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NONLINEAR LEAST SQUARES — AN AID TO THERMAL PROPERTY DETERMINATION

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16. Abstract

Nonlinear least squares techniques can be used to determine effective thermal conductivity values from experimental data. Comparisons between measured and predicted conductivity values indicate that the analytically determined values can be used with confidence in performing thermal protection system analyses. A study was performed to compare the relative efficiencies of different minimizing techniques; the method of Peckham was the most efficient.

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NONLINEAR LEAST SQUARES — AN AID TO THERMAL PROPERTY DETERMINATION

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SUMMARY

Nonlinear least squares techniques are applicable to solving problems associated with thermal property determination. Of the techniques discussed in this paper, the method of Peckham is shown to be the most efficient. Effective thermal conductivity values were determined using in-depth thermal response data from both atmospheric and reduced pressure tests. As shown, the predicted values compare favorably with measured thermal conductivity results. The results of this study show that the combination of nonlinear least squares and thermal analysis offers a more efficient tool for use in the design of experimental testing and in obtaining reliable thermal property information.

INTRODUCTION

The design and the development of a reusable thermal protection system for the space shuttle require detailed investigations of various material classes and configurations in addition to a knowledge of the thermophysical properties of the materials. These properties are normally obtained from standardized tests; however, before exhaustive property determination tests are conducted, it is desirable to perform thermal protection system analyses, because the results of these analytical studies can be used to minimize the number of materials to be considered.

Of special interest are analytical methods that permit the evaluation of thermal response data obtained from a single experiment. Many papers discussing the identification of parameters using nonlinear regression analysis and the inverse heat conduction problem are available (refs. 1 to 6). The calculation of the surface heat flux and the surface temperature from an in-depth temperature-history measurement is termed the inverse solution; the estimation of thermal property values from experimental in-depth temperature data is classified as a parameter identification problem. The motivation for the investigation presented in this paper was the work done by Pfahl and Mitchel (ref. 6) and by Williams and Curry (ref. 7).

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Pfahl and Mitchel indicated that a least squares technique could be used to obtain realistic values for thermal properties of ablating materials. The method they used was a variant of the method developed by Levenberg (ref. 8) and modified by Marquardt (ref. 9). Pfahl and Mitchel did not compare this method with other techniques. A comparison of the relative efficiency of different techniques in determining thermal properties is given in this paper. Also, it can be shown that meaningful property determination (that is, thermal conductivity) can be obtained from tests not designed to measure the thermophysical properties by using nonlinear least squares techniques.

SYMBOLS

a_i	coefficients for the effective thermal conductivity polynomial
F^2	sum of squares of the residuals
f	a vector of residuals to be minimized
f_k	the kth component of f
G	matrix of partial derivatives with components g_{ki}
g_{ki}	$\partial f_k/\partial x_i$
h	vector with components h_k
h_k	first term in the Taylor series expansion of f_k about x_o
K_c	thermal conductivity due to solid conduction
K_e	effective thermal conductivity
K_g	thermal conductivity of free gas
K_R	thermal conductivity due to radiation through a solid
K_{rs}	thermal conductivity due to solid conduction and radiation
L	thickness of the specimen
L_f	mean free path of molecule fibers
L_g	mean free path of gas molecules

N	backscattering cross section per unit volume
P	porosity of the specimen
S	sum of squares of the residuals to be minimized
T	temperature
T_{ij}	predicted temperature of the ith thermocouple at the jth time measurement
T^*_{ij}	measured temperature of the ith thermocouple at the jth time measurement
T_o	temperature of the specimen at the surface
T_2	temperature of the specimen at the back wall
TC_i^+	temperature above the nominal for the ith thermocouple
TC_i^-	temperature below the nominal for the ith thermocouple
W_j	a positive weighting factor for the jth constraint
x	a vector of control parameters
x_i	the ith control parameter or independent variable
x_j^H	highest permitted value for x_j
x_j^L	lowest permitted value for x_j
δ	correction to ξ along which S is minimized
ϵ_L	emissivity at the specimen back wall
ϵ_o	emissivity at the specimen surface
λ	scalar quantity to minimize S from ξ along δ
ξ	independent variables used to minimize S
σ	Stefan-Boltzmann constant

