FINAL REPORT

HIGH TEMPERATURE THERMAL CONDUCTIVITY MEASUREMENTS
OF UO_2 BY DIRECT ELECTRICAL HEATING

for

MASTER

Department of Energy
Safety Analysis Branch
Division of Reactor Development & Demonstration
Washington, D.C. 20545

by

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AC02-788T37213

Contract No. ~~EW-78-5-02-5079~~

October 1980

**ENGINEERING EXPERIMENT STATION
COLLEGE OF ENGINEERING
THE UNIVERSITY OF ARIZONA
TUCSON, ARIZONA**

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A Thesis Submitted to the Faculty of the

DEPARTMENT OF NUCLEAR ENGINEERING

In Partial Fulfillment of the Requirements
For the Degree of

MASTER OF SCIENCE

In the Graduate College

THE UNIVERSITY OF ARIZONA

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This thesis is being distributed as a final report in conjunction with DOE Contract No. EW-78-S-02-5079, High Temperature Thermal Property Investigations of Nuclear Reactor Fuels. The Thermal conductivity of UO_2 samples having specified stoichiometric composition has been determined using the electric heating technique previously developed in this department.

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ABSTRACT

This report contains further description of the investigation of high temperature properties of reactor type UO_2 pellets carried out with the Direct Electrical Heating (DEH) Facility at The University of Arizona.

Modifications to the experimental apparatus have been made so that successful and reproducible DEH runs may be carried out while protecting the pellets from oxidation at high temperature. X-ray diffraction measurements on the UO_2 pellets have been made before and after runs to assure that sample oxidation has not occurred.

A computer code has been developed that will model the experiment using equations that describe physical properties of the material. This code allows these equations to be checked by comparing the model results to collected data. The thermal conductivity equation for UO_2 proposed by Weilbacher has been used for this analysis. By adjusting the empirical parameters in Weilbacher's equation, experimental data can be matched by the code. From the several runs analyzed, the resulting thermal conductivity equation is

$$\lambda = \frac{1}{4.79 + 0.0247T} + 1.06 \times 10^{-3} \exp\left[\frac{-1.62}{kT}\right] - 4410. \exp\left[\frac{-3.71}{kT}\right]$$

where λ is in w/cm K, k is the Boltzman constant, and T is the temperature in Kelvin.

CHAPTER 1

INTRODUCTION

This report describes the continuing work that has been carried on with the Direct Electrical Heating Facility at The University of Arizona. An extensive report detailing the early work on this facility has been published (Himes 1979). A short discussion on the background of this method follows. If more description is necessary, consult either the report by Himes, or a work by Alexas and Lindner (1975). This report covers the solution of both experimental and analytical problems. Following the background discussion, the preparations necessary to enable successful experiments to be carried out are detailed (Chapter 2). Then some information and actual collected data from several experimental runs are given (Chapter 3). The analysis that is necessary to prepare the data for the model is detailed in Chapter 4. Then the preparations necessary to enable the model to adequately describe the physical response of the experiment are detailed (Chapter 5). The modeling chapter is followed by a discussion and presentation of the results of this study (Chapter 6). The report ends with Chapter 7 giving conclusions, recommendations, and a final summary.

1.1 Thermal Conductivity of Uranium Dioxide

A knowledge of the properties of uranium dioxide has become increasingly important due to the prevalence in the power reactor industry of fuels made of this material. A great many papers have been

published on the thermal conductivity of uranium dioxide. In addition, several papers summarizing the many investigations have also appeared and are most useful (Washington 1973, Brandt and Neuer 1976). The thermal conductivity of uranium dioxide depends on temperature, purity, stoichiometry, density, microstructure, and is also influenced by irradiation (Holden 1966). These many factors, plus the difficulty involved in taking measurements at high temperatures account for the scattered thermal conductivity data which is presented in the Thermo-physical Tables (Touloukian 1970). If only data for uranium dioxide specimens which closely resemble actual reactor fuel are taken, the scatter is greatly reduced, but still evident at higher temperatures (above 1600 C). Therefore, another study using a different method which is most applicable at high temperatures was undertaken. In addition, this investigation can collect data past the point where part of the material is molten, thereby gaining more information on a little known value--the thermal conductivity of molten uranium dioxide.

Many expressions modeling thermal conductivity equations have evolved from the various investigations. Some of these are purely mathematical using high order polynomial curves (Bates 1970), while others (Holden 1966, Washington 1973) often take a more common form such as

$$\lambda = \frac{1}{A + BT} + CT^3 \quad (1.1)$$

Other expressions use a mathematically best fit of data to find parameters for expressions derived from solid state physic ideas. The most likely form for this type of thermal conductivity equation is

$$\lambda = \frac{1}{\epsilon_1 + \epsilon_2 T} + \epsilon_3 T \exp\left(\frac{-\epsilon_4}{KT}\right) - \epsilon_5 \exp\left(\frac{-\epsilon_6}{KT}\right) \quad (1.2)$$

where K is the Boltzmann's constant, 8.61812×10^{-5} eV/K, T is the temperature in degrees Kelvin, and the 6 parameters (ϵ_i) are determined from experimental data and basic physics principles. This form of thermal conductivity equation with three terms was first proposed by Weilbacher (1972). The first term characterizes the phonon conduction, or lattice wave interactions. The second term is used to describe the electronic contribution to the thermal conductivity. This term has been the center of some controversy in the past, but new support has been added to its importance by MacInnes (1978) and R. Young (1979). The third term suggested by Weilbacher accounts for the leveling off of his thermal conductivity data at high temperatures. This term is used to represent the conduction decrease that occurs with the formation of lattice dislocations at high temperatures. Since little data have been successfully collected at very high temperature, there is still no strong corroboration for the inclusion of this last term. The values recommended for the coefficients of Eq. (1.2) by Weilbacher are:

$$\epsilon_1 = 5.25 \text{ cm K/w}$$

$$\epsilon_2 = 2.2 \times 10^{-2} \text{ cm/w}$$

$$\epsilon_3 = 9.58 \times 10^{-4} \text{ w/cm K}^2$$

$$\epsilon_4 = 1.13 \text{ eV}$$

$$\epsilon_5 = 4.18 \times 10^3 \text{ w/cm K}$$

$$\epsilon_6 = 3.29 \text{ eV}$$

Figure 1.1 shows a plot of Eq. (1.2) with these parameter values. The contribution of each of the three terms is also presented. The effect of the negative contribution from the third term can be seen above 2800 K. In another work, where many experimental results have been reviewed, Brandt and Neuer (1976) have accepted the three term idea proposed by Weilbacher (1972), but have obtained their constants for the first two terms by fitting a mean representation of the results of several investigators. The six terms Brandt and Neuer have chosen are:

$$\epsilon_1 = 4.39 \text{ cm K/w}$$

$$\epsilon_2 = 2.16 \times 10^{-2} \text{ cm/w}$$

$$\epsilon_3 = 1.12 \times 10^{-3} \text{ w/cm K}^2$$

$$\epsilon_4 = 1.18 \text{ ev}$$

$$\epsilon_5 = 4.18 \times 10^3 \text{ w/cm K}$$

$$\epsilon_6 = 3.29 \text{ ev}$$

Note that the last term of Eq. (1.2) is identical to Brandt and Neuer's. Figure 1.2 shows a comparison of the results of Eq. (1.2) with the two parameter sets used.

An objective of this research is to see if an equation of the form shown in Eq. (1.2) can be used to adequately fit the data that will be collected by the Direct Electrical Heating system. The values the parameters must have to fit these data over a wide temperature range will also be determined. Particular attention will be given to the data collected near melting so that information may be gained on the importance of the defect term.

Figure 1.1: UO_2 thermal conductivity from Eq. (1.2).

Figure 1.2. UO_2 thermal conductivity, Brandt's results compared to Weilbacher's results.

1.2 The Direct Electrical Heating Method

A Direct Electrical Heating (DEH) facility is a useful experimental tool. Commercial grade fuel pellets from the power reactor industry may be stacked and heated with this DEH facility so that conditions similar to actual reactor use may be obtained. Many different kinds of information may be gained from this type of experiment depending on the instrumentation that is set up. Because of the lack of reprocessing in this country, it is desirable to run fuel elements to a much higher burnup in a reactor core. Thus, there is an increasing interest in the mechanical behavior of the fuel pellets. In particular, investigations studying the fuel pellet-cladding interactions (pci) have been undertaken so that the causes of fuel element failure may be more readily understood (Kennedy, Christensen, and Eilbert 1979). The cracking phenomena that occurs with pellet heatup may have a large effect on the thermal conductivity from the fuel material to the coolant. Current models of pellet thermal expansion indicate expansion and contraction with temperature. It is possible that if characteristic vertical cracks appear, the pellet may not contract nearly so much on cooling. This keeps the gap smaller and may even keep part of the pellet in contact with the clad. DEH experiments might possibly be used to obtain useful information on the pellet's mechanical behavior, or on the pci problems.

This investigation will use the DEH facility in another way. Observation of the pellets while heating will be made (Section 3.3), but the experimental data collected will be used in trying to measure the thermal conductivity of the pellet material at high temperature. A

major difference between an actual nuclear heatup and an electrical heatup can be in the shape of the radial power distribution and hence the temperature profile of the heated pellets. For uranium dioxide, the nuclear heating produces much flatter profiles. This is easily explained by noting that the electrical conductivity (Section 5.2) rises rapidly with temperature. Then due to the higher center temperature, more current flows there causing a correspondingly higher joule heating. The steep temperature profile means that reasonably low surface temperatures will exist, even for fuel center temperatures near melting. The classical method of using a notch or hole to measure center temperature is not used in this research since center heating past melting is desired. With a hole or notch, the molten material would immediately slump out before information could be gained. Instead, the center temperature will be inferred using a computer code which models the experiment analytically. This code (MANTRA-III) uses an iterative technique to converge on a temperature profile that matches the experimental data collected. This code is described in Section 5.1 and Appendix A. The parameters of Eq. (1.2) will be adjusted so that MANTRA-III produces values that match experimental data over the range recorded. This can be done for each of the successful data runs, and averaged values of the parameters determined (Section 6.2).

CHAPTER 2

EXPERIMENTAL PREPARATIONS

The Direct Electrical Heating facility (DEH) was initially built and is described by Himes (1979). Many changes to the facility have been made so that further description is necessary here. The DEH equipment can be broken down into five general systems. Due to various problems in running the experiments, all five systems have been modified as necessary. A general description of each of these systems and the major changes made to them are given in the following sections.

2.1 Pellet Preparations

Three sets of uranium dioxide pellets were available for these experiments. One of these sets was immediately rejected due to its diameter being greater than its height. This set was received from Exxon Nuclear and contained 100 pellets. As will be discussed below, the area where pellets are joined can cause serious problems, so a reduction in the number of interfaces in the pellet stack is necessary. The pellets that will hereafter be called "thin" have dimensions that are generally around 1.27 cm long and 0.635 cm in diameter. This set came from Argonne National Lab and included 50 pellets. The other set, which is referred to as "thick," has diameters of 0.864 cm and are again around 1.27 cm long. They also came from Argonne National Lab, but were sent in 10 stainless steel clad fuel rods from the ZPR-ANL Development Program. All the pellets were removed from the rods when received.

The pellets are depleted uranium dioxide formed by cold pressing and sintering, the most common method of pellet manufacturing used in the power industry. The thick pellets are the most common size in use.

The surface condition of the pellets is important due to the nature of the DEH experiments. If pellets are used for nuclear heating the surface conditions are not as important in maintaining uniform heating. But for electrically heating a pellet stack, the quality of the pellet end surfaces becomes critical for trying to make good electrical and thermal contact. If the pellet interface is not flush, or only in partial contact, the electrical current will not flow evenly through the stack and uneven heatup will result. In addition, good surface quality was necessary for the X-ray diffraction measurements made as detailed in the next section.

The thick pellets were obviously not in very useful shape as delivered. Their ends were quite chipped and often concave. To correct these problems a surface grinding technique was tried. Several of the pellets were placed in a drum along with a solution of 600 grit Silicon Carbide, water, and crushed walnut shells. This mixture was then tumbled overnight. This process uniformly reduced the pellet diameter by 0.5 mm, but definitely enlarged the pellet surface pores. It was not used again. The process which proved most useful was an end grinding technique using a series of water bathed grinding tables. A geometrically correct holding jig for the pellets was made. They were then end ground into near perfect cylinders on these tables using first 150 grit, then 220 grit, and finally polished with 400 grit sandpaper.

The finished dimensions of one of these pellets was typically 1.07 cm in length with a 0.856 cm diameter.

The thin pellets were in much better initial condition, but they still required some end grinding. Another holding jig for these pellets was made and the same sandpaper grinding and polishing sequence was used. A typical thin pellet might have finished dimensions of 1.18 cm in length with a 0.637 cm diameter.

The density of the pellets could then be calculated since they were near perfect cylinders. Their dimensions were measured with a micrometer, and they were weighed with an analytical balance. The thick pellets typically had a density around 10.0, and the thin pellets 10.4 gm/cm³. The reason for lower densities of the thick pellets was obvious upon inspecting them under a microscope. Slices of the pellets were taken when needed using a 10,000 rpm, 4 mil diamond blade cutoff saw. Inspection of slices of the two pellets always showed that the thick pellets had more and larger pores distributed throughout their volume than the thin ones.

