HTD-Vol. 340, National Heat Transfer Conference
Volume 2
ASME 1997

APPLICATION OF REUSABLE INTERFACE TECHNOLOGY FOR THERMAL PARAMETER ESTIMATION[1]

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ABSTRACT

A Reusable Interface Technology is presented for application to thermal parameter estimation problems. It is applied to the estimation of thermal conductivity of compacted Al_2O_3 powder without binder. As temperature increases, the thermal conductivity of Al_2O_3 powder without binder decreases.

INTRODUCTION

Thermal parameter estimation using partial differential equation models in conjunction with experimental temperature measurements is slowly becoming an accepted way of estimating thermal properties such as specific heat, thermal conductivity, and emittance. This approach involves developing a computational model of the energy equation for the geometry/initial conditions/ boundary conditions of interest, predicting temperatures at temperature sensor locations, and choosing thermal properties such that a mean square error between data and model is minimized. Examples of this approach can be found in Pfahl (1970), Hills (1987), Courville and Beck (1987), Schisler (1988), Beck (1993), Dowding, et. al. (1995, 1996), and Blackwell, et. al. (1996a).

All of these approaches have a common feature; a thermal analysis code has been turned into a subroutine of a parameter estimation code. Each of these combined codes required a considerable amount of time to make source code modifications and to verify that the resulting code is error free. Once the thermal analysis code becomes a subroutine of the parameter estimation code, the connection between the original developers of the thermal analysis code and the new parameter estimation/thermal analysis code may be severed. This means that any future enhancements to the thermal analysis code may be difficult and time consuming to implement in the combined code.

A better approach is to isolate the interface mechanisms from the optimization and analysis codes such that both codes are allowed to evolve independently. That is, rather than modifying the source code of the thermal analysis package to convert it into a subroutine, allow the optimization and analysis systems to follow independent development paths and build reusable communication links between them. Moreover, if these isolated interface mechanisms are built in a general, reusable manner, then the amount of work required to update the interfaces for new code versions can be minimized and sometimes eliminated entirely. This approach is designated Reusable Interface Technology.

In many organizations, the trend is toward commercial thermal analysis software. Not every organization can afford the luxury of maintaining their own thermal analysis software. Consequently, the end user may not have access to source code for the thermal analysis module. In this case, making the thermal analysis code into a subroutine of the parameter estimation code is not only difficult to maintain, it is likely infeasible. These observations point clearly to the need for an alternative approach to parameter estimation involving complex physical models. Reusable Interface Technology satisfies this need.

OVERVIEW OF REUSABLE INTERFACE TECHNOLOGY

In order for the thermal analysis code development to be independent of the optimization code development, it is desirable to employ a flexible, reusable communication mechanism which does not require modification of either the thermal analysis or the optimization packages. This approach will ensure that the two codes are always compatible and will allow the two development teams to work independently of each other. The DAKOTA iterator toolkit [Eldred, et. al. (1996a, 1996b) and DAKOTA] implements Reusable Interface Technology within an object-oriented frame-

1. This work was supported by the United States Department of Energy under Contract DE-AC04-94AL85000.
2. Distinguished Member of Technical Staff, Fellow ASME.
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work of “plug-and-play” libraries of iterative algorithms, system-level strategies, and simulation interfaces.

In DAKOTA, simulation interfaces are implemented in terms of communication protocols, such as CORBA, MPI, and file-based I/O, and specialized function evaluation interfaces, such as the Application Interface, the Test Function Interface, the Approximation Interface, and the Multidisciplinary Optimization Interface. The simplest example of a DAKOTA interface is the Application Interface, which utilizes system calls and file-based I/O for process spawning and data communication, respectively. The Application Interface approach is sufficient for this parameter estimation application since the thermal analysis and optimization programs are executed on the same machine.

A schematic of the Application Interface is given in Figure 1. The Application Interface isolates application specifics from an iterator method by providing a generic interface for the mapping of a set of parameters (e.g., a vector of design variables) into a set of responses (e.g., an objective function, constraints, and/or sensitivities). Housed within the Application Interface are three pieces of software. The input filter program (“IFilter”) provides a communication link which transforms the set of input parameters into input files for the simulator program. The simulator program reads the input files and generates results in the form of output files or databases. Finally, the output filter program (“OFilter”) provides another communication link through the recovery of data from the output files and the computation of the desired response data set. Generally, the application developer (e.g., the thermal parameter estimation investigator) will develop these input and output filters for the particular analysis code of interest using whichever programming or scripting language is most convenient. If care is taken to develop quality filter programs, then libraries of input and output filters can be built up over time, thereby maximizing reuse and minimizing reinvention. Moreover, the amount of work required to update the filter programs for new analysis and optimization package versions can be minimized and sometimes eliminated entirely.