σ_T standard temperature deviation

ϕ penalized performance index

$\tilde{\phi}$ performance index to be minimized

ψ_j constraints placed on ϕ

THEORETICAL FORMULATION

Several numerical optimization methods and nonlinear least squares techniques were examined to determine the relative efficiency of each technique in determining thermal conductivity. The techniques ranged from simple ones such as adaptive creep and steepest descent to sophisticated techniques such as those devised by Peckham (ref. 10) and Powell (ref. 11). The two most efficient techniques, which were developed by Powell and Peckham, reduced the number of function evaluations by more than 600 and 1000 percent, respectively, when compared to Davidon's (ref. 12) method. All minimizing techniques examined did not require special formulations for the perturbation equations but used numerical procedures to obtain the effects of parameter variations. An implicit thermal model was used with these techniques. The primary difference in the efficiencies of the numerical optimization techniques and the methods based on the nonlinear least squares are shown in the difference in the basic formulation.

Numerical Optimization

The general nonlinear optimization problem is concerned with finding the extremum of a performance index of the form

$$\tilde{\phi} = \tilde{\phi}(x) \tag{1}$$

where x is an n dimensional vector with components x_j, subject to an m vector of constraints

$$\psi_j = \psi_j(x) \tag{2}$$

The x_j are independent variables (control parameters) the values of which are to be determined such that equation (1) is an extremum subject to the constraints in equation (2). If the constraints are applied directly to the independent variable

$$x_j^L \leq x_j \leq x_j^H \tag{3}$$

where $j = 1, 2, \ldots, m$, then a region of control space is defined within which the solution must lie. Problems involving equality constraints can be treated as unconstrained problems by replacing the actual performance index with a penalized performance index ϕ, where

$$\phi = \tilde{\phi} + \sum_{j=1}^{m} W_j \psi_j^2 \tag{4}$$

If the W_j values are sufficiently large in magnitude, minimization of equation (1) subject to the constraints of equation (2) is equivalent to the minimization of the unconstrained performance index defined by equation (4). By means of this approach, search techniques for finding unconstrained minima can be applied in the solution of constrained minima.

Various numerical procedures have been developed to solve parameter optimization problems. Most of the search techniques were based on the reduction of the multidimensional control space to a succession of steadily improving searches along a vector. Thus, the search technique can be thought of as a one-dimensional search technique. The numerical search for the minimum of $\tilde{\phi}$ can be performed in a local region by most methods, but none can guarantee the global minimum. The object of these numerical methods is to isolate the minimum performance index as rapidly as possible, often without knowledge of the characteristics of the response surfaces. A measure of the effectiveness of the various search techniques used in this report is the number of evaluations required to locate the minimum.

Least Squares

In the least squares formulation, a vector of variables $x = x_1, x_2, \ldots, x_n$ is defined for which a minimum value for S is to be determined, where

$$S = \sum_{k=1}^{m} \left[f_k(x)\right]^2 \tag{5}$$

In a linear approximation

$$f_k = h_k + \sum_{i=1}^{n} g_{ki} x_i$$

or in matrix notation

$$f = h + Gx \tag{6}$$

The value of x at the minimum (x_o) is given by

$$G^T G x_o = -G^T h \tag{7}$$

If the gradients g_{ki} are available, these equations can be solved for x_o. Because, in general, the f_k are not linear in x, x_o will not be the true minimum and is used for the starting value of x for the next iteration. At this point, equation (7) represents the standard solution to the least squares problem and $G^T G$ is positive definite because x is assumed not to be at a stationary point. Also

$$\frac{\partial}{\partial \lambda} S(\xi + \lambda\delta)\Big|_{\lambda=o} < 0 \tag{8}$$

because ξ is not a stationary point of S. To guarantee convergence, a positive value of λ may be developed to minimize $S(\xi + \lambda\delta)$ (for example, λ_m) then $\xi + \lambda_m\delta$ will approximate the minimum. If the second-order partial derivatives are not zero, the quadratic convergence depends on having the magnitude of the correction of the same order as the functions. An error in the derivatives by δ is acceptable and does not jeopardize convergence. In any case, the least squares method hinges on the approximation that the second-order partial derivatives can be ignored in the simulation. The term is of order δ if f_k is linear in the variables; and, in all other cases, the convergence of the procedure will only be linear. The correction to ξ is calculated by solving equation (7). In the iterative procedure, $\xi + \lambda_m\delta$ is chosen as the new starting point. Therefore, in the least squares formulation, an advantage is gained because the local effects of the gradient are directly related to each control parameter; however, in multivariable optimization, only the composite effect is observed.