2.2 Pellet Stoichiometry

A major problem in running this type of experiment is controlling the oxidation of the uranium dioxide during the heatup. As has been reported in many papers, the thermal properties of uranium dioxide change with different O/U ratios. In general, the thermal conductivity decreases as the O/U ratio increases. The dissolved oxygen can be considered to disrupt the lattice introducing scattering centers, therefore increasing the phonon resistance (Roberts 1961,

Washington 1973). Therefore, a good deal of work was done to verify that the pellet stoichiometry remained near constant. This was done using an X-ray Diffractometer system in conjunction with a linear recorder available in the Metallurgical Engineering Department. A General Electric X-ray tube using a copper target and a nickel filter was used to supply a beam of X-rays with a discrete wavelength. A special sample holder was built to hold a pellet so that an end of it would be exactly in the center of the beam at the center of the instrument. This sample holder allowed a reproducible geometry each time an experiment was set up. To get useful results, the pellets were end polished or sliced and end polished as mentioned in the previous section.

This setup allowed data to be collected from which the lattice constants of the uranium dioxide could be obtained. The measured diffraction angles were used with the Miller Indices of the crystal structure (Selected Powder Diffraction Data for Metals and Alloys 1978), in two methods of obtaining precise lattice parameters. The calculations, involving a least squares data fit (Young 1962) and an extrapolation to gain the lattice parameter, were carried out by a program put together for this research called XRAY. It is presented in Appendix B. The extrapolation methods used and a discussion of the technique involved in measuring lattice parameters is presented in a text by Nuffield (1966).

There is a direct correlation between the lattice parameter and the O/U ratio of the specimen as shown in Figure 2.1 (Holden 1966). A similar curve is presented by Ishii and Naito (1967). Uranium dioxide

Figure 2.1. Lattice constant vs. O/U ratio.

has the fluorite crystal structure and as oxygen is absorbed into the lattice, the distance between the atoms is decreased. Thus by measuring the lattice constant before and after an experiment, a good indication of specimen oxidation can be obtained.

2.3 Gas Supply System

This system supplies the inert atmosphere that bathes the pellets during heating so that oxidation will be prevented. A new one-quarter inch thick neoprene seal was added to the baseplate of the bell jar. The penetrations of the bell jar were all resealed so that positive pressures as well as a vacuum could be tolerated. Most

importantly, bell jar clamps were added to securely fasten the bell to the base plate seal for operating in the positive pressure mode.

The system can now have a vacuum drawn on it, or the inert gas supply, the argon, can be used to supply greater than atmospheric pressure inside the bell jar. This insures that any gas leaks that occur will be argon out rather than oxygen in. A highly sensitive pancake detector was used to insure that no contamination from the uranium dioxide pellets escaped the bell jar while operating in the positive pressure mode.

2.4 Pellet Support

Maintaining a highly uniform and sturdy pellet stack was a critical factor for successful experiments. Uneven heating or non-uniform current flow through the stack will create the effect of higher local temperature causing increased current flow and therefore more localized heating. This current tunneling or cascading effect will eliminate any successful data taking. Therefore, several things were done to keep the pellets supported properly.

A device for smoothly raising and lowering the top electrode was added so that the placement of the pellet stack could go more smoothly. The adjustments that control the top and bottom electrodes were checked before each run to ensure that they came together correctly. The graphite end pieces that support the pellet stack between the electrodes and allow for even current flow take a good deal of abuse during high power runs. Several new sets of these were milled with carefully ground ends to keep the stack flush with the end pieces.

The end grinding of the pellets was very effective in creating uniform pellet stacking. The interfaces between the pellets were the critical points of contact for each stack. A thin film of graphite powder was used at the interfaces for improved conductivity and a general smoothing of the stack. Insertion of any instrument probes into the interfaces between the pellets caused problems in smooth heatups and was therefore discontinued.

2.5 Power Supply

The power supply used is the same as that described by Himes (1979). It is capable of 160 volts maximum at low currents, and at least 100 amps at low voltages. New and heavier duty filter capacitors were added to the instrument after the old ones burned out.

Some practice is necessary in using this power supply due to the time delay in its response. In particular, close attention to the pellet heatup is necessary to prevent what will commonly happen, the "run away." This is the phenomena whereas the pellet starts to heat, its conductivity rapidly increases allowing more current to flow through it and thus a more rapid heating. The response time of the power supply is such that the current is not limited quickly enough and this "run away" sequence can take less than 5 seconds to melt the stack down.

2.6 Instrumentation

Only three data values were needed for each step of the run: voltage, current, and surface temperature. Due to the adjustments

necessary and the fast pace of the runs, the data and other observations were voice recorded for later transcription into a lab book.

The voltage was measured across a central pellet using high temperature probes fixed in place. The probes were made with chiseled end points from thermocouple wires. These end points were placed under compression against the interfaces of the central pellet as can be seen in the photographs in Chapter 3. Often two independent sets of voltage probes were used to take independent measurements. Digital readout voltage meters were used.

The current through the stack was commonly measured with an internal shunt in the power supply. The voltage over this shunt was read with a digital electrometer. To back up this current measurement in the later runs, an external, high power, in-line shunt was placed in the positive line between power supply and the DEH system. The voltage from this shunt was measured with a heavy duty deflection meter. This shunt-meter combination used was matched, and therefore gave very reliable measurements from mid through high power.

The surface temperature was measured with a recently calibrated optical pyrometer. The pyrometer was powered with a small power supply rather than a battery. Since the pellets are viewed through a window, recorded temperatures need to be corrected not only for uranium dioxide surface emittance, but also for the glass window transmittance (Section 5.4).

The heated stack was periodically photographed during the run. This supplied further information on hot spot effects, pellet cracking,

voltage probe contact, and pellet integrity. Some of these photographs are presented in the next chapter.

CHAPTER 3

THE EXPERIMENTS

The Direct Electrical Heating Experiments were run periodically over a 15 month period. As new modifications were added or new pellet preparation techniques tried, experiments would be run to test them. In general, a run takes about two to three hours after it is set up to go. Fourteen runs were recorded in the DEH lab book. The general procedures for these runs will be given followed by some run descriptions.

3.1 Experimental Procedures

The procedures varied somewhat from run to run as techniques were improved and new modifications tried. The general procedures that follow would most closely fit the final data taking runs. These procedures can be divided into three sections, the equipment setup, the heatup, and the data collection.

The equipment setup involves constructing the pellet stack. As was mentioned in Section 2.4, this must carefully be done to have a decent run. The voltage probes were then fixed in place using their mechanical support and bending the probe wires. The bell jar was cleaned up, particularly the viewing window, and placed into position. The bell jar fasteners were tightened slightly so that a vacuum could be drawn. At maximum vacuum the fasteners were slightly tightened again. The volume was then purged with argon gas. A second vacuum and purge was completed and this time the gas flow is left on and adjusted to the

desired flow rate. The vacuum pump was turned off and the pressure in the bell jar controlled with a needle valve in the outlet gas line. The system pressure was generally set for 3 to 5 psig. The gas system was then left alone with only minor adjustments to keep the pressure constant. The camera, tape player, and meters were then set up.

The power supply was turned up to its maximum of 160 volts to start the heatup. The heatup is considered to be the time from when the power is turned on until the pellet stack glows visibly. This process turned out to be an important part of each run. Problems with the heatup often indicate that the stack was not constructed well enough and that problems would likely occur during the remainder of the run. In addition, care was taken during the latter part of the heatup to keep power supply "run aways" from ruining the pellet stack. The power supply was turned down after pellet heatup was noticed. For a well constructed three or four pellet stack, heatups would normally take around 15 minutes.

After the initial heatup the pellet stack was bright enough to start taking surface temperature measurements. The lowest fuel surface temperature measurements that could be taken with the pyrometer were around 800 degrees C. From 800 to 1000 degrees C, some pellet hot spot irregularities generally were evident, particularly around the pellet interfaces and the voltage probe contacts. These problems generally disappeared above 1000 degrees C and an even heatup was obtained. The experiment response from the time of even heatup to shutdown was generally very good. A step increase in power was made and the pellet state generally stabilized on current, voltage, and surface temperature

values around half a minute later. The measurements were taken when steady, and the power increased again. This was continued until it was decided to halt the experiment usually one or two hours after started. A shutdown was made when some of the DEH system parts were overheating, or when the pellet stack was bubbling molten uranium out cracks in the side. The last run went step by step to higher temperatures until the stack collapsed.

3.2 Experiment Check Runs

DEH Runs 1 through 9 were all made to become familiar with the equipment and to test system modifications. Such changes as positive pressure, pellet geometry, stack construction methods, voltage probe placement, gas flow patterns, and style of graphite end pieces were all worked out during these initial runs.

DEH Run 2 had a power supply run away take place during initial heatup. The run away resulted in some melting of the stack. There was a definite current path after this which caused completely uneven heatup. After this initial run away, when the power was increased the current either peaked and dropped back or another run away started. A steady state of high heating could not be achieved.

DEH Run 5 was made with the vacuum inside the bell jar held as low as possible, but with no argon gas flow. This was done to supply an oxidized pellet for the X-ray diffraction measurements. From the time the power was turned on, the pellet only lasted 20 minutes before it had crumbled away from the contacts, thus showing severe and rapid oxidation.

DEH Run 6 was terminated at a relatively low power level because of smoke from the power supply. DEH Run 7 had just gotten past initial heatup when one of the filter capacitors exploded smoking up the room, but identifying the problem with the power supply.

3.3 The Data Taking Runs

DEH Runs 10 through 14 were all made to collect data for analysis. Some information on each of these five runs follows. In these runs, one of the middle pellets of the stack was called the measured pellet since all data collected refers to it.

Run 10 was made using the thin pellets for a three pellet stack. Newly milled graphite end pieces were used. These end pieces had a somewhat larger diameter (1.28 cm) than previous sets that were used. After a very slow heatup that took nearly an hour, and some initial hot spot problems with the bottom pellet, an even heatup was achieved. The power was step increased until uneven heatup across the middle pellet prevented accurate surface temperature measurements from being taken. The run was shut down at that point. Table 3.1 gives some general information on the measured pellet and this run.

Table 3.1. DEH Run 10 Pellet Information

Specimen label	N4
length	1.1814 cm
diameter	0.6306 cm
density	10.38 g/cc
Max current read	33.4 amps
Max temperature	1545°C

Pellet N4 was sliced and end polished after Run 10 so that the X-ray diffraction equipment could be used to measure its lattice constant. This was done for comparison to unheated samples to check for any stoichiometry changes (see Section 6.1).

Figures 3.1, 3.2, and 3.3 are presented to show the actual data that were collected. (The current correction, described in Section 4.1, has been applied before the data were plotted. This holds true for the presented data for all the runs.) Each data point was a steady position achieved after a small power increase. Thus, the data points were collected in time sequence from low temperatures to high. Three figures are shown to illustrate how each of the data types relates to the other. Figure 3.1 also shows the approximate time scale for the DEH experiments. This same type of time scale holds for all of the runs, but will only be included here. It is the time from when the power is first turned on through the initial heatup and the first visible lighting of the stack, allowing pyrometer measurements, to the final shutdown of the power.

DEH Run 11 used the thick pellets in a four pellet stack. The second pellet from the top was the measured one. The same graphite end pieces were used again. This run was photographed at various points from heatup to shutdown. A heatup was achieved in 15 minutes. Early in the run, a very bright spot appeared in the bottom pellet (Figure 3.4). This bright spot, representing a superheated area, gradually moved upward through the stack during the run. As the bright spot moved into the measured pellet (Figure 3.5), the effect on the data could clearly be seen. As shown in Figure 3.6, at a surface temperature of around

Figure 3.1. Run 10, current vs. temperature data points with an approximate time scale.

Figure 3.2. Run 10, voltage vs. temperature data points.

Figure 3.3. Run 10, voltage vs. current data points.

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Figure 3.6. Run 11, current vs. temperature data points.

1200°C, the bright spot caused a rapid upward drift of temperature for only a small current gain. These unexplained phenomena made the collected data unacceptable. Table 3.2 gives general information on the measured pellet.

Table 3.2. DEH Run 11 Pellet Information

Specimen label	T2
length	1.0541 cm
diameter	0.8585 cm
density	10.032 g/cc
Max current read	43.5 amps
Max temperature	1477°C

An inspection of the stack was made while it was being dismantled. The top graphite end piece had a severe vertical crack running through it causing it to split apart when removed. All four of the pellets were fused together. With some force the top two snapped free, but the bottom two remained fused together. The measured pellet was end polished and run on the diffractometer.

DEH Run 12 had a stack made up of three of the thin pellets. Newly milled graphite end pieces with a smaller diameter (0.978 cm) were used. The heatup took around 25 minutes. There were slight bright spots at each of the interfaces during the early part of the run, but these disappeared at higher power levels. A consistently uniform brightness (see Figure 3.7) over most of the run allowed useful data to be collected. The brightest area of the stack was generally in the

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middle of the center pellet (Figure 3.8), and was very noticeable during the latter part of the run. This brighter area expanded both upwards and downwards at the higher power levels. The run was shut down when a molten extrusion appeared from a crack in the side of the top pellet (Figure 3.9). As can be seen from Figure 3.9, the top half of the pellet stack ended up quite a bit hotter than the bottom half. General run information is given in Table 3.3.

The pellet stack was again fused together. The bottom pellet was snapped off with some force, but the top two remained together. Obvious melting signs were seen at the interface ends where the bottom pellet came off. The melting signs occurred in a fairly uniform ring. The top pellet's surface showed a great deal of change. The smooth dull surface that the pellets normally have had been changed to a sparkly exterior with obvious damage from too much heat showing up at its upper section. The collected data are presented in Figures 3.10, 3.11, and 3.12.