This mapping of parameters to responses provides generic information to the iterator/estimator (the data flows are abstract and method-independent), and the application and implementation specifics are hidden. This encapsulation of complexity through abstract APIs is an essential part of providing a flexible and extensible capability for systems analysis in general, and thermal parameter estimation in particular. Furthermore, having hidden the specifics of the simulation and systems analysis in use, the abstract data flows between iterator and simulation enable application of the full suite of DAKOTA capabilities on the problem of interest. Various capabilities can be selected among methods for parametric analysis, optimization, uncertainty quantification, or parameter estimation, and these methods may be used in a complementary fashion to address a variety of engineering issues in design, surety, estimation, and nondeterministic analysis. The availability of suites of methods increases the chances of success, leads to experimentation, and enhances understanding. In addition, production usage and leading-edge research are both supported. Whereas novice users may employ a single algorithm using files and system-calls on a single machine, advanced users may employ multi-method strategies (e.g., hybridization, sequential approximate optimization, optimization under uncertainty) employing the latest asynchronous communication protocols for distributed and massively parallel computing.

DETAILS OF REUSABLE INTERFACE TECHNOLOGY

For the simple Application Interface discussed previously, the names of the input filter, analysis, and output filter executables are provided in the DAKOTA input. These executables will be invoked by the DAKOTA system synchronously and in immediate succession (asynchronous execution of multiple parallel processes is also available but is not used here). The specific form and function of these executables is entirely independent of the DAKOTA system and can be implemented in whichever programming or scripting language is most convenient. These details are presented next.

All the calculations presented here were run on UNIX™ work stations. A shell script was used run the various codes in sequence. The Output Filter was a FORTRAN code that reads data files containing the experimental temperatures and the computed temperatures, computes the mean square error S, and writes S to a file to be read by the iterator.

The input filter is somewhat more complicated. The input to a large scale finite element, finite difference, or finite volume code

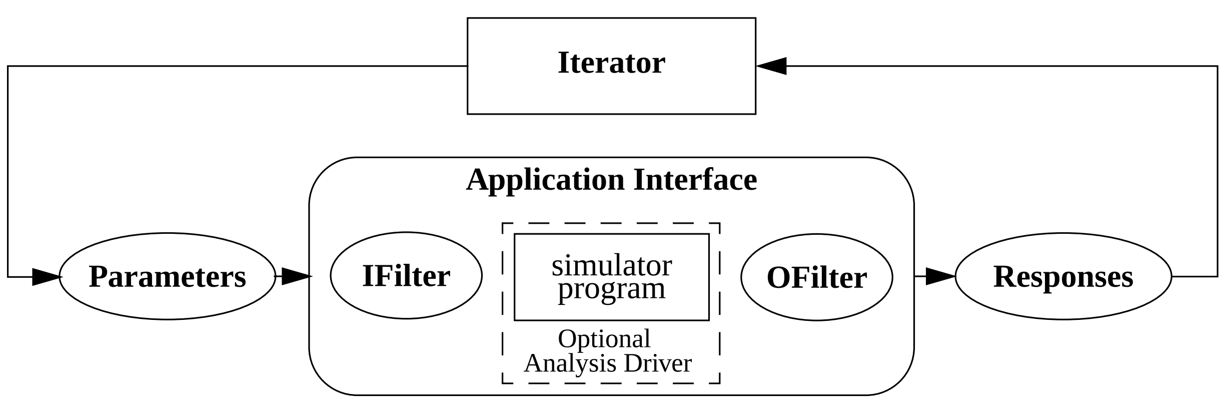

Figure 1: Reusable interface technology-the Application Interface.

has a certain amount of structure to it. For each simulation, this input deck has to be rebuilt automatically without human intervention. This involves inserting the latest parameter values into the appropriate location in the input data file. The UNIX™ facilities **sed** and **awk** could be used to perform some of these operations. Instead, we chose to use an algebraic preprocessor APREPRO (Sjaardema, 1992) which allows one to build an input deck in symbolic form. For example, if the unknown thermal conductivity at temperature T_1 is given the symbolic name {cond_1} in the input file and a 2nd file containing the line {cond_1 = 0.417} is read by APREPRO, the output from APREPRO will be a line containing the number 0.417. In effect, APREPRO replaces an alpha string by a numeric string. This code was originally developed to aid in the preparation of multiple input data files for parameter studies, and was ideally suited for the task at hand. The output from the iterator is a list of the latest parameters along with an alpha-numeric identifier; a simple FORTRAN code was written to translate the parameter list into a string that can be read by APREPRO.