THE CONDUCTIVITY PROBLEM

The material investigated in this study is a rigidized fibrous insulation. The porosity and transparence of the material permits heat transfer to occur by conduction and radiation. Analytical studies (ref. 13) have shown that the effective thermal conductivity K_e can be expressed as

$$K_e = K_c + K_R \tag{9}$$

where K_c is the conductivity due to conduction and K_R is the conductivity due to radiation. The conductivity due to radiation is given by

$$K_R = \frac{\sigma L \left(T_o^4 - T_L^4\right)}{\left(\frac{1}{\epsilon_o} + \frac{1}{\epsilon_L} - 1 + NL\right)\left(T_o - T_L\right)} \tag{10}$$

where σ is the Stefan-Boltzmann constant, T_o and T_2 are the bounding surface temperatures, ϵ_o and ϵ_L are the bounding surface emittances, L is the sample thickness, and N is the backscattering cross section per unit volume. A more complete expression (ref. 14) that includes the contribution by gas conduction is given by

$$K_e = K_{rs} + \frac{K_g}{P}\left(\frac{L_f}{L_f + L_g}\right) \tag{11}$$

where K_{rs} is the contribution by solid conduction and radiation, K_g is the conductivity of free gas, P is the porosity, and L_f and L_g are the mean free paths of molecule fibers and gas molecules, respectively. The effective conductivity can be expressed as a polynomial in temperature with coefficients composed of unknown property values. The model used in this study is

$$K_e = a_o + a_1 T + a_2 T^2 + a_3 T^3 \tag{12}$$

where the unknown coefficients a_i are to be determined such that the difference between the desired temperatures and the predicted temperatures is a minimum. If T_{ij} is the temperature at the ith thermocouple and jth time measurement, the least squares problem is to minimize

$$S(a_0, a_1, a_2, a_3) = \sum_{j=1}^{m} \sum_{i=1}^{n} \left(T_{ij} - T^*_{ij}\right)^2 \tag{13}$$

where T^*_{ij} is the desired temperature.

The optimization problem is to minimize

$$\phi = \tilde{\phi} + \sum_{K=1}^{n \times m} W_j \psi_j^2 \tag{14}$$

where $\psi_j = T_{ij} - T^*_{ij}$ with $K = i + (j - 1)n$ and $\tilde{\phi} = 0$.

EFFICIENCY STUDY

Several numerical optimization techniques and nonlinear least squares techniques were used to solve the thermal conductivity problem. The standard least squares and most of the numerical optimization techniques either converged too slowly to be of use or did not converge at all. The only numerical optimization scheme evaluated that was of value to the current investigation was Davidon's method. However, it was necessary to adjust the initial metric to account for the large derivatives. The successful least squares techniques that were examined were a least squares with a Levenberg correction, the method developed by Powell, and the method developed by Peckham. With all these techniques, realistic values of effective thermal conductivity as a function of temperature were achieved for an analytical test model subjected to a low heating rate with an acceptable tolerance of $\pm 0.1°$ R for each temperature prediction. Typical results for Powell's method are shown in table I. The least squares techniques were superior to Davidon's method in achieving convergence. Davidon's method required 229 function evaluations to achieve convergence compared to 61 for Levenberg, 39 for Powell, and 21 for Peckham (table II). To differentiate better between the least squares techniques, an additional analytical test was simulated using a higher heating rate with an acceptable tolerance of $\pm 2°$ R for each temperature prediction. Again, Peckham's method was superior in achieving convergence, with only 17 function evaluations as compared to 31 for Powell (table III).

ERROR ANALYSIS

Results using numerically generated data show that least squares techniques can be used to calculate thermal properties. For the analytical verification studies, the same mathematical formulation controls the thermal model for both the generation of data and the prediction of thermal conductivity. However, under actual test conditions, some of the assumptions used in formulating the mathematical model are violated. For instance, with a one-dimensional thermal model, it is impossible to account for any two-dimensional conduction that may exist. Because the thermal conductivity is independent of the test conditions, any differences observed in the calculated thermal conductivity values may be attributed to measurement errors, such as errors caused by uncertainties in the location of the thermocouple. Accordingly, an investigation was performed to determine the effects of variations in thermocouple location on thermal conductivity.