DEH Run 13 used the thick pellets in a three high stack. The contact surfaces of the graphite end pieces were milled smooth again and reused. Two separate voltage probes and meters were used. Two separate current measuring instruments were used, with the additional meter operating off a shunt that was placed external to the power supply. This backup and very reliable current meter was used for Run 14 as well. It showed that a current correction was needed as described in Section 5.1. A normal heatup for this run took about 25 minutes. Usable data were recorded until shutdown as the stack brightness stayed reasonably uniform. Shutdown was again made shortly after a visible

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Table 3.3. DEH Run 12 Pellet Information

Specimen label	N8
length	1.1811 cm
diameter	0.6304 cm
density	10.40 g/cc
Max current read	66.2 amps
Max temperature	1660°C

Figure 3.10. Run 12, current vs. temperature data points.

Figure 3.11. Run 12, voltage vs. temperature data points.

Figure 3.12: Run 12; voltage vs. current data points.

molten extrusion appeared from a vertical crack in the top pellet. Post heatup inspection revealed obvious melting in the pellet centers, and the top two pellets remained fused together. The general run information is given in Table 3.4. The data collected for this run are presented in Figures 3.13, 3.14, and 3.15.

Table 3.4. DEH Run 13 Pellet Information

Specimen label	A5
length	1.2116 cm
diameter	0.8644 cm
density	9.948 g/cc
Max current read	80 amps
Max temperature	1600°C

DEH Run 14 was made with a four pellet stack using the thick pellets. The graphite end pieces were milled smooth and reused. A single digital voltmeter was used to switch between two sets of voltage probes. A good deal of trouble was encountered while trying to get through the heatup. The heatup problems were finally passed after an hour into the run. The middle part of the run showed even heatup with early severe cracking at the bottom of the stack (Figure 3.16). The power was step increased and data were collected past the point where visible molten extrusions appeared (Figure 3.17). The run was shut down when the stack integrity was failing and flashes of molten material were being ejected. General information on the measured pellet is given in Table 3.5. The data collected are presented in Figures 3.18, 3.19, and 3.20.

Figure 3.13. Run 13, current vs. temperature data points.

Figure 3.14. Run 13, voltage vs. temperature data points.

Figure 3.15. Run 13, voltage vs. current data points.

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Table 3.5. DEH Run 14 Pellet Information

Specimen label	A8
length	1.1862 cm
diameter	0.8641 cm
density	9.987 g/cc
Max current read	80 amps
Max temperature	1700°C

Figure 3.18. Run 14, current vs. temperature data points.

Figure 3.19. Run 14, voltage vs. temperature data points.

Figure 3.20. Run 14, voltage vs. current data points.

Inspection of the pellets during the dismantling of the stack showed all of them having major structural changes due to melting. All pellets showed molten extrusions, with the entire center portion of the top pellet having been ejected from the stack. The ejected uranium dioxide metal globules were collected and are stored with the other pellets. The top graphite end piece remains fused to the upper electrode. The surface of the top pellet showed the same change to a sparkly surface that was evident in Run 12.

3.4 Run Comparisons

Three of the five data taking runs were probably successful. Run 11 was rejected as mentioned in the previous section. Run 14 is suspect since its data do not show the same tendencies as the data from the other runs. The heatup problems experienced may have adversely affected the remainder of the run.

Runs 10 and 12 both used thin pellets and show very similar data. Figure 3.21 graphically compares every third point of the data collected. As can be seen, it is a very favorable comparison lending some confidence to the data. The sharp rise in the data curve where surface temperature remains near constant with increasing current shows clearly. This same rise is evident in Run 13, but in a different place since this and Run 14 were both made with the thick pellets. Figure 3.22 compares some of the data from these two runs. It shows a good comparison over the lower range, but at about 1450°C the curves split. Again, the difficulties with Run 14 may have affected its data collection.

Figure 3.21. Thin pellet runs, data comparison.

Figure 3.22. Thick pellet runs, data comparison.

Other comparisons were evident through the runs. The initial heatup was usually somewhat difficult with careful manipulation of the controls necessary for a smooth heatup with no runaway. The unusual heatup problems that occurred with Run 14 are not explained. As can be seen in the run photographs, horizontal cracks always appeared at the ends of the stack just above and below the graphite end pieces. A corresponding darkened area showed up here as well indicating that the increased linear heat transfer near the graphite end pieces caused severe thermal differences in the pellet stack that account for the cracking. Vertical cracks along the center pellets also always appeared. These cracks occurred at higher temperatures and were likely from the differential expansion experienced radially through the pellets due to the extremes of temperature from surface to center. It was through these cracks that the molten material extruded. The upper end of the pellet stack always showed the greatest damage from high heatups. This was likely due to reduced cooling since the surrounding argon at this point had already been greatly heated by the lower pellet area. The increased heating of the upper area was also demonstrated since the upper pellets generally remain fused together.

CHAPTER 4

DATA ANALYSIS

The data collected for this experiment were taken two different ways. After preparing a pellet for a DEH run, its physical characteristics are measured. Then during the DEH run experimental data are collected as described and presented in the previous chapter. The accuracy of the physical measurements made on the pellets is quite good, especially when compared to the various experimental and theoretical uncertainties involved. The following sections describe what is done to correct a systematic error that appeared, and to reduce the random experimental error inherent in all data collection.

4.1 Current Correction Factor

The digital current metering system built into the power supply gives readings to the tenth of an amp and is sensitive enough to register current from 0.1 amps up. An external and independent current measuring system revealed an increasing positive error in the digital meter's reading as the power was increased. This showed up for two different runs with two different external shunt-meter sets. The two current readings stay the same up to around 5 amps then slowly start to diverge. This is attributed to the joule heating of the wire used as an internal sense resistor in the power supply.

To calculate a correcting equation that could be applied to all of the current readings obtained in the various runs, a curve fitting

approach was used. The digital meter's current readings, I , were plotted against the external shunt-meter readings, A . A quadratic equation was fit to these points using a nonlinear, least squares curve fitting program. This was done for Runs 13 and 14 with the resulting correction equation being very nearly the same. The current correction factor used is

$$A = -4.117 \times 10^{-2} + 0.9871xI - 8.38 \times 10^{-4} \times I^2 \quad (4.1)$$

for $I > 5$ amps

where I is the measured current and A is the actual current.

4.2 Curve Fitting Data

The data collected during the DEH experiment are taken on a point by point basis. To reduce the random errors of the data acquisition and to obtain a general smoothing of the resulting data, a curve fitting technique was again used.

The data plots (as presented in Section 3.3) generally show two distinct regions. The lower region curve fit gives either voltage or current for a given temperature. A cubic equation gave the best fit for current versus temperature, while a linear equation generally is the best fit to the voltage versus temperature data. These two expressions are presented for Run 13 as an example. They are shown in Figures 4.1 and 4.2. The lower section best fit curve for Run 13 is

$$A = -90.815 + 0.2961 T - 3.1943 \times 10^{-4} T^2 + 1.1747 \times 10^{-7} T^3 \quad (4.2)$$

for $T \leq 1440^\circ\text{C}$

Figure 4.1. Run 13 data showing current vs. temperature curve fit.

Figure 4.2. Run 13 data showing voltage vs. temperature curve fit.

where T is the observed temperature in degrees celsius, as presented in the data plots. The expression for the best fit to the voltage versus temperature curve for the lower section of Run 13 is

$$V = 28.821 - 0.01664 T \quad (4.3)$$

for $T \leq 1440^{\circ}\text{C}$

The upper section can no longer use temperature to find the data points as can be seen in the current-temperature or voltage-temperature data plots. For this section of the curves the current was made the controlling variable and the corresponding temperature or voltage were obtained for a given current. The temperature-current fit shown in the upper section of Figure 4.1 is from the following equation.

$$T = 1523.5 - 4.3434 A + 0.0182 A^2 + 6.6914 \times 10^{-4} A^3 \quad (4.4)$$

for $T > 1440^{\circ}\text{C}$

The voltage versus current fit required the use of a third figure since, for the upper range voltage cannot be obtained from temperature. The upper range of the voltage-current data is shown in Figure 4.3 with the best fit curve through it. The equation for this best fit is as follows.

$$V = 0.3222 - 0.2315 A + 1.9697 \times 10^{-3} A^2 + 1.956 \times 10^{-8} A^3 \quad (4.5)$$

Thus, the voltage and current are obtained by specifying a temperature up to some cutoff point, then the voltage and temperature are obtained for a specific current value. The cutoff point used is the temperature where the high and low range curves meet. This value was obtained

Figure 4.3. Run 13 data showing voltage vs. current fit for upper range of data.

graphically from an expanded plot of the area of intersection as shown in Figure 4.4.

Figure 4.4. Expanded view of Figure 4.1 showing cutoff value where upper range curve starts.

CHAPTER 5

MODEL PREPARATION

To find the thermal conductivity of uranium dioxide from data collected during the direct electrical heating of the samples, an analytical technique has been developed using a computer code called MANTRA-III. A general description of the code function is given in the following section. For a more detailed description and a listing of the code, see Appendix A. MANTRA-III is made up of several models which describe the response of the material during the electrical heating. Some detail on these models and where they come from is given in the sections following the general code description.

5.1 Code Description

MANTRA-III is the third major version of the code written for this investigation. A summary flowchart of MANTRA-III is presented in Figure 5.1. Some discussion of the starting values and data is given at the end of this section. The selection of data points is made from the curve fits obtained (previous chapter). The number of data points and their position on the curve are specified by the input data. An example of a set of five data points is given in Figure 5.2. From these points, five temperature profiles can then be constructed and are shown in Figure 5.3. The profiles are constructed by choosing a center temperature and using the thermal conductivity equation to find the temperature drop between nodes. The power dissipated by each nodal

Figure 5.1. MANTRA-III summary flowchart.

Figure 5.2. Run 13 data with current vs. temperature fit showing the data points used to generate the profiles of Figure 5.3.

Figure 5.3. Example profile set from Run 13 data showing temperature regions.

volume is determined from the electrical conductivity equation. An iteration is performed on the center temperature until the surface temperature calculated matches that observed. Then the power from each nodal volume is summed up and divided by voltage to get a calculated current. It is this current that is compared to measured current giving the error of interest. The current errors are squared so that negative or positive have equal importance. The squared current errors from each of the profiles are then summed to get an overall error called SSQ. It is this value that is minimized by MANTRA-III.

The temperature given in Figure 5.2 is the observed surface temperature. After being corrected to actual surface temperature, it will correspond to the outside point of a temperature profile given in Figure 5.3. MANTRA-III is capable of automatically determining which parameters of the thermal conductivity equation to optimize, or will optimize a particular parameter if specified in the input. If the code is optimizing all the parameters, the profile set is divided up into temperature regions as shown in Figure 5.3. MANTRA-III can work with from 1 to 5 regions or 1 to 5 profiles depending on user specifications. The temperature region division is made since the profile set covers such a wide range of temperatures. At the lower range different parameters of the thermal conductivity equation will have effect than at the high range. The division is made in even increments between the center temperature of the hottest profile and the surface temperature of the coolest profile, which are the temperature extremes for the profile set. The code will then find the most sensitive parameters of each region. If the sensitivity of the first two parameters is nearly

the same, both of them will be adjusted for this region. Each time an adjustment to a parameter is made, all of the data points have a new temperature profile constructed for them. The profiles in the example have 25 nodes, which was the most common number used in this study. Up to 50 nodes may be specified for the code. If there are 25 temperature nodes, then the pellet is divided into 24 nodal volumes. Each of these nodal regions has an equal volume and lies between two annular rings made up by the temperature nodes. This can be seen in Figure 5.3 by the nodes getting closer together as they get further from the center.

A data input file based on information from Run 13 will be used to illustrate the code operation. This data file is presented in Table 5.1. "TBEG" thru "AEND" all refer to values from the curves that have been found to fit the data as shown in Section 4.2. If "TTNC" is a negative value, then "TEND" must be smaller than the beginning temperature, "TBEG." Since the observed surface temperature is the value represented in the curve fits and plots, degrees Celsius is used here.

The next 8 values give the voltage fit for curve one, from temperature, and curve two, from current. Two parameters for the curve fit give a linear equation while four give a cubic fit. The best fit for current versus temperature is given for curve one followed by curve two where temperature is calculated from a given current value.