EXPERIMENTAL PROCESSING FURNACE

As a demonstration of this methodology, we will estimate the thermal conductivity of compacted Al_2O_3 powder without binder present. Figure 2 is a schematic of the furnace designed to study the binder burnout phase of ceramic processing. The heating element was fabricated from a hollow threaded ceramic rod 0.635 cm ID, 1.27 cm OD (0.25 in ID, 0.5 in OD) with 16 turns/in of 24 gauge nichrome wire. The volume of the hollow portion of the heating element was filled with zirconia insulation (compacted to a density of approximately 96 Kg/m^3, 6 lbm/ft^3) in order to minimize convection losses from the heater inner surfaces. The active length of the heating element was 9.843 cm (3.875 in). In order for both the electrical leads to begin and end at the bottom of the heating element and to minimize potential cross-talk from stray electromagnetic radiation, a twin parallel thread arrangement was used (e.g., like a striped barber pole). Additional details of the furnace can be found in Blackwell, et.al. (1996b).

When this processing furnace was originally designed, no consideration was given to using it to estimate thermal conductivity. Consequently, it was not optimized for thermal conductivity measurements; some of these deficiencies are discussed in a subsequent section. After preliminary binder burnout experimental results were obtained, it was decided to attempt to extract thermal conductivity information from the temperature measurements. This paper presents the results of the thermal conductivity estimation.

SAMPLE PREPARATION

The green ceramic samples were prepared by pressing a powder compact of spray dried 94 wt% Al_2O_3 powder containing 3 wt% of a 50/50 mixture (by weight) of methylcellulose and hydroxypropylcellulose binder. Ceramic annuli of approximately 6.7 cm (2.64 in) outside diameter, 2.0 cm (0.79 in) inside diameter, and 1.3 cm (0.51 in) tall were formed by uniaxial pressing ~ 100 gm of powder in a 7.4 x 2.2 cm (2.91 x 0.87 in) stainless steel die cavity followed by isostatic pressing. Die pressing pressure of 4.4 MPa (638 psi) was used in combination with isostatic pressing pressure of 35.4 Mpa (5134 psi) to produce ~ 57% relative density compacts for testing. Fifteen type E thermocouples (0.0127 cm (0.005 in) diameter) were placed radially along the interface between adjacent samples. The primary measurement locations were along the interface between two nominally identical samples. A total of ten thermocouples were used at this primary location, two rays of five each with the two rays being 180 degrees apart. The spacing was approximately equal for each ray and the two rays were nominally identical. In reporting the data, each of the 5 pairs of thermocouples at the same radial location was averaged and reported as five thermocouples. One thermocouple was placed on

