least-squares techniques.

The set of programs that computes thermal conductivity at a fixed temperature has many similarities with those used for a vertical window. The left-hand side of Eqs. (4) and (6) are identical; in the right-hand side the computation of v_u of Eq. (6) is similar to the computation of $\partial T/\partial t$ of Eq. (4). From a practical point of view computations in a vertical or in a horizontal window are just options in the group of computer programs to process experimental temperature profiles.

The main advantages of the computational technique at a constant temperature are

(a) the use of regions of profiles with steep temperature gradients, where heat conduction is the dominant physical process;

(b) the use of different locations on the surface of the specimen, averaging potential problems of one location with other points on the surface of the specimen;

(c) the complementarity with the other approach (vertical window) with the possibility of extracting more information from the same set of profiles; and

(d) the possibility to check the independence of thermal conductivity from the temperature gradient.

Some disadvantages of this technique are as follows.

(a) Thermal conductivity is measured at one temperature only, so several computations and a fit of λ vs T are needed for evaluating the temperature dependence of λ.

(b) An estimate of the temperature derivative of thermal conductivity is useful for the computation. The term including $d\lambda/dT$ is generally small, therefore the estimated value does not influence much the computation. In the case of gross discrepancies between the estimated value and the final result, iterative computations might be necessary.

In conclusion, computations in tube-space seem to be the best solution in extracting all the information on thermal conductivity from the temperature profiles. Operation with a vertical window provides thermal conductivity over a wide temperature range; operation with a horizontal window computes λ at a constant temperature but may extract the information from regions where heat conduction is the dominant physical process.

4. COMPUTER SIMULATIONS

The evaluation of thermal conductivity from experimental temperature profiles always require large amounts of numerical calculations. Some round-off errors are inevitable, but the main concerns are either software errors in the complex computer programs or wrong assumptions in the numerical computation model. For instance, if the temperature profile in the (vertical or horizontal) window is not representable by a third-degree polynomial, then the space derivatives will be computed incorrectly and the width of the window may influence this error. A certain amount of subjective judgement is often necessary when selecting the best fittings for temperature vs time or position vs time. Least-squares fittings are presently

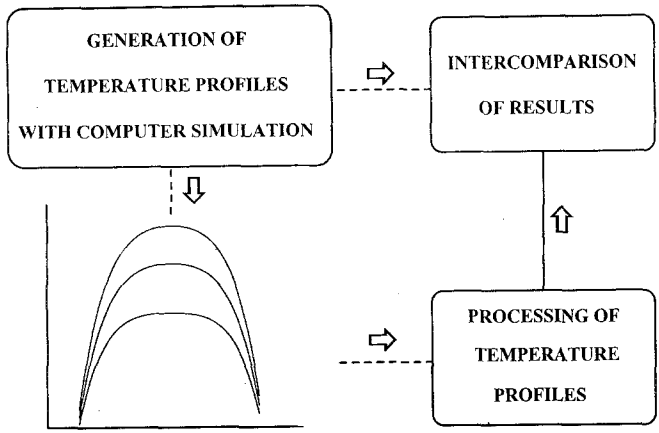

Fig. 7. Block diagram of computer simulations.

implemented either with polynomials or with splines, and the function selection may influence the computed results.

The capability of the computer programs to evaluate correctly the thermal conductivity from the temperature profiles was assessed by performing some computer simulations and data processing of simulated profiles as shown in Fig. 7.

A computer program that simulates the dynamic heating experiment was prepared. This program presently performs simulations in tube-space;

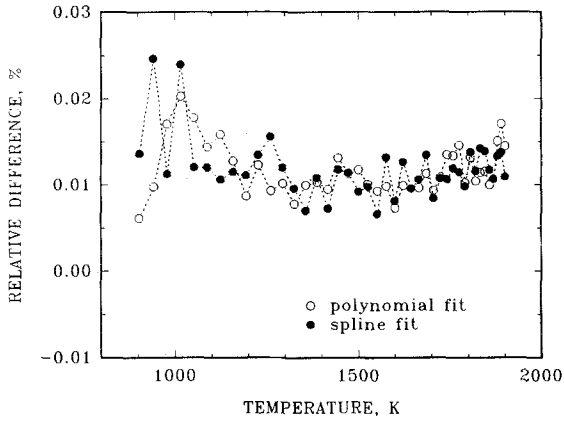

Fig. 8. Relative difference between assumed and computed thermal conductivity in a simulated heating experiment. Calculations performed with a vertical window using different functions for fitting temperature vs time.

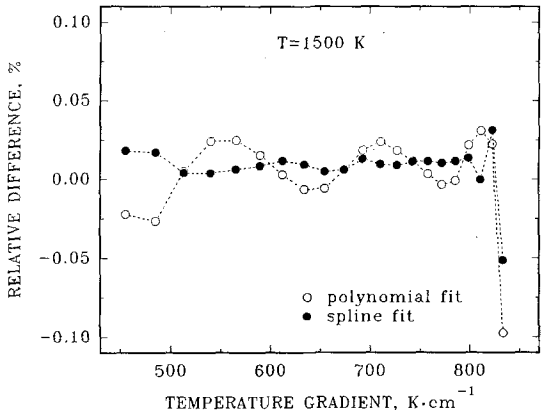

Fig. 9. Relative difference between assumed and computed thermal conductivity in a simulated heating experiment. Calculations performed with a horizontal window at 1500 K using different functions for fitting space vs time.

a more complex version operating in absolute space is in preparation. From the input data (thermophysical properties, geometrical quantities, initial and boundary conditions, experimental conditions), a set of simulated temperature profiles is generated. The smooth profiles (free from noise and known numerically for the entire length of the specimen) are then fed to the data processing programs to recompute thermal conductivity. The results of recomputations of λ from these computer simulations for a vertical window and for a horizontal window are presented in Figs. 8 and 9, respectively. When operating on simulated computer profiles (smooth and free of noise), both polynomials and splines are adequate and provide similar results. Recomputations of thermal conductivity with a vertical window show a slight positive bias (of the order of 0.015%) with all relative differences being between 0.005 and 0.025% (see Fig. 8). The same recomputations for a horizontal window show typical relative differences in the band $\pm 0.025\%$, with one point with a maximum relative difference of -0.1% (see Fig. 9).

5. CONCLUSIONS

The evaluation of thermal conductivity from a set of temperature profiles obtained in a dynamic experiment is not a trivial task. Computations in absolute space are possible but require large amounts of interactive computer time. Simpler computation techniques are available when operating in tube-space and the procedures to obtain thermal conductivity as a

function of temperature (vertical window) or at a constant temperature (horizontal window) have been described in detail. For the latter method, a new form of the partial differential heat transfer equation has been presented.

Computer simulations of heating experiments in tube-space indicate it is possible to compute thermal conductivity from simulated temperature profiles with adequate precision, the computational error being less than 0.1%. Further work in this area is necessary, both to obtain the profiles in absolute space and to simulate the cooling phase of the experiment, because profiles collected during cooling depend only on three properties (heat capacity, hemispherical total emittance and thermal conductivity) and heat conduction becomes an important factor as cooling progresses.

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