The six initial thermal conductivity equation parameters are given next. Those shown in Table 5.1 are from the set chosen by Brandt and Neuer (1976) as described in Section 1.2. The electrical

Table 5.1. Input Data File

```

13      MRUN, THE DEH RUN # (I2)
1000.   TBEG, STARTING TEMP, CELSIUS (F6.1)
1550.   TENDC, ENDING TEMP, CELSIUS (F6.1)
50.     TINC, TEMPERATURE INCREMENT (F6.1)
1440.   TCUT, TEMP WHERE CURVE TWO STARTS
5.0     AINC, CURRENT INCREMENT FOR CURVE TWO
30.0    AEND, ENDING CURRENT VALUE
+2.8821E+01  **      BMDX BEST FIT FOR VOLTAGE
-1.6635E-02  ****      VCONST(1 TO 4)
              ****      CURVE ONE, V FROM T
              **
9.3222      **      CURVE TWO, V FROM A
-2.2149E-01  ****      VCONST(5 TO 8)
1.9697E-03   ****
1.9560E-08   **
-9.0815E+01  **      BMDX BEST FIT FOR CURRENT
2.9610E-01   ****      ACONST(1 TO 4)
-3.1943E-04  ****      CURVE ONE, A FROM T, (E11.4)
1.1747E-07   **
1.5235E+03   **      CURVE TWO, T FROM A
-4.3434      ****      ACONST(5 TO 8)
1.8199E-02   ****
6.6914E-04   **
4.39         **      THE INITIAL THERMAL CONDUCTIVITY PARAMS
+2.1600E-02   CT(1) TO CT(6)
+1.1E00E-03   (E11.4)
1.1800
+4.1800E+03
3.29
9.646        CE(1) ELECTRICAL CONDUCTIVITY
-2.0870E+04  CE(2) MODEL PARAMETERS
1.2310E+07   (E11.4)
-6.4840E+09  SIX POSITIONS AVAILABLE

0.001        EPS      SSO CONVERGENCE LIMIT (E11.4)
0.4322       RO      PELLET OUTER RADIUS, CM
1.2116       LRT     PELLET LENGTH, CM
0.907        TD      THEORETICAL DENSITY
25           N       # OF RADIAL NODES FOR SURF
1            NPRO     # OF SIMULTANEOUS PROFILES TO WORK WITH
4            NREG     # OF TEMP REGIONS THE PROFILES DIVIDED INTO
0            ONEPAR   IF ONE PARAMETER ONLY IS TO BE OPTIMIZED
0.1          STEP    THE INITIAL STEP SIZE FOR OPTIMIZATION
0.001        SMIN    THE MINIMUM STEP SIZE FOR OPTIMIZATION

```

conductivity parameters remained constant for this investigation and are those given in Section 5.3.

"EPS" puts a limit on the smallest SSQ value that is needed. It has only been reached with single profile sets.

"RO," "LRT," and "TD" are all measured physical properties of the pellet of interest as given in Section 3.3.

"N" gives the number of nodes the profiles are divided into. This value could be from 15 to 50. More accuracy is achieved with more nodes, but at the cost of much longer computer run times. "NPRO" can be from 1, for single profiles, up to 5, for the largest sets. "NREG" gives how many temperature regions will be used and also is between 1 and 5. "ONEPAR" is set to zero if automatic parameter optimization is wanted. Otherwise it has a value from 1 to 6 depending on which particular parameter is to be used. If "ONEPAR" is anything but zero, "NREG" defaults to 1 region since no decision on sensitivity of the parameters is needed. "STEP" gives a value for the percentage of change a parameter is incremented each time. The value 0.1 means initially each time a parameter is incremented in either direction, it will change by 10%. This step size is decreased as the optimization progresses until "SMIN" is reached.

5.2 Thermal Conductivity Model and Porosity Correction

The thermal conductivity model used is given in Eq. (1.2) and explained in Section 1.1. This equation calculates thermal conductivity for uranium dioxide of theoretical density up to melting. Since this investigation allows the central region of the pellet to melt, a value

for the thermal conductivity of molten uranium dioxide is needed. R. A. Young (1979) suggested that there will be a factor of five increase in the thermal conductivity as the material melts. Thus, at the melting temperature, the thermal conductivity is calculated from the present parameter values and increased by the factor of five. There is no porosity correction applied to the molten material. The thermal conductivity is lower for less dense materials since the thermal resistance of small gaps in the material is greater than the resistance through the material itself. This reduction in thermal conductivity is accounted for by the porosity correction factor.

Washington (1973) performed a literature survey and recommended one of two relationships be used depending on sample porosity.

$$\lambda/\lambda_o = 1 - \alpha p \quad \text{where } \alpha = 2.5 \quad (5.1)$$

for $p \leq 10\%$

or

$$\frac{\lambda}{\lambda_o} = \frac{1 - p}{1 + \beta p} \quad (5.2)$$

where $\beta = 2.0$ for $p > 10\%$

where λ_o is the uncorrected thermal conductivity value, and p is the porosity, defined as

$$p = 1 - TD \quad (5.3)$$

with TD being the per cent of theoretical density for the particular sample. It is likely that the effect of porosity is also temperature dependent. An equation showing this is as follows (Alexas and Lindner, 1975).

$$\lambda/\lambda_0 = 1 - \alpha p \quad (5.4)$$

$$\text{where } \alpha = 2.6 - (0.5 \times 10^{-3})(T - 273)$$

$$\text{for } 873 \text{ K} < T < 3073 \text{ K}$$

Brandt and Neuer (1976) averaged the porosity information they obtained from a literature survey to come up with the same result as Eq. (5.4). Since this equation is commonly agreed on in the various papers, and since it seems most complete, it will be used in this investigation.

The thermal conductivity equation, Eq. (1.2), and its porosity correction, Eq. (5.4), are located in the subroutine THERM of the code MANTRA-III. The thermal conductivity is used to find the temperature drop across each nodal volume when constructing the profiles.

5.3 Electrical Conductivity Model

An accurate electrical conductivity model for uranium dioxide is very important for the type of analysis used in this research. Fortunately, for the high temperature range, good agreement has been reached among various investigators. Bates (1967) has proposed the following equation, which is generally used.

$$\sigma = \exp\left[a + \frac{b}{T} + \frac{c}{T^2} + \frac{d}{T^3}\right] \quad (5.5)$$

$$\text{for } T > 1300 \text{ K}$$

where: $a = 9.646$

$$b = -2.087 \times 10^4$$

$$c = 1.231 \times 10^7$$

$$d = -6.484 \times 10^9$$

This equation gives σ , the electrical conductivity in $\text{ohm}^{-1} \text{cm}^{-1}$.

Alexas and Lindner (1976) constructed a sixth order polynomial to fit their electrical conductivity data. Their equation when plotted also very favorably matches Bates's equation. This investigation will then use Eq. (5.5) which is plotted in Figure 5.4.

Due to the unreliability of electrical conductivity equations at lower temperature, Eq. (5.5) limits the lower end of the data range that can be investigated. The electrical conductivity equation is in the subroutine named ELECT of the code MANTRA-III. It is used to find the power dissipated in the annular ring of each node.

5.4 Surface Temperature Correction

An observed surface temperature in degrees Centigrade of the uranium dioxide pellet was measured using an optical pyrometer. To get the actual surface temperature from this measurement a correction for emitted light must be used. Starting with Planck's law for blackbody radiation and using a value of 65 microns for the wavelength of the emitted light, the following correcting equation was found (Kreith, 1973).

$$T_a = \left[\frac{1}{T_o} + \frac{\ln E_w}{22135} \right]^{-1} \quad (5.6)$$

T_o is the observed temperature in Kelvin, T_a is the actual surface temperature, and E is the product of the uranium dioxide surface emissivity and the glass transmittance. The transmittance of the window is assumed to have a constant value of 0.93.

Figure 5.4. Electrical conductivity of UO_2 .

There are not many papers reporting the emittance of uranium dioxide. On reviewing several papers, Brandt and Neuer (1976) present a plot of emissivity vs. temperature. An Argonne National Lab report, "Properties for LMFBR Safety Analysis" (1976), recommends the same data that Brandt and Neuer used in their figure. Alexas and Lindner (1976) used a correlation relating emissivity to temperature that most closely fit their results. This correlation matches the figure presented by Brandt and Neuer fairly well, and will be used in this research.

$$\epsilon = 1.645 - 3.9215 \times 10^{-4} T \quad (5.7)$$

for $1900 < T < 3100 \text{ K}$

and

$$\epsilon = 0.9 \quad \text{for } T < 1900 \text{ K} \quad (5.8)$$

This calculation is carried out in the program MANTRA-III in the function subroutine TREAL.

5.5 Thermal Expansion Correction

Two sources for the thermal expansion coefficient of uranium dioxide will be cited. Both of these are recommended values from literature surveys. The expansion equation given in "Properties for LMFBR Safety Analysis" (1976) for uranium dioxide is

$$\frac{\Delta L}{L_0} \% = 6.8 \times 10^{-4} (T-273) + 2.9 \times 10^{-7} (T-273)^2 \quad (5.9)$$

$$\text{for } 273 \text{ K} < T < 3138 \text{ K}$$

where L_0 is the initial dimension. The book by Holden (1966) gives an equation that is very similar except for the leading term.

$$\frac{\Delta L}{L_0} \% = 1.723 \times 10^{-2} + 6.797 \times 10^{-4} (T-273) + 2.896 \times 10^{-7} (T-273)^2 \quad (5.10)$$

for 1250 K < T < 2500 K

The first correction factor given, Eq. (5.9), is the one used in MANTRA-III. It covers a wider range and seems more reasonable at lower temperatures.

The expansion equations are given for a particular temperature, but obviously the heated pellets have a temperature profile that is highest in the center and lowers toward the pellet surface. The expansion corrections should then be made with the pellet's bulk average temperature. This average temperature could be obtained from the final profile, but the corrected pellet dimensions should be known before the final profile is obtained. The approach used in MANTRA-III is to get this value from voltage and current measured at the temperature of interest. This is done by finding the average electrical conductivity, σ , from the basic electrical relationships, initially neglecting the expansion.

$$P = VI = V^2/R \quad \text{and} \quad R = L/\sigma A \quad (5.11)$$

where: L = pellet length

V = voltage measured

I = current measured

A = pellet cross sectional area, πr^2

Substituting for R and A and solving for the average electrical conductivity yields

$$\sigma = IL/V\pi r^2 \quad (5.12)$$

The bulk average temperature is then obtained from this by solving the electrical conductivity equation for temperature. Thus a cubic equation that can be rewritten as follows

$$gT^3 = CT^2 + dT + f \quad (5.13)$$

where g is defined as

$$g = \ln \sigma - b \quad (5.14)$$

and

$$b = 9.646$$

$$c = -2.087 \times 10^4$$

$$d = 1.231 \times 10^7$$

$$f = -6.484 \times 10^9$$

which are the parameters for the electrical conductivity equation shown in Section 5.3 (Bates, 1967).

A straightforward Newton-Raphson iterative method is used to find the solution to the cubic Eq. (5.13). This is done in the sub-routine THEXP of the code MANTRA-III.

CHAPTER 6

RESULTS

Some description has been given of how the data were collected and curve fitted, and what the computer code, MANTRA-III, can do. There are a great many methods that can be used in analyzing the data with this code. After many trials, the result sequence given in the following section was established. The second section presents the final thermal conductivity results while the last section of this chapter gives some of the results from the X-ray diffractometer analysis.

6.1 Result Method

After a particular data file is prepared, an initial thermal conductivity parameter set is chosen. MANTRA-III is set to operate with single profiles and automatic optimization. Some manipulation of the initial thermal conductivity parameter set may be necessary to get MANTRA-III to generate the wanted profiles without running into unstable temperature solutions. The starting temperature is set to 1000°C or greater because of the limit on the electrical conductivity equation. MANTRA-III is then run with 50°C increments so that it will construct a temperature profile for each data point up to where center melting is reached.

There are usually only two occurrences that will stop a run of MANTRA-III abnormally. A "non-convergence error" will appear if the final profile has too large a central molten portion which corresponds

to severe central melting of the pellet during the experiment. The nonconvergence comes about during the iterations of center temperature to match observed surface temperature. If "unstable temperature solutions" are hit by MANTRA-III it will try to adjust the temperature parameters to remedy the situation. If it cannot, an "unstable solution error" will discontinue the run. This occurs when the values chosen, or sometimes incremented to, will not allow solutions to match observed data. The instability comes about when a small change in a thermal conductivity parameter value causes the surface temperature of the constructed profile to get unreasonably large, or small.

In analyzing the data sets from each run, two different initial thermal conductivity parameter sets were specified as input. These were Weilbacher's and Brandt's as given in Section 1.2. The single profile set for Run 13, Brandt's parameters, is presented in the following two figures. This profile set successfully ran from a starting observed temperature of 1000°C all the way up to center melting, which stopped the run. Eleven profiles were constructed of which ten are displayed. Figure 6.1 shows profiles 2 through 7 and Figure 6.2 shows profiles 6 through 11. The code does construct the temperature profiles to be flat across the center of the pellet, but limitations on the computer graphics do not allow this to show.

The resulting parameters and current errors that were obtained for each profile are presented in Table 6.1. It can be seen that parameter 2 is the only one that changed for every profile, while parameter 1 changed for the low profiles and parameter 6 for the high. These results came from MANTRA-III in the automatic optimization mode

Figure 6.1. Low temperature profiles from Run 13.

Figure 6.2. High temperature profiles from Run 13.

Table 6.1. Run 13 Single Profile Results

Obs. Temp	Cent. Temp	Current	Parameters ^a				Error
			1	2	4	6	
1000°C	1802 K	3.32	4.39	2.160E-2	1.18	3.29	
1050	1897	3.90	4.403	3.986E-2	1.571	3.29	0.26
1100	1953	4.74	--	4.384E-2	--	--	-2.6E-2
1150	2015	5.91	4.430	3.879E-2	1.591	--	3.2E-2
1200	2122	7.51	--	3.422E-2	--	--	-2.5E-2
1250	2281	9.63	--	3.098E-2	--	--	-1.6E-2
1300	2504	12.36	4.452	2.853E-2	1.768	3.251	3.0E-2
1350	2674	15.78	--	2.588E-2	--	2.958	-2.0E-2
1400	2925	19.98	--	2.552E-2	--	2.293	-3.0E-2
1441 ^b	3092	23.00	--	2.534E-2	1.944	3.654	2.0E-2
1431	3137	28.00	--	2.529E-2	1.923	3.695	-2.6E-2
			--	2.963E-2	1.881	3.735	-9.7E-3

^aParameters 3 and 5 were not changed.