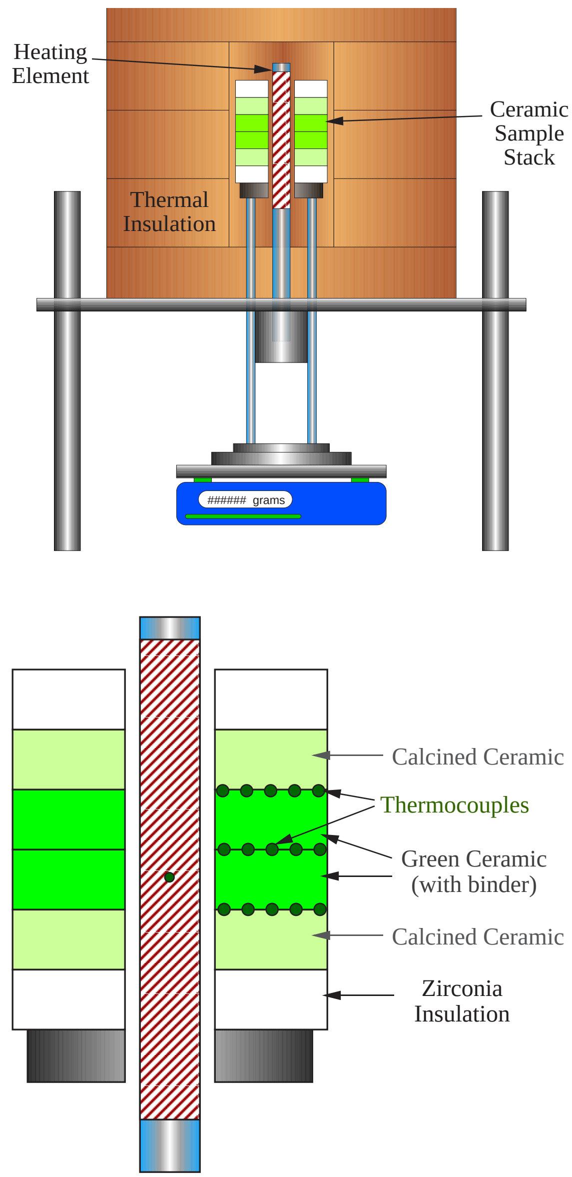

Figure 2: Schematic of binder burnout furnace with heating element, green ceramic, insulation and thermocouple locations identified.

the inside surface of the threaded ceramic rod heater, at an axial location approximately equal to the primary measurement interface. Four additional thermocouples were placed at other locations in the sample stack to give information on the asymmetry of the temperature profile. The thermocouple numbering scheme is shown schematically in Figure 3.

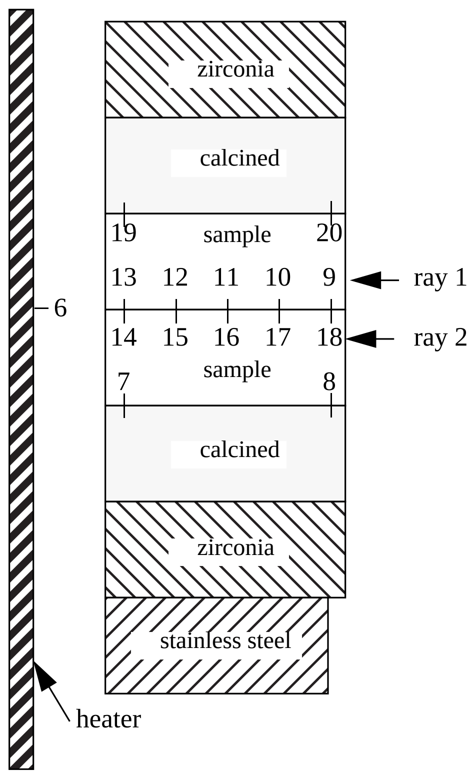

Figure 3: Schematic of axisymmetric model showing approximate thermocouple locations and numbering.

Since the weight of the sample stack was to be monitored continuously during the binder burnout phase of the experiment (although not reported here), a gap was maintained between the sample stack and any surrounding material. A computer controlled data acquisition system was used to read the thermocouples and to control the 200 W power supply.

TEST PROCEDURE

All samples were prepared with binder present (see section above). The test procedure was to power the heater in a predetermined manner and thermally drive the binder from the samples. Thermocouple temperatures and heater power were monitored continuously. After a test duration of approximately 6 hours, the sample temperature was of the order of 800 K and all the binder had been removed. Separate Thermogravimetric Analysis (TGA) experiments indicated that all the binder had been removed by the time the temperature reached 800 K. The power was then turned off and the assembly was allowed to cool overnight. Without altering the experimental setup, the heater was powered a second time and temperatures were again recorded; this experiment provided data from which the thermal conductivity of the green body without binder was estimated and will be reported here. The heater power history was chosen to produce sample temperature histories prototypical to those used during the binder burnout phase of industrial ceramic processing. If the temperature rise rate is too large, finished parts tend to crack. If the temperature rise rate is too small, productivity is reduced.