This investigation consisted of (1) comparing different conductivity values at different heating rates using the same specimen and (2) using similar data at different times when results from only one test were available. The results of this investigation indicate that it may be possible to assess the directional effects of errors in thermocouple location. The following procedure was used to assess the effects of errors in thermocouple location. A positional error for the ith thermocouple, which produces a temperature above the nominal, was designated as TC_i^+; conversely, TC_i^- designates a positional error that produces a temperature below nominal. Nominal means that there is no positional error in the thermocouple location. A positional error equivalent to the thermocouple wire diameter (0.01 inch) was assumed. Four thermocouples are used; the fourth is maintained at its nominal position. This allows for the following four different cases to be examined for both TC_1^+ and TC_1^-.

1. Case a: TC_2^+, TC_3^+
2. Case b: TC_2^+, TC_3^-
3. Case c: TC_2^-, TC_3^-
4. Case d: TC_2^-, TC_3^+

Of primary interest are the results obtained for TC_1^+ (cases c and d) and for TC_1^- (cases a and b). These combinations result in the largest least squares error and associated errors in the predicted thermal conductivity. Typical results for heating rates of 15, 20, and 30 Btu/ft^2-sec are shown in figures 1 and 2. In general, the results for figure 1 give lower values of conductivity than would be predicted using nominal thermocouple locations. The conductivity increased with increasing heating rate at the higher temperatures for this case. Conversely, the results shown in figure 2 indicate that the highest values of conductivity were obtained using the lower heating rates and that these values were greater than would be predicted using nominal thermocouple locations.

EXPERIMENTAL VERIFICATION

Convective Tests

Thermal evaluation tests have been conducted in the NASA Manned Spacecraft Center 10-megawatt arc-heated facility on test models fabricated from LI-1500, a surface-insulation material that is being developed for potential application on the space shuttle. The primary objective of the tests was to demonstrate the reusability of the material system for temperatures between 2500° and 3000° R. The test specimens were 4-inch-diameter flat-faced cylinders with a nominal thickness of 2 inches. Each model contained chromel/alumel thermocouples installed in depth to allow monitoring of the thermal response of the material. The tests were conducted over a range of gas enthalpy levels from 4000 to 6000 Btu/lb, heat transfer rates from 12 to 22 Btu/ft^2-sec, and model impact pressure levels from 0.0023 to 0.0027 atmosphere. Three test runs identified as tests 302, 304, and 308 were selected as typical. The heating rates for these tests were 14.2, 16.8, and 21.4 Btu/ft^2-sec, respectively. Conductivity values predicted on the basis of these tests are shown in figure 3. Tests 302 and 304 were in close agreement and had a standard temperature deviation σ_T of 2.2° and 2.6° R, respectively. Test 308 had a σ_T value of 9.6° R but provided conductivity values that closely approximated experimentally determined values, indicating that an error could exist in the in-depth position of the thermocouples. Based on the previous analyses of these positional error effects, the thermocouple locations were changed in the thermal model. Predicted thermal conductivity values are shown in figure 4. The corresponding values of σ_T were 1.7°, 3.2°, and 7.3° R for tests 302, 304, and 308, respectively.

Radiant Tests

A series of radiant heating cycles were performed on a specimen of the surface-insulation material in radiant-lamp facility at a pressure of 1 atmosphere. The specimen was a 4-inch-diameter flat-faced cylinder instrumented with four 0.01-inch-diameter chromel/alumel thermocouples. Four thermocouples were located in the center of the specimen at depths of 0.30, 0.50, 1.0, and 1.5 inches from the heated surface. The thermocouple junction was placed on a 0.50-inch-diameter cylindrical plug of LI-1500 that was inserted into the specimen. The other thermocouples were installed in the same manner, using four LI-1500 plugs for the installation. The thermocouple wires were carefully located around the circumference of the plugs and extended out of the bottom of the specimen.

Predicted thermal conductivity results using the 1-atmosphere radiant test data are shown in figure 5 for maximum times of 540, 600, and 740 seconds. Significant variations in thermal conductivity predictions using these various times were obtained.

The previous analysis for errors in thermocouple location was used as a guide, and the thermocouple locations were changed in the thermal model. Conductivity results obtained from these revised locations are shown in figure 6. A comparison of figures 5 and 6 shows that the standard temperature deviation σ_T has been reduced by approximately 50 percent and a better correlation of conductivity values was obtained.