^bReached curve two.

with a limit on SSQ of 0.001. This limit stopped the optimization for all but the first profile which reached its minimum obtainable error for this thermal conductivity parameter set.

Some of the interesting results from this profile set should be pointed out. The last two profile results given in Table 6.1 have come from the upper curve fit of the data as described in Section 4.2. Thus according to these calculations performed by MANTRA-III, central melting of the fuel pellet was reached at about the same observed surface temperature as that region shown in the data curves of Section 3.3 where the surface temperature has started to remain near constant with increasing current. The upper profile in Figure 6.2 clearly shows that a central molten region has been achieved since the temperature has levelled off near the center. More interestingly, this upper profile shows surface temperature about the same as the previous profile. This corresponds with moving on to curve two of the data fits. Tables 6.2 and 6.3 give the data that the profiles were constructed from, showing numerically that center melting has been attained while surface temperature is not increasing. Figures 6.1 and 6.2 and Tables 6.2 and 6.3 also show the increased radius of the sample due to thermal expansion.

These kinds of profile sets can be constructed from a variety of initial thermal conductivity parameter sets. Once the current error for a data point is small enough, the resulting profiles will be quite similar regardless of the thermal conductivity parameters. However, a full profile set like that presented in this section is not so easily obtained. Usually, unstable solutions or nonconvergence errors will occur until a suitable initial thermal conductivity parameter set is

Table 6.2. MANTRA-III Printout, Profile 10

PROFILE 10: TOBS= 1441.4C, VOLTAGE= 5.04V, CURRENT= 23.00AMPS		
TSURF= 1738.5K, CURRENT ERROR=-2.527E-02		
RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	3092.0	0.0000
.0904	2787.5	24.5176
.1279	2640.3	15.2368
.1566	2534.8	11.2798
.1808	2449.2	9.0542
.2022	2376.2	7.4940
.2215	2312.3	6.3175
.2392	2255.5	5.3969
.2557	2204.2	4.6588
.2712	2157.7	4.0566
.2859	2115.0	3.5581
.2999	2075.7	3.1408
.3132	2039.2	2.7880
.3260	2005.3	2.4871
.3383	1973.6	2.2287
.3502	1943.9	2.0052
.3617	1916.0	1.8108
.3728	1889.6	1.6407
.3836	1864.7	1.4913
.3941	1841.1	1.3593
.4043	1818.7	1.2423
.4143	1797.3	1.1382
.4241	1777.0	1.0452
.4336	1757.5	.9619
.4429	1738.9	.8860

Table 6.3. MANTPA-III Printout, Profile 11

PROFILE 11: TOBS= 1430.8C, VOLTAGE= 4.39V, CURRENT= 28.00AMPS TSURF= 1727.7K, CURRENT ERROR=-9.680E-03		
RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	3137.0	0.0000
.0906	3112.4	22.5196
.1282	2911.3	19.5107
.1570	2769.5	14.1172
.1813	2654.0	10.9483
.2027	2555.4	8.7727
.2220	2469.0	7.1612
.2398	2392.4	5.9265
.2563	2323.8	4.9597
.2719	2261.7	4.1904
.2866	2205.2	3.5701
.3006	2153.5	3.0641
.3139	2105.9	2.6474
.3268	2062.0	2.3010
.3391	2021.2	2.0108
.3510	1983.2	1.7659
.3625	1947.7	1.5578
.3737	1914.4	1.3800
.3845	1883.2	1.2271
.3950	1853.7	1.0950
.4053	1825.9	.9804
.4153	1799.5	.8804
.4251	1774.5	.7929
.4346	1750.7	.7159
.4440	1728.1	.6470

found. Similar single profile sets were obtained for the two sets of initial thermal conductivity parameters for DEH Runs 10, 12, 13, and 14. The results from the single profile sets were then used as a starting point in determining the best set of parameters for each run.

To find a resulting best parameter set for one of the DEH runs, a set of five profiles was worked with at once. These were spaced out so that the five data points from the best fit curve cover the entire range of data collected to just below melting. This is similar to what is shown in Figure 5.2, except the data points would be spread out from about 1000°C to where the two curves intersect. The initial thermal conductivity set comes from values obtained from the single profile results, if they allow a solution to all five profiles to be reached. If not, fewer profiles of lower temperature will have to be tried first so that a workable initial thermal conductivity parameter set may be determined. This was the case for Run 13. The interim 4 profile set results are presented in Appendix A. The thermal conductivity parameter results from that run were then used as the initial set for the five profile run. The following is repeated again; two basic starting sets for each run were obtained, the one from Weilbacher's and the one from Brandt's suggested parameters.

Table 6.4 presents the automatic optimization sequence that was gone through in obtaining the smallest errors for the five profile set of Run 13 starting with Brandt's parameters. As shown, the minimum SSQ achieved is 15.08. Notice that the error for Profile 1 is the largest. Profiles 3 and 4 have negative errors yet Profile 5 is back to a positive error. Midway through the optimization sequence the

Table 6.4. MANTRA-III Printout, Run 13 Optimization

THE OPTIMIZING								

			#--CURRENT ERRORS--#					
REG	PAR	VALUE	SSQ	1 PROFILE	2 PROFILE	3 PROFILE	4 PROFILE	5 PROFILE
1	4*	1.50	17.83	2.942	1.927	-.2477	-1.678	1.606
1	4	1.23	63.56	2.809	1.759	-.5546	-2.771	-6.678
#			253.9	3.234	2.318	.6422	1.137	15.37
3	2*	3.268E-02	31.94	2.124	.8142	-1.806	-4.156	-2.498
3	2	2.674E-02	70.81	3.947	3.259	1.838	1.452	6.255
#								
STEP REDUCED TO .0100								
1	6*	3.38	18.65	2.943	1.928	-.2454	-1.658	1.861
1	6	3.31	16.97	2.941	1.926	-.2506	-1.702	1.284
1	4*	1.35	18.81	2.961	1.946	-.2021	-1.540	1.960
1	4	1.38	16.13	2.922	1.902	-.2947	-1.850	.6772
2	4	1.39	16.05	2.905	1.880	-.3355	-1.986	.1259
2	2*	2.941E-02	16.48	2.995	2.001	-.1573	-1.795	.5127
2	2	3.000E-02	16.38	2.817	1.762	-.4515	-2.252	-.2578
#								
STEP REDUCED TO .0010								
1	4*	1.39	16.39	2.904	1.878	-.3394	-2.077	7.3298E-02
1	4	1.39	16.03	2.907	1.882	-.3316	-1.973	.1790
1	6	3.31	16.03	2.907	1.882	-.3319	-1.976	.1457
2	4	1.39	16.01	2.909	1.884	-.3279	-1.962	.1992
2	2*	2.974E-02	16.02	2.900	1.872	-.3456	-1.989	.1606
2	2	2.968E-02	16.32	2.917	1.896	-.3102	-2.014	.2378
#								
TRY SECOND MOST SENSITIVE PARAM								
1	6*	3.27	16.40	2.907	1.883	-.3312	-2.067	-.1664
1	6	3.34	16.15	2.910	1.886	-.3251	-1.939	.5113
2	2*	2.941E-02	16.51	2.998	2.005	-.1494	-1.770	.5864
2	2	3.000E-02	16.27	2.820	1.766	-.4440	-2.229	-.1850
3	4*	1.37	16.19	2.926	1.907	-.2860	-1.823	.7654
3	4	1.40	16.76	2.892	1.863	-.3661	-2.166	-.3118
4	1	4.50	16.00	2.901	1.874	-.3426	-1.963	.1725
1	6	3.34	15.23	2.902	1.875	-.3399	-1.717	.4829
2	2	3.000E-02	16.18	2.814	1.757	-.4560	-2.228	7.7380E-02
3	4	1.40	16.27	2.886	1.854	-.3780	-2.088	-3.9212E-02
4	1	4.54	15.20	2.894	1.865	-.3547	-1.736	.4544
1	6	3.37	16.33	2.895	1.866	-.3525	-1.962	.7044
2	2	3.000E-02	16.20	2.806	1.747	-.4707	-2.249	4.9069E-02
3	4	1.40	16.28	2.878	1.843	-.3928	-2.108	-6.6774E-02
4	1	4.59	15.17	2.886	1.854	-.3696	-1.756	.4255
1	6	3.37	15.85	2.887	1.855	-.3674	-1.983	4.1149E-02
2	2	3.000E-02	16.23	2.798	1.736	-.4856	-2.269	2.0489E-02
3	4	1.40	16.30	2.870	1.833	-.4077	-2.129	-9.4402E-02
4	1	4.63	15.14	2.878	1.844	-.3846	-1.776	.3964
1	6	3.37	15.86	2.879	1.845	-.3825	-2.004	1.0048E-02
2	2	3.000E-02	16.26	2.790	1.726	-.5006	-2.290	-8.3622E-03
3	4	1.40	16.33	2.862	1.822	-.4227	-2.150	-.1227
4	1	4.68	16.03	2.870	1.833	-.3400	-2.045	.3670
STEP REDUCED TO .0010								
1	6*	3.34	15.16	2.878	1.844	-.3845	-1.774	.4248
1	6	3.34	16.07	2.878	1.844	-.3850	-2.026	.3676
2	2*	2.974E-02	16.04	2.869	1.832	-.3424	-2.050	.3557
2	2	2.968E-02	15.17	2.887	1.856	-.3671	-1.751	.4371
3	4*	1.35	16.08	2.876	1.842	-.3887	-2.037	.3420
3	4	1.39	15.16	2.880	1.846	-.3808	-1.763	.4513
4	1	4.64	15.14	2.877	1.843	-.3863	-1.778	.3934
1	6	3.34	16.07	2.877	1.843	-.3865	-2.028	.3646
2	2	2.968E-02	15.17	2.886	1.855	-.3686	-1.753	.4342
3	4	1.35	15.15	2.879	1.845	-.3823	-1.765	.4484
4	1	4.64	15.14	2.876	1.842	-.3878	-1.780	.3905
1	6	3.34	16.07	2.876	1.842	-.3881	-2.030	.3617
2	2	2.968E-02	15.16	2.885	1.854	-.3702	-1.755	.4312
3	4	1.35	15.15	2.878	1.844	-.3839	-1.767	.4454
4	1	4.65	15.13	2.876	1.841	-.3894	-1.782	.3875
1	6	3.34	16.06	2.875	1.840	-.3896	-2.032	.3588
2	2	2.968E-02	15.16	2.884	1.852	-.3717	-1.757	.4283
3	4	1.39	15.15	2.877	1.843	-.3854	-1.769	.4425
4	1	4.65	15.13	2.875	1.839	-.3909	-1.784	.3846
1	6	3.34	16.06	2.875	1.839	-.3911	-2.034	.3558
2	2	2.968E-02	15.16	2.884	1.851	-.3732	-1.759	.4253
3	4	1.39	15.10	2.876	1.842	-.3268	-1.771	.4395
4	1	4.66	15.10	2.876	1.841	-.3283	-1.773	.4365
1	6	3.34	15.08	2.875	1.840	-.3286	-1.775	.4077
2	2	2.968E-02	15.15	2.884	1.852	-.3710	-1.750	.4484

REACHED LIMIT OF OPTIMIZATION TRIES

* INDICATES DIRECTION WAS CHANGED

INDICATES REGION WAS SKIPPED

84a

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Profile 5 error was very small, yet the overall SSQ was reduced more by allowing 5's error to increase some so the Profile 4 error would reduce more. This particular optimization sequence was stopped due to a limit placed on the number of optimization tries.

Parameters 3 and 5 never show up in the automatic optimization due to their lesser importance, or sensitivity, in the thermal conductivity equation tried. Therefore, the next step in gaining a final parameter set is to run MANTRA-III so that each of these parameters will be tried individually. This is done by setting "ONEPAR" of the input file to either 3 or 5, and putting the new values obtained for parameters 1, 2, 4, and 6 into the initial thermal conductivity set.

6.2 Thermal Conductivity Results

The four data taking runs were analyzed using MANTRA-III with the method described above. The final thermal conductivity parameter sets obtained when Weilbacher's values were used as the starting point are given in Table 6.5 along with these starting values for comparison. The asterisk denotes values that are far from the same parameter values of the other runs, and will be omitted in gaining an overall parameter set.

Figure 6.3 graphically presents the data from Table 6.5. The solid line represents Weilbacher's results while the dotted lines are results from this research. The DEH Run 14 curve is not depicted due to the very high SSQ that resulted as shown in Table 6.5. The results of each of the three terms of Eq. (1.2) are broken out and plotted

Table 6.5. Final Parameter Sets (Weilbacher's)

Run	10	12	13	14	Weilb
SSQ	14.4	10.9	17.0	107.	
1	6.218*	5.281	5.308	5.228	5.25
2	4.338E-2	4.190E-2	2.594E-2	2.363E-2	2.2E-2
3	9.580E-4	9.580E-4	1.129E-3	5.251E-3*	9.58E-4
4	1.465	1.905	1.683	2.287*	1.13
5	4256.	4640.	3899.	4705.	4180.
6	3.740	3.754	3.547	3.788	3.29

Figure 6.3. Thermal conductivity results from Table 6.5 with Weilbacher's results for comparison.

separately in Figures 6.4, 6.5, and 6.6 where the solid line is again Weilbacher's results for comparison.