EXPERIMENTAL RESULTS

Representative experimental temperature results are shown in Figure 4. For this experiment, the heater power varied linearly

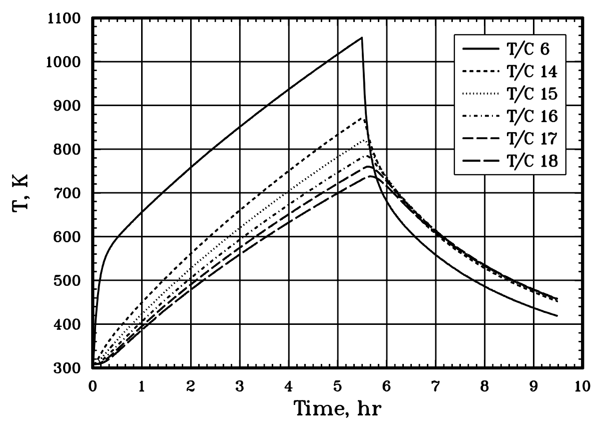

Figure 4: Heater and sample temperature history for green body without binder.

with time over the range of 25-56 W. The heater temperature rises very rapidly over the first 20 minutes of the experiment. Thereafter, the temperature rise rate of the heater is slightly less than linear. After the power is turned off, the heater temperature drops rapidly to values below the sample temperature. This is because of the small amount of energy stored in the heater relative to that stored in the sample stack as well as enhanced heat loss down the heater assembly.

THERMAL CONDUCTIVITY ESTIMATION TECHNIQUE

Parameter estimation techniques were used in this study to estimate the thermal conductivity from the temperature measurements. This technique involves developing a (numerical) model of the experimental configuration. In this case, it was assumed that the heat conduction was 2-D axisymmetric with the energy equation being given by

$$\rho C \frac{\partial T}{\partial t} = \nabla(k \nabla T) + \dot{g}''' . \tag{1}$$

This equation was solved numerically using a fully implicit Galerkin Finite Element Method, Gartling and Hogan (1994). The mesh consisted of 1975 nodes, 1787 4-node quadrilateral elements, and 189 radiation enclosure surfaces; details of the mesh are given in Figure 5. The open region between the heater assembly and the sample stack was treated as a radiation enclosure problem with a non-participating medium and was solved using the net-radiation method as described in Siegel and Howell (1981).

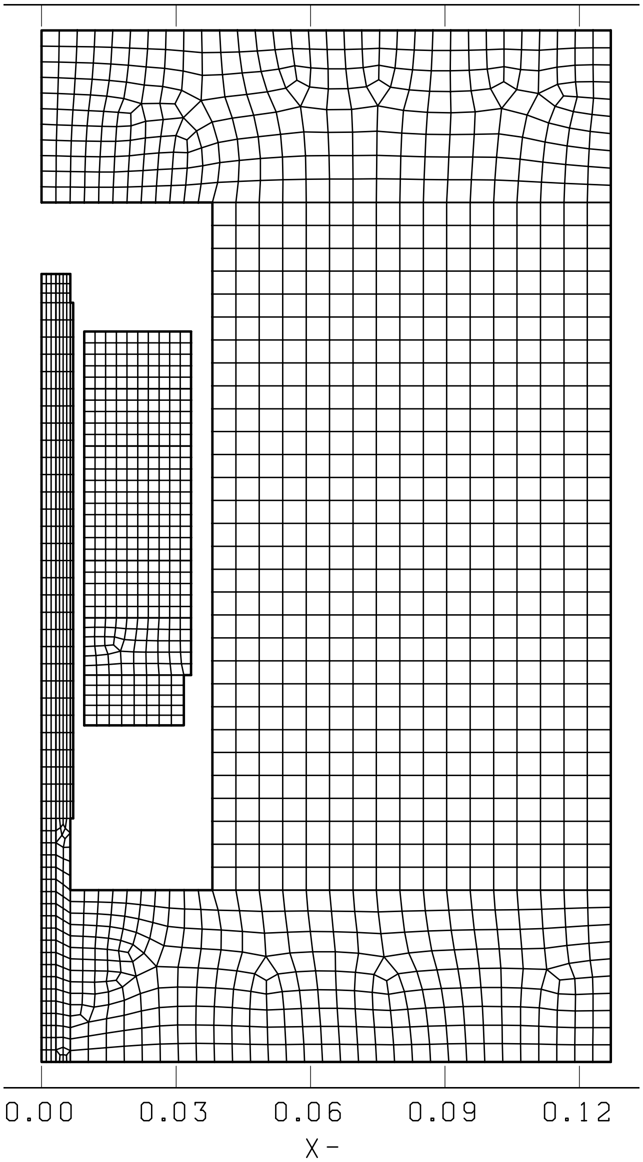

Figure 5: Finite element mesh used in the thermal model of the binder burnout furnace.