Thermal Conductivity Tests

For comparative purposes, thermal conductivity values obtained by guarded-hotplate and radial in-flow apparatus (ref. 15) are shown in figures 3 to 6. Although the values of thermal conductivity obtained using nonlinear least squares do not agree at every point with the values obtained by these standard experimental methods, the general agreement is considered good. It should be noted that the arc-jet and radiant tests were designed to show material thermal response and reusability and the thermocouples were installed to provide secondary information. However, analyses made using the measured guarded-hotplate conductivity values will not reproduce the in-depth thermal response; analyses using the values determined by the nonlinear least squares analysis will reproduce the response. Finally, because the tested materials were early prototype specimens, some differences in the thermal conductivity values may be attributed to variations in material.

CONCLUSIONS

Nonlinear least squares techniques can be readily applied to solving the difficult and realistic problems associated with thermal property determination. The results obtained can be used with confidence for thermal protection system design analysis. The most successful nonlinear least squares technique, which was one developed by Peckham, used an implicit thermal model to solve the heat equation. The effects of positional errors in the thermocouple location were significant; but, when these errors were accounted for in the thermal analysis, the least squares error could be reduced. By taking the positional errors into account, meaningful thermophysical property values can be determined from simply instrumented tests.

Thermal conductivity values were obtained from the in-depth thermal response of experimental models as a function of temperature at both atmospheric and reduced pressures. These values compared well with values measured directly. This study illustrates the capability and applicability of the least squares program for property determination. Although the theory and numerical methods are not new, it is believed that the combination of nonlinear least squares and thermal analysis offers a new, more efficient tool to be used in the design of experimental testing and a rapid technique for obtaining reliable thermal property information required in the preliminary design of a thermal protection system.

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908-42-02-00-72

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TABLE I. - COMPARISON OF PREDICTED CONDUCTIVITY BY POWELL'S METHOD TO ACTUAL CONDUCTIVITY FOR LI-1500 USING TEMPERATURE-TIME HISTORY OF A THERMOCOUPLE

Temperature, °R	Conductivity, Btu/ft-hr-°R	Predicted conductivity, Btu/ft-hr-°R	Error, percent
660	0.0277	0.0275	0.72
860	.0324	.0324	.00
1260	.0439	.0446	-1.59
1960	.0745	.0762	2.28
2460	.1102	.1093	-.82
2960	.1583	.1534	-3.10

TABLE II. - COMPARISON OF EFFICIENCY OF NONLINEAR MINIMIZING TECHNIQUES IN SOLVING FOR THERMAL CONDUCTIVITY

Method	Number of iterations	Number of function evaluations
Davidon	10	229
Levenberg	12	61
Powell	10	39
Peckham	14	21

TABLE III. - COMPARISON OF EFFICIENCY OF NONLINEAR LEAST SQUARES TECHNIQUES IN SOLVING FOR THERMAL CONDUCTIVITY

Method	Number of iterations	Number of function evaluations
Levenberg	32	161
Powell	9	31
Peckham	12	17

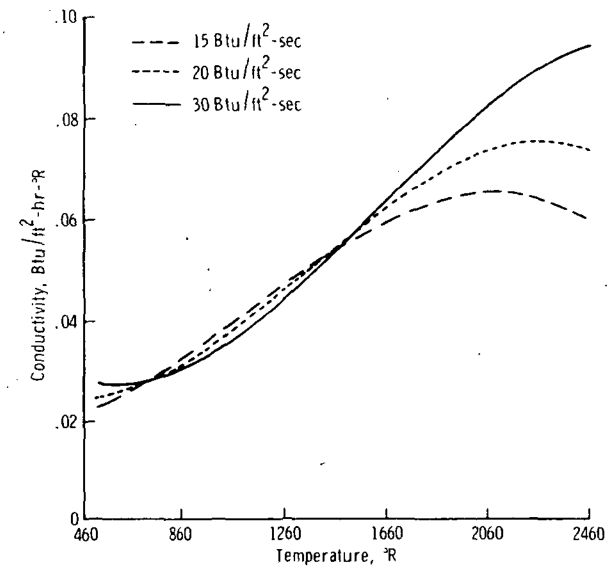

Figure 1. - The effects of thermocouple location error on thermal conductivity for different heating rates for TC_1^+, case d.