Table 6.6 presents the final parameter sets that resulted from the 4 runs when Brandt's parameters (last column) were used as the starting set. As before, the asterisk denotes a value to be neglected in overall averages. The Run 14 SSQ is even larger for this group than last and Run 14 curves will again be omitted. Figure 6.7 presents the results from Eq. (1.2) with these parameter sets. Figures 6.8, 6.9, and 6.10 give the results from each of the three terms of the thermal conductivity equation. For all of these figures, the solid line comes from Weilbacher's results.

All of the six resulting parameter sets from Runs 10, 12, and 13 are shown together in Figure 6.11. Runs 10 and 12 were made with thin pellets while Run 13 used the thicker ones. The lower temperature range grouping of the results is fairly good, but there is certainly some scattering at the higher temperature range.

There are many different ways an overall best average set of parameters could be achieved. After looking at and plotting some of these, the method chosen was to average all of the parameters given in Tables 6.5 and 6.6 except the values marked with an asterisk. The final six parameters obtained is given in Table 6.7. The thermal conductivity curve that results from these values put into Eq. (1.2) is shown in Figure 6.12 along with Weilbacher's results as the solid line.

Figure 6.13 shows the breakdown of the resulting thermal conductivity into its three parts for both Weilbacher's and this

Figure 6.4. Phonon term results from Table 6.5 with Weilbacher's results for comparison.

Figure 6.5. Electron term results from Table 6.5.

Figure 6.6. Defect term results from Table 6.5.

Table 6.6. Final Parameter Sets (Brandt's)

Run	10	12	13	14	Brandt
SSQ	10.3	16.3	15.0	194.	
1	4.39	4.346	4.656	4.329	4.39
2	4.187E-2	4.620E-2	2.971E-2	2.526E-2	2.16E-2
3	1.036E-3	1.079E-3	1.122E-2	1.106E-3	1.12E-3
4	1.609	1.648	1.385	1.627	1.18
5	6394.*	4607.	4486.	4303.	4180.
6	3.927	3.630	3.336	3.981	3.29

Figure 6.7: Thermal conductivity results from Table 6.6 with Weilbacher's results for comparison.

Figure 6.8. Phonon term results from Table 6.6 with Weilbacher's results for comparison.

Figure 6.9: Electron term results from Table 6.6.

Figure 6.10. Defect term results from Table 6.6.

Figure 6.11. Thermal conductivity results from the six final parameter sets of Tables 6.5 and 6.6.

Table 6.7. Overall Average Parameter Set

Parameter	Value
1	4.79
2	2.47E-2
3	1.06E-3
4	1.62
5	4410.
6	3.71

Figure 6.12. The thermal conductivity results from the overall average (OA) parameter set given in Table 6.7.

Figure 6.13. The phonon (P), electron (E), and defect (D) terms of the overall average (OA) parameter set given in Table 6.7 compared to Weilbacher's (W) results.

average set. "WP" indicates Weilbacher's parameters for the phonon term. Similarly, "OAD" indicates the overall average parameters for the defect term.

6.3 X-ray Diffractometer Results

X-ray diffraction measurements were made on the uranium dioxide samples through Run 10. In several cases a pellet was examined both before and after it was heated for comparison. The highest five diffraction angles were always used in the program XRAY to get consistent results. Two extrapolation methods were used: the Nelson-Riley and the cotangent method (Nuffield, 1966). These two methods usually gave very close results. When these results varied substantially, the data were assumed to be incorrect. DEH Run 5 was made to intentionally oxidize a pellet for analysis with the diffraction technique. Table 6.8 gives some results of the diffractometer analysis. For detail see Appendix B. Pellet B41 showed a definite decrease in lattice parameter due to the heating in the bell jar without argon purge. The other three samples reported were from the only runs where acceptable measurements were made on the same pellet before and after heating. Many other heated and unheated pellets were measured with similar results. As can be seen in the table, the lattice parameter for pellets N4 and B5 remained inside the error bounds before and after heating. Pellet T5 showed a slight decrease, but not enough to indicate anything other than experimental error might be present. The majority of measurements made on both heated and unheated pellets fell between the limits presented by sample T5.

Table 6.8. Diffractometer Results

Pellet	Lattice Parameter	DEH Run
B41	$5.4703 \pm .0018$	unheated
	$5.4685 \pm .0007$	5 (oxidized)
B5	$5.4696 \pm .0009$	unheated
	$5.4705 \pm .0009$	6
T5	$5.4705 \pm .0008$	unheated
	$5.4691 \pm .0004$	9
N4	$5.4702 \pm .0006$	unheated
	$5.4703 \pm .0007$	10

CHAPTER 7

CONCLUSIONS

The modifications made to the equipment and procedures were successful in allowing consistent data collection for the DEH runs. The problem of pellet oxidation has been controlled. The experiment does allow temperatures to be reached where center region melting of the pellet occurs. The "crucible effect" of the individual pellets is evident in that the outer shell of the sample will contain the inner molten region with only slight leakage through vertical thermal expansion cracks. This holds true up to very high power densities, until the pellet stack collapses.

The code MANTRA-III does allow analysis of the experiments and predicts the occurrence of central pellet melting. This seems to occur when the observed surface temperature becomes constant with increasing current as shown in the data plots of Section 3.3. The parameter optimization was successful for 3 of the 4 good data taking runs. The sum of the SSQ's achieved for these three runs when starting with Weilbacher's parameters is 42.3 while for Brandt's it is 41.6. This indicates no preference for starting with either set, and likely, no matter what successful starting parameters are chosen the resulting SSQ will be about the same. The above statement will probably hold true for this particular equation; Weilbacher's equation, Eq. (1.2). If another

were tried that gave lower overall SSQ's, it could be deemed a better thermal conductivity equation.

Some comments may be made on Eq. (1.2) from the resulting thermal conductivity parameter sets obtained. In the figures of the preceding chapter where the parts of the thermal conductivity equation are separated, it can be seen that each of the three terms of the run results has a smaller value than Weilbacher's results. In particular, the contribution of the electron term for this equation seems to be much less than anticipated. This, of course, is also the case for the overall average of the results and can clearly be seen in Figure 6.13.

Data have been collected past central melting and some of the single profiles constructed contained some nodes that were at melting. This indicates that the factor of five thermal conductivity jump used to get a value at melting was successful in allowing MANTRA-III to make some calculations in the molten regime. Until this factor of five jump was included, no success in generating a slightly molten profile was achieved.

7.1 Recommendations

After all the modifications were made and the analysis technique worked out, it was found that only three successful data taking runs had been made. More are needed, particularly for the thick pellets. Analysis of experiments that reach melting could possibly give a better value for molten thermal conductivity than is now available. A major point would be to make some minor changes to the MANTRA-III code so that it would use a particular value for molten uranium dioxide but would

allow the radius of the central molten regime to move so that the data curves could be tracked with the code to their end points. A particular radius of the molten region could then be predicted by the code for the highest heatup achieved. The measured pellet from each run could then be sliced and the molten radius measured to see if the prediction is accurate.

It seems that there is still some room to try other thermal conductivity equations to see if the overall SSQ of the runs can be reduced. Perhaps a trial of Weilbacher's equation with the third term omitted might better indicate the importance of the defect term.

Due to the flexibility of a six parameter thermal conductivity equation, more work could be done with finding a single best set of parameters for the data obtained.

Some success was met in using the factor of five jump to get temperature profiles to include a central molten region. More work should be done with this idea by using differing thermal conductivity jumps or differing values of the molten electrical conductivity.

7.2 Summary

This report describes the work that was carried out to get meaningful thermal conductivity results from a Direct Electrical Heating of uranium dioxide pellets. Experimental equipment and techniques were modified so that successful data taking runs past central melting of the pellet stack may be consistently carried out. The modeling code MANTRA-III has been developed so that temperature profiles from 1250 K to melting may be constructed. MANTRA-III also finds an overall best set

of thermal conductivity parameters for a particular run by analyzing data over the entire range collected (to melting) rather than a particular point.

It is shown that these techniques and codes do provide a method for determining the thermal conductivity of the solid material and an estimate of its molten thermal conductivity as well. Five data-taking runs were carried out. Three of these turned out satisfactorily and allowed best thermal conductivity parameter sets to be determined. From these an overall average thermal conductivity parameter set is suggested. Data from the DEH experiments has been collected well past central melting of the pellets. With new analysis techniques or modifications of the analytical methods described in this report, the molten data gathered might yield the thermal conductivity value of molten uranium dioxide.

APPENDIX A

MANTRA-III CODE

The idea for this type of code, and the original code, MANTRA, were from the research which preceded this investigation (Himes, 1979). The code has been almost totally changed with only the subroutines SURF and ELECT remaining similar to what they were. This code now contains 1 function subroutine, 7 subroutines, the controlling program (MANTRA), and is about 750 lines long. A list of the program divisions in a hierarchy of how they are connected is presented in Figure A.1. Each of the separate routines will then be presented and described in the following sections. Finally, an example output is presented in the last section.

A.1 MANTRA

MANTRA is the controlling program that reads in the data file and calls up the subroutines as necessary. An example of an input data file is presented in Table 5.4. "TAPE3" is used to hold just the final profiles so that they can easily be transferred for plotting.

After reading in and printing the input values, and the initializing of appropriate variables, this program finds the initial information necessary to build up the temperature profiles. The data (surface temperature, current, voltage) for a profile are determined from the appropriate curve, the function subroutine TREAL is called to get the corrected surface temperature in Kelvin, the average electrical

Figure A.1. MANTRA-III subroutine connection.

conductivity is found, then THEXP is called to get the bulk average temperature and from this, the thermal expansion correction. This is done for one profile at a time until the set is complete. (A five-profile set is now maximum, as set by the Dimension Statement.) The information on the profile set is then printed out.

To construct the initial profiles, SUMSQ is called. (SUMSQ actually delegates the work to the lower subroutines, see Figure A.1.) If during the profile construction some type of error occurs, MANTRA has two sections to try and manipulate the thermal conductivity parameters so that a good solution (meaning a good profile) may be achieved. Checks are made to see if central melting occurs on some profile other than the hottest. MANTRA-III is not now capable of handling more than two or three nodes of melting. Checks are also made to see if a specified end value is reached.

When the checks are passed and an initial profile set is obtained, the optimization section is reached. (This section actually starts with the statement label 190, the previous lines are headings to be done once only.) The general idea of what is done in using the entire profile set is presented in Section 5.1 and will not be repeated here. In determining how the parameters are to be moved, when the step size is decreased, and when no more improvement is possible requires a rather extensive set of checks and command routing as can be seen in the listing which accompanies this discussion. To determine which parameters are to be moved, the subroutine SENSIT is called. Each time a parameter is changed, a new set of profiles is constructed to determine if the change is good. Again, SUMSQ is called to do this.

SUMSQ returns the current error for each particular profile and the sum of these current errors squared, SSQ, which is the value MANTRA is trying to minimize.

When the minimum SSQ has been achieved, or when SSQ has gone below "EPS," a predetermined limit set in the input file, MANTRA prints out the final profiles and information.

A.1.1 Program Listing

```

PROGRAM MANTRA(INPUT,OUTPUT,TAPE2=OUTPUT,TAPE3)
INTEGER OP,ALTER,ONEPAR
DIMENSION VCONST(8),ACONST(8),TSC(12),SIG(12),CF(12),ERR(12)
DIMENSION TREG(5),KP(12),TAV(5),AREAL(12),MDIR(6)
DIMENSION OP(4),SIGN(6),THOLD(12),IMP(6),CTH(6)
COMMON/B1/T(12,50),R(12,50),Q(12,50),N,V(12),CL(12),MUN
COMMON/B2/HET,HLTA,IS(12),IPKINI,KSUMF(12),TM(12)
COMMON/B3/CT(6),TD,CE(6)
C---THE INCREMENTING FUNCTION FOR THE PARAMETERS
PINC(J)=CT(J)*STEP*SIGN(J)*CT(J)
C-----
C---READ IN INPUT
C-----
      READ 13,MRUN,TBEGC,TENDC,TINC,TCUT,AINC,AEND
      READ 23,(VCONST(K),K=1,8)
      READ 23,(ACONST(K),K=1,8)
      READ 33,(CT(K),K=1,6)
      READ 33,(CE(K),K=1,6)
      READ 43,EPS,RAD,HIGH,TD
      PER=100.0*TD
      READ 53,N,NPRD,NREG,ONEPAR,STEP1,SMIN
      RI=0
      IF(ONEPAR.GT.0)NREG=1
      FORMAT(1(I2,/,),5(F6.1,/,),F6.1)
13      FORMAT(7(E11.4,/,),F11.4)
23      FORMAT(5(E11.4,/,),E11.4)
33      FORMAT(3(E11.4,/,),E11.4)
43      FORMAT(12,/,3(I1,/,),F7.5,/,F7.5)
53      C-----
      C---PRINT INPUT INFORMATION
      C-----
      PRINT 7,MRUN,TBEGC,TENDC,TINC,TCUT,AINC,AEND
      PRINT 17,(VCONST(K),K=1,8),(ACONST(K),K=1,8),(CT(K),K=1,6)
      PRINT 27,(CE(K),K=1,6)
      PRINT 37,RAD,HIGH,RI,PER,N,NPRD,NREG,ONEPAR
7      FORMAT(1H1,/,10X,22(1H-),/,10X,
1      *---FROM DEH RUN #*,I2,*---*,/,10X,22(1H-),
2      //,15X,*STARTING AT OBSERVED TEMPERATURE OF *,F6.1,2X,
3      *AND ENDING AT *,F6.1,* CELSIUS*,/,20X,
4      *THE TEMPERATURE INCREMENT USED IS *,F6.1,
5      //,15X,*THE CUTOFF TEMPERATURE WHERE CURVE TWO STARTS IS*,
6      F7.1,/,20X,*THE CURRENT INCREMENT IS*,F4.1,
7      * AND THE MAX CURRENT ALLOWED IS*,F5.1)
17      FORMAT(///,15X,*THE CONSTANTS GIVEN BY THE BMDX *,
1      *FIT FOR VOLTAGE FROM TEMPERATURE ARE:*,/,20X,4(1PE11.4,3X),
2      //,15X,*CONSTANTS FOR CURVE TWO, VOLTAGE FROM AMPS:*,/,20X,
3      4(1PE11.4,3X),/,15X,*THE CONSTANTS FOR THE CURRENT FIT, *,
4      *AMPS FROM TEMP:*,/,20X,4(1PE11.4,3X),/,15X,*CONSTANTS FOR*,
5      * CURVE TWO, TEMP FROM AMPS:*,/,20X,4(1PE11.4,3X),
6      ///,15X,*THE SIX INITIAL THERMAL CONDUCTIVITY PARAMS ARE:*,/,
7      20X,6(1PG11.4,2X))
27      FORMAT(///,15X,*THE INITIAL ELECTRICAL CONDUCTIVITY *,