The thermal conductivity was assumed to be a linear function of temperature and of the form

$$k(T) = k_1\frac{(T-T_2)}{(T_1-T_2)} + k_2\frac{(T-T_1)}{(T_2-T_1)} \qquad (2)$$

with k_1 and k_2 being the parameters to be estimated, corresponding to the temperatures T_1 and T_2 respectively. This approach is preferable to estimating the slope and intercept of the *k* vs. *T* curve because of potential differences in order of magnitude of the parameters being estimated. The two temperatures T_1 and T_2 correspond to the nominal minimum and maximum temperature of the experimental data. The procedure is to select k_1 and k_2 such that the least square error between the experimental temperature measurements $Y_i(x_j)$ and the model results $T_i(x_j)$

$$S = \sum_j \sum_i [Y_i(x_j) - T_i(x_j)]^2 \qquad (3)$$

is minimized.

Since the heater was a threaded rod with nichrome wire wound in the thread grooves, the effective heater emittance was not known. Consequently, the heater emittance was estimated.The emittance of the green body without binder was also treated as an unknown and was estimated from the temperature data. A total of four unknown parameters were estimated from the experimental temperatures.

The model was driven by the electrical energy dissipated in the heater volume. The source term was computed by taking the measured heater power and dividing by the volume of the heater in the model.

COMPUTATIONAL RESULTS

Thermal conductivity results will be presented for an experiment in which the heater power varied linearly from 25 W to 56 W over approximately 6 hours. The cool down portion of the experiment was not modeled because the thermal model did not include a convective heat loss to a bulk fluid (air at atmospheric pressure) node inside the radiating cavity. As long as the heater was powered, this heat loss could be assumed negligible; when the heater power is turned off, this assumption is no longer valid.

A comparison between the experimental and the computational results at the sensor locations for the converged parameter values are shown in Figure 6. There is reasonably good agreement between model and data for the 5 thermocouples (each being an average of 2 thermocouples) at the interface between the samples. However, the predictions for the heater thermocouple are not in as

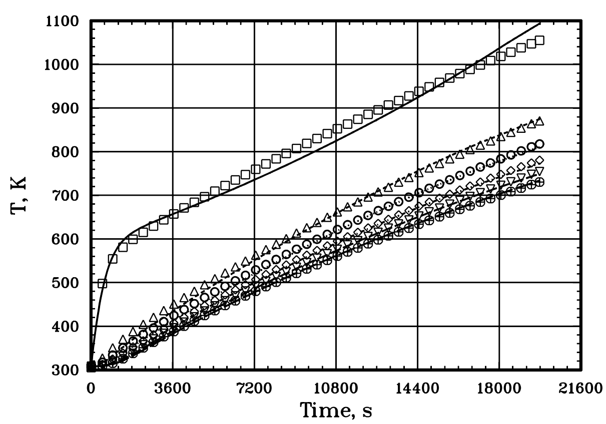

Figure 6: Comparison between experimental and computational results for converged parameter values; thermocouples are at sample interface and numbers are same as those in Figure 4; symbols represent data (444 points, not all shown).

good agreement. In fact, the slope of the predicted heater temperature (at late time) is increasing while the experimental data indicates that the slope is decreasing. This suggests that the model has bias in it; a possible explanation is that heat loss from the heater by means of convection within the radiating cavity is not accounted for.

There are four remaining thermocouples to be compared with the model; in Figure 3, these are identified as 7, 8, 19, and 20. For the results presented here, T/C 8 did not function properly. Figure

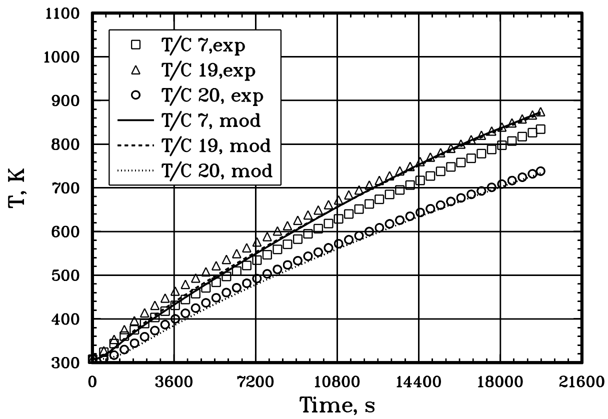

Figure 7: Comparison between model and experiment for asymmetry thermocouples.