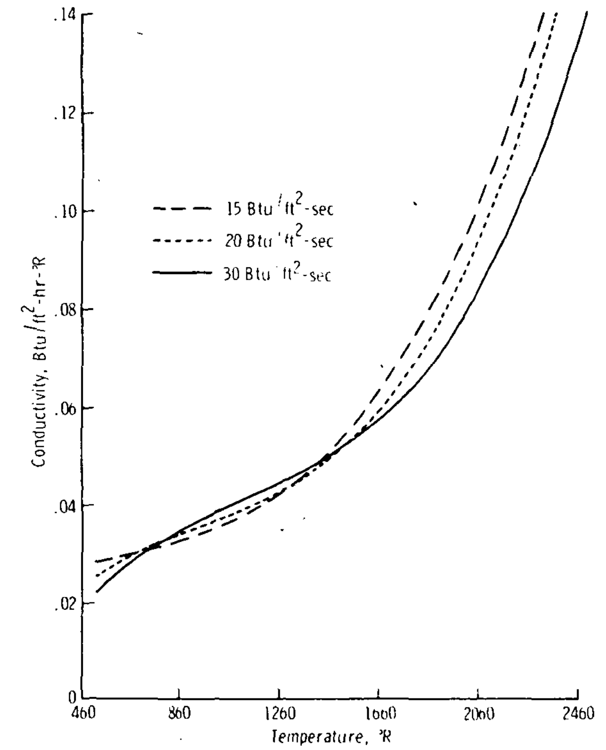

Figure 2. - The effects of thermocouple location error on thermal conductivity for different heating rates for TC_1^-, case b.

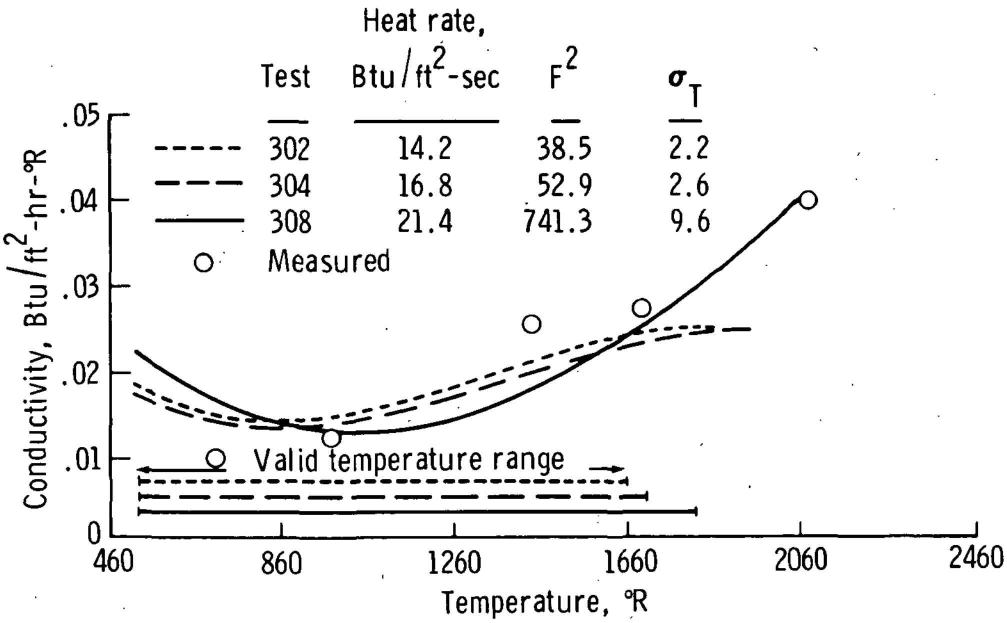

Figure 3. - Calculated values of thermal conductivity at reduced pressure (arc-jet test data).