```

```

2  *PARAMETERS ARE:*,//,20X,8(1PG11.4,2X))
37  FORMAT(//,10X,*SAMPLE CHARACTERISTICS:*,//,20X,*RADIUS:*,
1  F10.5,* CM.*/,//,20X,*ACTIVE LENGTH:*,F10.5,* CM.*/,//,
2  20X,*CENTRAL VOID RADIUS:*,F10.5,* CM.*/,//,
3  20X,*INITIAL FRACTION OF THEORETICAL DENSITY:*,F10.5,* PERCENT*,
4  //,10X,*PROFILE INFO:*,//,20X,*INITIAL NUMBER OF NODES:*,I2,
5  //,20X,*WORKING WITH *,I1,* PROFILES AND *,I1,* TEMP REGIONS*,
6  //,20X,*THE PARAMETER OPTIMIZATION CODE: *,I1)
C---INITIALIZE COUNTERS AND FLAGS
DD 15.K=1,6
15  SIGN(K)=1.0
    NPCUT=0
    TSCD=TBEGC-TINC $ NP=0 $ NPST=1-NPRO $ ALTER=0
    MOP1=0 $ MOP2=0 $ MS1=0 $ MTWD=0 $ IAMP=0
5    NPST=NPST+NPRO $ STEP=STEP1 $ JSUM=0
    M2=0
C---
C--SETTING UP THE PROFILES
C-----
C--GET PROFILE POINTS
    NEND=NPST+NPRO-1
    TBEG=TSCD+TINC
10    DO 70.NP=NPST,NEND
        THOLD(NP)=1.0
        IF(IAMP.EQ.1)GO TO 20
        TSCD=TSCD+TINC
        GO TO 30
20    A=A+AINC
C--CHECK IF TEMP OR AMP LIMITS ARE PASSED
30    IF(TINC.LT.0)GO TO 32
        IF(TSCD.GT.TENDC.AND.ALTER.GT.0)GO TO 400
        IF(TSCD.GT.TENDC)GO TO 80
        IF(A.GT.AEND)GO TO 400
        GO TO 35
32    ALTER=-1
        IF(TSCD.LT.TENDC)GO TO 400
C--GET DATA POINTS FROM CURVE FITS
35    IF(IAMP.EQ.1)GO TO 50
        IF(TSCD.GE.TCUT)GO TO 40
C--CALCULATE VOLTAGE AND CURRENT FROM BMDX BEST FIT EQUATIONS
C-----CURVE ONE
    V1=VCONST(1)+VCONST(2)*TSCD+VCONST(3)*TSCD**2+VCONST(4)*TSCD**3
    A=ACONST(1)+ACONST(2)*TSCD+ACONST(3)*TSCD**2+ACONST(4)*TSCD**3
    GO TO 60
C--FIND STARTING CURRENT VALUE 1ST TIME CURVE TWO IS USED
40    A=ACONST(1)+ACONST(2)*TCUT+ACONST(3)*TCUT**2+ACONST(4)*TCUT**3
    IA=A $ A=IA $ IAMP=1 $ NPCUT=NP
C--CURVE TWO, CALCULATE VOLTAGE & TEMP FROM CURRENT
50    V1=VCONST(5)+VCONST(6)*A+VCONST(7)*A**2+VCONST(8)*A**3
    TSCD=ACONST(5)+ACONST(6)*A+ACONST(7)*A**2+ACONST(8)*A**3
60    AREAL(NP)=A $ V(NP)=V1 $ TSC(NP)=TSCD
C--CALL TO GET CORRECTED SURFACE TEMPERATURE
    TS(NP)=TREAL(TSCD)
    TS1=TS(NP)
C--CALCULATE AVERAGE ELECT. CONDUCTIVITY WITH THIS DATA
    SIG(NP)=(AREAL(NP)*HIGH)/(3.14159*V(NP)*RAD**2)
C--GET CORRECTION FACTOR AND MEAN TEMPERATURE OF PELLET
    SIG1=SIG(NP)
    CALL THEXP(SIG1,CF1,TS1,TMEAN)
    CF(NP)=CF1
    TM(NP)=TMEAN $ RSURF(NP)=CF(NP)*RAD $ CL(NP)=CF(NP)*HIGH

```

```

70      CONTINUE
      GO TO 90
C--CHECK IF LIMIT IS PASSED BY END PROFILE
80      ALTER=ALTER+1
      IF (NP.EQ.NEND) GO TO 120
      GO TO 400
C--PRINT INFORMATION ON THE PROFILE SET
90      PRINT 47,NPRO
      DO 100 NP=NPST,NEND
      IF (NP.LT.NPCUT.OR.NPCUT.EQ.0) GO TO 95
      PRINT 59,NP,TSC(NP),AREAL(NP),V(NP)
      GO TO 98
95      PRINT 57,NP,TSC(NP),AREAL(NP),V(NP)
98      PRINT 67,SIG(NP),TH(NP),CF(NP)
      PRINT 77,RSURF(NP),CL(NP),TS(NP)
100     CONTINUE
47      FORMAT(1H1,/,10X,****INFORMATION ON THE SET OF *,
2       1I,*,PROFILES=****,/)
59      FORMAT(//,5X,***PROFILE NUMBER *,I2,****,/,10X,
2       *(NOW ON CURVE TWO)*,/,10X,
3       *MEASURED VALUES*,/,15X,*TEMPERATURE:*,T30,F6.1,* C*,
4       /,15X,*CURRENT: *,T30,F5.2,* AMPS*,/,15X,*VOLTAGE:*,
5       T30,F5.2,* VOLTS*)
57      FORMAT(//,5X,***PROFILE NUMBER *,I2,****,/,10X,
2       *MEASURED VALUES*,/,15X,*TEMPERATURE:*,T30,F6.1,* C*,
3       /,15X,*CURRENT: *,T30,F5.2,* AMPS*,/,15X,*VOLTAGE:*,
4       T30,F5.2,* VOLTS*)
67      FORMAT(10X,*PELLET AVERAGE VALUES:*,/15X,
1       *ELECTRICAL COND.**,F8.5* (1/ohm cm)/15X,*TEMPERATURE**,
2       5X,F8.2,* K*,/15X,*EXPANSION CORRECTION**,F8.5)
77      FORMAT(10X,*CORRECTED VALUES*,/15X,*radius**,F8.5,* CM*,
2       /,15X,*LENGTH**,F8.5,* CM*,/15X,*SURF TEMP**,F8.2,* K*)
C--CALL TO GET INITIAL PROFILES AND SSQ, THE SUM OF THE CURRENT
C--ERRORS SQUARED
110     CALL SUMSQ(AREAL,ALTER,NPRO,SSQ1,NPST,ERR)
C--CHECK IF MAX SURF TEMP AVAILABLE IS LESS THAN ACTUAL
C--THAT IS, WHEN "MLTA">0. CHECK FOR UNSTABLE SOLUTION, MUN.
      MFROM=0 $ JP=0
      IF (MLTA.GT.0) GO TO 130
      IF (MUN.GT.0) GO TO 440
      MU1=0 $ MOP2=0 $ MS1=1 $ MTWO=0
C--CHECK IF MELTING WAS REACHED BY OTHER THAN END PROFILE
      IF (ALTER.GT.0) GO TO 120
C--SAVING FIRST VALUES
      SSQST=SSQ1
      DO 115 K=1,6
115     CTH(K)=CT(K)
      GO TO 190
120     IF (ALTER.GT.1) STOP
C--ALTER PROFILES TO GET BELOW MELTING OR END LIMIT, ADD MORE NODES
      TINC=TINC*0.6
      PRINT 97,TINC
      TSCD=TBEG-TINC
      N=N+10
      ALTER=ALTER+1
      GO TO 10
C--FOR THE MLTA CASE, ADJUST THE OVERALL MOST SENSITIVE PARAM
C--IN A PARTICULAR DIRECTION TO INCREASE CALCULATED SURF TEMP
125     MFROM=1
130     NP=MLTA
      T1=TH(NP)

```

```

      IF(NP.EQ.NHOLD)GO TO 135
      CALL SENSIT(NOTE,T1,OP)
      MPAR=OP(1)
      IF(JP.EQ.OP(1))SIGN(JP)=-1.0*SIGN(JP)
135    IF(NP.LT.NHOLD)GO TO 140
      IF(T(NP,N).LT.THOLD(NP))GO TO 140
      THOLD(NP)=T(NP,N) $ NHOLD=NP
      GO TO 150
140    SIGN(MPAR)=SIGN(MPAR)*(-1.0)
150    CT(MPAR)=PINC(MPAR)
      PRINT 107,NP,T(NP,N),TS(NP),MPAR,CT(MPAR)
      IF(MFROM.EQ.1)GO TO 270
      GO TO 110

C-----
C--PARAMETER OPTIMIZATION FOR THE SET OF PROFILES
C-----
C--PRINT REGION INFO AND OPTIMIZATION HEADINGS
160    M2=1 $ JP2ND=0
      DO 165 K=1,6
165    SIGN(K)=1.0
      PRINT 127,(CT(K),K=1,6)
      PRINT 117,T(NEND,1),(TREG(K),K=1,JE),T(NPST,N)
      PRINT 247,(TAV(K),K=1,NREG)
      DO 170 K=NPST,NEND
170    KP(K)=K
      PRINT 137,(KP(K),K=NPST,NEND)
      PRINT 147,SSQ1,(ERR(K),K=NPST,NEND)
      GO TO 230
C--RETRYING MOST SENSITIVE PARAM, FLAG
180    PRINT 287
      STEP=STEP1/10.0
      JP2ND=3
C--INITIALIZE AND DIVIDE PROFILE SET INTO NREG REGIONS
190    M3=0
      IF(SSQ1.LT.0.1.AND.JP2ND.NE.2)GO TO 350
200    IMPROV=1
      DO 195 K=1,6
195    IMP(K)=0
      DO 205 K=1,6
205    MDIR(K)=0
210    TREG1=(T(NEND,1)-T(NPST,N))/NREG
      IF(NREG.EQ.1)GO TO 225
      JE=NREG-1
      DO 220 JA=1,JE
      TREG(JA)=T(NEND,1)-TREG1*JA
220    TAV(JA)=TREG(JA)+TREG1/2.0
225    TAV(NREG)=T(NPST,N)+TREG1/2.0
C--CHECK IF HEADINGS NEEDED (FIRST TIME THROUGH)
      IF(M2.NE.1)GO TO 160
230    JR=1
C--CALL TO FIND TWO MOST SENSITIVE PARAMS FOR REGION
C--"JR" IS REGION #, AND "JP" IS PARAM #
250    TSEN=TAV(JR)
      IF(ONEPAR.GT.0)JP=ONEPAR
      IF(ONEPAR.GT.0)GO TO 255
      CALL SENSIT(NOTE,TSEN,OP)
      JP=OP(1)
      IF(JP2ND.EQ.2)JP=OP(2)
      IF(JP.EQ.0)GO TO 320
255    IF(JP.EQ.JPHOLD.AND.IMPROV.EQ.0)GO TO 300
C--SAVE PARAM VALUE, STEP PARAM