7 presents a comparison between the model and data for those thermocouples designed to measure asymmetry in the sample temperature field. In the design of the experiment, it was hoped that the temperature field would be symmetrical about the interface between the two samples. This means that thermocouples 7 and 19 would be identical as would thermocouples 8 and 20 (in Figure 3). The experimental data shows that T/C 7 is lower than T/C19 while the model results lie nearly on top of each other. The physical asymmetry of the sample stack is consistent with the experimental results; a stainless steel washer is on the bottom of the stack but not on the top. There is also more heat conduction down the heater than up because of its construction. The trend of the model results is consistent with the experimental data; however, the predicted magnitude of the effect is not as great as the data indicates. The model and experiment for T/C 20 are in good agreement.

The results presented in Figure 6 and Figure 7 do not allow a very detailed comparison between the model and the data. A plot of the temperature residuals (defined as the experiment - model results) is a much better indicator. The temperature residuals corresponding to Figure 6 are presented in Figure 8. The heater temperature residual (T/C 6) stands out because of its magnitude. The other residuals are smaller but do not display the characteristics of a well designed experiment. Ideally, the temperature residuals should be randomly distributed around zero; clearly, this is not the case in Figure 8. The temperature residuals presented in Dowding, et. al. (1995, 1996) are examples of a well designed experiment. The temperature residuals corresponding to the results in Figure 7 are presented in Figure 9. The residual for T/C 7 is the largest; it is felt that this is due to model bias for the heat conduct-

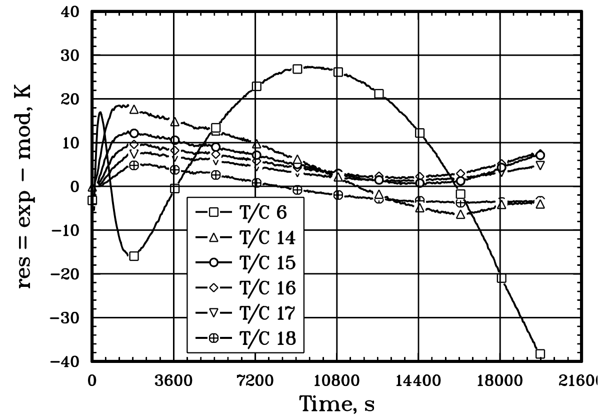

Figure 8: Temperature residuals for heater and sample interface thermocouples.

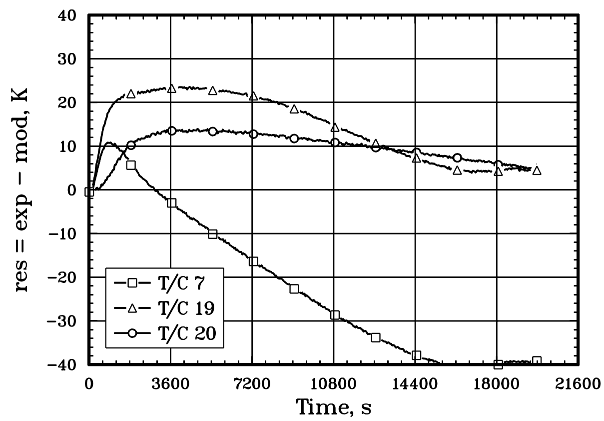

Figure 9: Temperature residuals corresponding to the results of Figure 7.

ed down the heater. Some simplifying assumptions about the heat loss from the bottom of the heater were made and it appears that they may not be valid. T/C 19 also has large residuals. The estimated parameter values are given in Table 1.

parameter	value
ε_g	0.999
ε_w	0.657
k_1 at 273 K	0.417 W/m-K
k_2 at 973 K	0.0517 W/m-K

Table 1. Converged value of parameters; dimensionless finite difference gradient parameter was 0.005.

The emittance of the green body without binder requires some discussion. The optimization package has the capability of specifying bounds on the parameter values. Physically, the emittance must be less than unity; the bounds used for this study was 0.999. The fact that the optimizer converged to the upper bound is evidence that the model has bias.