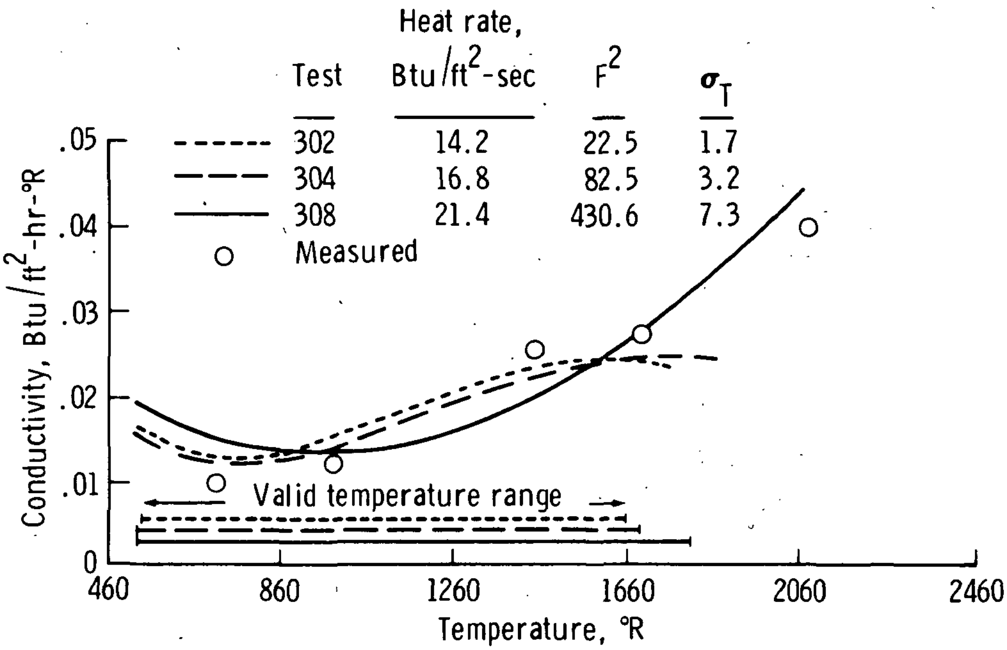

Figure 4. - Calculated values of thermal conductivity at reduced pressure with thermocouple locations analytically translated (arc-jet test data).

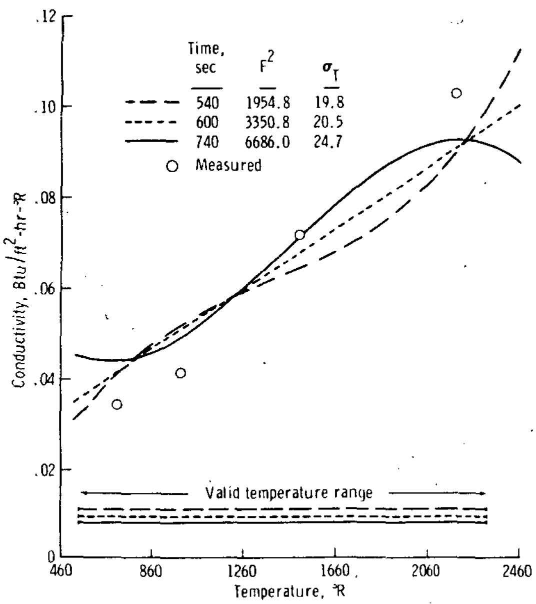

Figure 5. - Calculated values of thermal conductivity at atmospheric pressure (radiant test data).

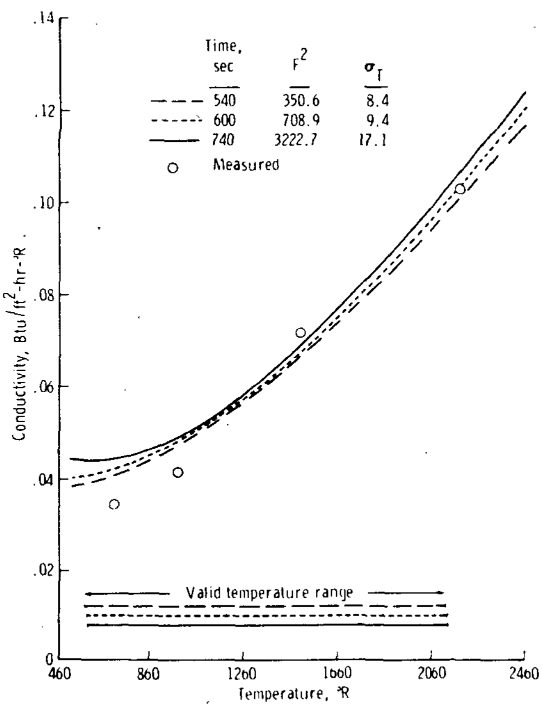

Figure 6. - Calculated values of thermal conductivity at atmospheric pressure with thermocouple locations analytically translated (radiant test data).