In non-linear parameter estimation, it is advisable to examine the sum-of-squares function in the vicinity of the optimized values. This can give some confidence that a global minimum was achieved. For the four parameters considered here, these results are given in Figure 10. Each parameter value has been translated

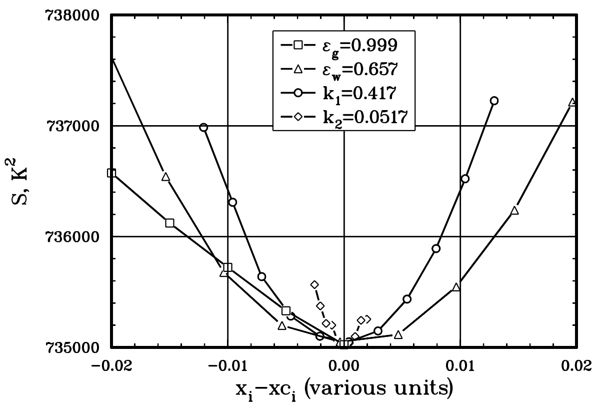

Figure 10: Sum-of-squares function as a function of parameter values; note scaling to put converged solution at 0.0.

so that an abscissa of 0.0 corresponds to the converged solution. For ε_g, S does not exhibit a minimum, as discussed earlier. The parameters ε_w and k_1 appear to be well behaved, as evidenced by the classical smooth bowl shape. The parameter k_2 does not appear to be as well behaved; however, S did not vary significantly with k_2 for the range considered.

For the converged solution presented here, 15 iterations were required with 120 function evaluations. Each function evaluation took approximately 40 minutes of CPU on a Sun SPARC 20™ work station.

PRACTICAL COMMENTS RELATIVE TO THE UTILIZATION OF THIS METHODOLOGY

The parameter estimation approach presented is certainly not a foolproof technique. Comments included here are intended to aid someone else attempting to perform calculations similar to those presented here.

The use of gradient based optimization techniques requires that the solution be smooth in the parameter space. Since we used finite difference methods to compute gradients, some of our early solutions were not sufficiently smooth for the optimizer to converge properly. For example, the initial time step we chose was related to the data sample rate (approximately 45 sec). We found that this was not small enough to produce smooth derivatives with respect to all parameters, even though the temperature field appeared smooth to the eye. Eventually, we settled on a maximum time step of 10 sec; this produced acceptable results at the expense of long run times. It was felt that the reason for the small time steps was related to the fact that the conduction/radiation solution was solved in a sequential manner instead of fully coupled. This problem goes away if the time step is sufficiently small. Given ample computing resources, the parameter estimation should be repeated with smaller allowable time steps to see if the converged values are sensitive to this parameter. For future work, we are considering analytical based methods to compute sensitivity coefficients.

This experiment was not designed with parameter estimation in mind. Consequently, the experimental configuration is not optimum in any sense. If one was not concerned with real time sample weight measurements, then the sample stack would probably have been in intimate contact with the insulation in the furnace. This would eliminate any impact that the radiative properties of the heater and sample would have on the estimated sample conductivity.

For a problem driven by a source (or heat flux boundary condition), it is possible to estimate heat capacity and thermal conductivity simultaneously. No sensitivity coefficient studies were performed for this experimental configuration to see if both heat capacity and thermal conductivity could have been estimated. For optimal experimental design, the reader is referred to Beck and Arnold (1977).

The thermal model contained eight different materials. With the exception of those properties being estimated in this study, all other material properties were obtained from handbooks. No study was done to estimate the sensitivity of these results due to uncertainties in the handbook property values. A better strategy would be to design a parameter estimation experiment with as few different material as possible and choose materials that were well characterized.

SUMMARY

The concept of Reusable Interface Technology has been discussed relative to estimating coefficients of partial differential equations. This approach allows communication between the analysis code (pde solver) and the optimization code to take place in a flexible, reusable manner. The development of these two code modules can proceed independent of each other. As new code versions are released, they can be integrated into the parameter estimation process with ease. This Reusable Interface Technology approach will allow one to perform optimization/parameter estimation using codes for which you do not have access to the source code of the analysis code (i.e., commercial analysis codes).

The techniques has been applied to the estimation of the thermal conductivity of Al_2O_3 powder without binder, valid over the temperature range of 300-800 K. The conductivity of the Al_2O_3 powder without binder decreases with increasing temperature.

ACKNOWLEDGMENTS

The following people at Sandia National Laboratories contributed to this project: R. J. Cochran developed the original finite element model; R. E. Hogan provided modifications to the thermal analysis code, and K. G. Ewsuk and J. Cesarano III acquired the experimental data used here.

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