```

```

260      CTHOLD=CT(JP) $ JPHOLD=JP
      CT(JP)=PINC(JP)
C--GET NEW PROFILES AND PRINT VALUES
270      CALL SUMSQ(AREAL,ALTER,NPRO,SSQ2,NPST,ERR)
      JSUM=JSUM+1
      IF(JSUM.GT.65)GO TO 375
      IF(MUN.GT.0)GO TO 430
      IF(MOP1.GT.0)SSQ1=SSQ2
      MOP1=0 $ MOP2=0 $ MS1=0 $ MTWD=0
      IF(MLTA.GT.0)GO TO 125
      PRINT 157,JR,JP,CT(JP),SSQ2,(ERR(K),K=NPST,NEND)
C--IS SSO IMPROVING
      IF(SSQ2.LE.SSQ1)GO TO 310
C--GET PARAM BACK
      CT(JP)=CIHULU $ IMPROV=0
      IF(IMP(JP).GT.1)GO TO 320
C--CHANGE DIRECTION AND DEL FLAW
      IF(MDIR(JP).EQ.1)GO TO 320
      SIGN(JP)=SIGN(JP)*(-1.0)
      PRINT 217
      MDIR(JP)=1 $ GO TO 260
C--PRINT REGION SKIPPED SYMBOL
300      PRINT 257 $ GO TO 320
C--CHECK IF SSO HAS REACHED LIMIT
310      SSQ1=SSQ2 $ IMPROV=1 $ IMP(JP)=IMP(JP)+1
      IF(SSQ1.LT.EPS)GO TO 380
C--DOES 2ND REGION PARAM NEED TO BE STEPPED, THEN CHECK FOR OUTSIDE REGION
315      IF(JP2ND.EQ.2)NOTE=1
      IF(NOTE.EQ.2)GO TO 330
320      IF(JR.EQ.NREG)GO TO 340
      JR=JR+1 $ GO TO 250
C--CHANGE TO SECOND PARAM
330      JP=OP(2)
      NOTE=1 $ M3=M3+1 $ GO TO 260
C--IF IMPROVEMENT IS SEEN AT THIS STEP SIZE, CONTINUE
340      IF(IMPROV.EQ.1) GO TO 210
C--REDUCE STEP SIZE
350      STEP=STEP/10.0
      IF(STEP.LT.SMIN)GO TO 360
      PRINT 207,STEP $ GO TO 200
C--CHECK IF 2ND PARAM SHOULD BE TRIED
360      IF(M3.GE.6)GO TO 370
      IF(JP2ND.GT.1)GO TO 370
      JP2ND=2
      PRINT 277
      STEP=STEP/10.0
      GO TO 190
C--SHOULD PARAM 1 BE RETRIED
370      IF(JP2ND.EQ.2.AND.IMP(JP).GT.1)GO TO 180
      GO TO 380
C-----
C--PRINT FINAL PROFILE INFO
C-----
375      PRINT 307
380      IF(SSQST.GT.SSQ1)GO TO 395
      DO 385 K=1,6
385      CT(K)=CTH(K)
395      CALL SUMSQ(AREAL,ALTER,NPRO,SSQ1,NPST,ERR)
      IF(MELT.EQ.1)PRINT 87
      PRINT 167,NPRO,SSQ1,(CT(K),K=1,6)
      PRINT 237,T(NEND,1),(TREG(K),K=1,JE),T(NPST,N)

```

```

      PRINT 247, (TAV(K), K=1, NREG)
      DO 390 NP=NPST, NEND
      PRINT 177, NP, TSC(NP), V(NP), AREAL(NP), TS(NP), ERR(NP)
      PRINT 187, (R(NP, K), T(NP, K), Q(NP, K), K=1, N)
C---WRITE PROFILES ONTO A TAPE
      WRITE(3, 197) HRUN, NP, TSC(NP)
      WRITE(3, 187) (R(NP, K), T(NP, K), Q(NP, K), K=1, N)
390    CONTINUE
C---STOP IF MELTING HAS BEEN REACHED
      IF (MELT.EQ.1) STOP
      GO TO 5
400    PRINT 227 $ STOP
C---FOR THE UNSTABLE CASE, MOVE PARAMS TO GAIN STABILITY
430    CT(JP)=CTHOLD $ MFROM=1
440    NP=MUN
      T2=TM(NP)
      CALL SENSIT(NOTE, T2, OP)
      IF (JP.EQ.OP(1).AND.IMP(JP).GT.0) GO TO 490
      IF (JP.EQ.OP(1)) SIGN(JP)=SIGN(JP)*(-1.0)
      IF (OP(1).EQ.MOP1) GO TO 450
445    MOP1=OP(1)
      NPAR=OP(1) $ GO TO 460
450    IF (OP(2).EQ.MOP2) GO TO 470
      NPAR=OP(2) $ MOP2=OP(2)
460    CT(NPAR)=PINC(NPAR)
      IF (MTWO.EQ.1) CT(NPAR)=PINC(NPAR)
      PRINT 267, NPAR, CT(NPAR)
      MUN=0
      IF (MFROM.EQ.1) GO TO 270
      GO TO 110
470    IF (MS1.EQ.1) GO TO 480
      MOP1=0 $ MOP2=0
      MS1=1
      MSS1=OP(1) $ MSS2=OP(2)
      SIGN(MSS1)=SIGN(MSS1)*(-1.0)
      SIGN(MSS2)=SIGN(MSS2)*(-1.0)
      GO TO 445
480    IF (MTWO.EQ.1) STOP
      MTWO=1 $ MS1=0
      GO TO 445
490    PRINT 297 $ IMPROV=0
      GO TO 315
C-----
C---GENERAL OUTPUT FORMATS
C-----
87    FORMAT(/, 15X, '***CENTER MELTING HAS BEEN REACHED***')
97    FORMAT(/, 10X, '***ALTERING PROFILES** TINC IS NOW *, F5.1)
107   FORMAT(10X, 'MLTA FOR PROFILE*I2,*, SURFACE TEMP: CALCULATED=*,
2     F8.2, 3X, 'ACTUAL=*, F8.2, /, 13X, 'CHANGED PARAM *I1* TO *1PG11.4)
117   FORMAT(/, 5X, 'INITIAL TEMP REGION BOUNDS FOR THE SET OF *
2     *PROFILES:*, /, 5X, 7(F7.1, 3X))
127   FORMAT(/, 10X, 'PARAMETER STARTING VALUES:*, /, 6X, 6(1PG11.4))
137   FORMAT(1H1, 5X, 3H***, 'THE OPTIMIZING*, 3H***, /, 6X, 20(1H-), /,
2     T35, **--CURRENT ERRORS--**, /, 1X, 'REG PAR VALUE=T25, *SSO*, T34,
3     S(I2, * PROFILE*, 4X))
147   FORMAT(3X, T22, 6(1PG11.4, 3X))
157   FORMAT(T2, I1, T6, I1, T10, 1PG10.3, T22, 6(G11.4, 3X))
167   FORMAT(1X, 20(1H-), /, 1X, 1H*, * INDICATES DIRECTION WAS *
2     *CHANGED*, /, 1X, 1H*, * INDICATES REGION WAS SKIPPED*,
3     /, 3X, 10(1H*), **FINAL INFORMATION ON THE SET OF *, I1,
4     * PROFILES*, 10(1H*), /, 4X, *SUM OF CURRENT ERRORS SQUARED=*,

```

```

5      G10.3, //10X, *PARAMETER VALUES*, /5X, 6(1PG11.4))
177   FORMAT(///, 2X, *PROFILE *I2, 1H:, * TOBS=*F7.1, *C, *
2      * VOLTAGE=*F5.2, *V, * CURRENT=*F6.2, *AMPS*, /, 14X,
3      *TSURF=*F7.1, *K, *, * CURRENT ERROR=*1PG10.3, /, 3X,
4      *RADII (CM)*, T18, *TEMP (K)*, T30, *POWER DENS (W/CM3)*
187   FORMAT(3X, F7.4, T18, F7.1, T34, F8.4)
197   FORMAT(//5X, *DEH RUN *I2, *, PROFILE *I2, 1H:, * TOBS=*F7.1, *C, /,
2      3X, *RADII (CM)*, T18, *TEMP (K)*, T30, *POWER DENS (W/CM3)*
207   FORMAT(10X, *STEP REDUCED TO*, F7.4)
217   FORMAT(1H, T7, 1H)
227   FORMAT(//, 10X, *END VALUE REACHED==*STGP*)
237   FORMAT(/, 5X, *TEMP REGION BOUNDS FOR THE SET OF *
2      *PROFILES:*, /, 5X, 7(F7.1, 3X))
247   FORMAT(3X, *AVS*, T11, 5(F7.1, 3X))
257   FORMAT(1X, 1H#)
267   FORMAT(10X, *DUE TO UNSTABLE TEMP SOLUTION, *
2      *CHANGED PARAM*, I2, * TO *, 1PG11.4)
277   FORMAT(10X, *TRY SECOND MOST SENSITIVE PARAM*)
287   FORMAT(10X, *BACK TO MOST SENSITIVE PARAM*)
297   FORMAT(10X, *UNSTABLE TEMP SOLUTION REACHED*)
307   FORMAT(/, 10X, *REACHED LIMIT OF OPTIMIZATION TRIES*)
      END

```

A.2 THEXP and TREAL

THEXP is satisfactorily explained in the listing of it on the following page. Its purpose is to calculate the bulk average temperature and from that the thermal expansion corrections. The origin of the equations used in this subroutine are given in Section 5.5.

TREAL calculates the true pellet surface temperature from that observed with the optical pyrometer. The equations given to do this are described in Section 5.4.

A.2.1 THEXP and TREAL Listings

```

      SUBROUTINE THEXP(SIG,CF,TS,TM)
      COMMON/B3/CT(6),TD,CE(6)
C--THE ITERATION FUNCTIONS
      F(X)=(-G*X**3)+CE(2)*X**2+CE(3)*X+CE(4)
      FP(X)=(-3.0*G*X**2)+2.0*CE(2)*X+CE(3)
C--THIS ROUTINE CALCULATES THE BULK AVERAGE TEMP OF THE PELLET BY
C--SOLVING THE ELECTRICAL CONDUCTIVITY EQUATION. NEWTON-RAPHSON
C--ITERATION IS USED ON BATES'S ELECT. COND. EQUATION. THIS
C--AVERAGE TEMP IS THEN USED TO GET THE PELLET THERMAL EXPANSION
C--CORRECTION FACTOR.
C--THE INITIAL TEMP GUESS
      X=2000.0 $ ITER=0 $ ER=1.0
      G=ALCG(SIG)-CE(1)
C--LGDP TO GET SOLUTION
10      ITER=ITER+1
      X2=X-F(X)/FP(X)
      DIF=ABS(X2-X)
      IF(DIF.LT.ER)GO TO 20
      IF(ITER.GT.20)GO TO 90
      X=X2 $ GO TO 10
C--CONVERGED ON MEAN TEMP, KELVIN. CALCULATE CORRECTION FACTOR, CF.
20      TM=X2
      CF=1.0+6.8E-6*(TM-273.16)+2.9E-9*((TM-273.16)**2)
      RETURN
C--FOR NO TM CONVERGENCE, ESTIMATE A VALUE
90      PRINT 3,X2,X
      X2=TS+300.0
      GO TO 20
3       FORMAT(/,5X,*NO CONVERGENCE FOR TM, USE ESTIMATE*,/,
2       5X,*LAST TEMP VALUES WERE*,F8.2,* AND*,F8.2)
      END

```

```

      FUNCTION TREAL(T)
C--OBSERVED TEMP IN KELVIN
      TD=T+273.16
C--UD2 EMISSIVITY
      E=0.9
      IF(TD.LE.1900)GO TO 10
      E=1.645-3.9215E-4*TD
C--GLASS TRANSMITTANCE
10      TAU=0.93
C--CORRECTED SURFACE TEMP
      A=1.0/TD
      B=ALDG(E*TAU)/22135.4
      TREAL=1.0/(A+B)
      RETURN
      END

```

A.3 SENSIT

For a given temperature and a particular set of thermal conductivity parameters, SENSIT determines the order of sensitivity of the parameters. This is done so that MANTRA will not move a parameter that has little or no effect while in the automatic optimization mode. SENSIT works for Weilbacher's equation now, Eq. (1.2). For some other equation, a new set of partial derivatives would need to be determined and put in. The comment lines marked "CZZZ" set aside the partial derivatives to be changed. This particular partial derivative set calls for a value of the thermal conductivity to be known. This is obtained by calling THERM.

A.3.1 SENSIT Listing

```

      SUBROUTINE SENSIT(NOTE,TSEN,OP)
C---THIS SUBROUTINE CHECKS THE SIX PARAMETERS TO DETERMINE THEIR
C---ORDER OF SENSITIVITY, THEN CHOOSES WHICH TO OPTIMIZE. THIS
C---IS DONE FOR ANY SET OF PARAMETERS SENT ALONG WITH THE
C---CORRESPONDING TEMPERATURE.
      INIL68 P,OP
      DIMENSION C(6),SP(6),OP(4),P(6)
      COMMON/B3/CT(6)
C---BOLTZMAN'S CONSTANT
      BK=8.61812E-05
C---GET THE THERMAL CONDUCTIVITY FOR THIS SET, THC
      T=TSEN
      CALL THERM(T,THC)
C---THESE SENSITIVITY FUNCTIONS COME FROM THE PARTIAL
C---DERIVATIVE OF EACH PARAMETER W.R.T. THE THERMAL CONDUCTIVITY
C---EQUATION, THE SENSITIVITY OF PARAMETER 1, ETC.: "SP(1)"

```

```

CZZZ1
A1=THC*((CT(1)+CT(2)*T)**2)
SP(1)=CT(1)/A1
SP(2)=CT(2)*T/A1
A3=EXP(-CT(4)/(BK*T))
SP(3)=(CT(3)*T/THC)*A3
SP(4)=CT(3)*CT(4)*A3/(THC*BK)
A5=EXP(-CT(6)/(BK*T))
SP(5)=CT(5)*A5/THC
SP(6)=CT(5)*CT(6)*A5/(THC*BK*T)

CZZZ2
C--FIND THE ORDER OF THE MAGNITUDE OF THE SENS. FUNC.
DO 100 K=1,6
100 C(K)=SP(K)
DO 105 I=1,6
IF(C(1).LT.C(2))GO TO 30
IF(C(1).LT.C(3))GO TO 40
IF(C(1).LT.C(4))GO TO 50
IF(C(1).LT.C(5))GO TO 60
IF(C(1).LT.C(6))GO TO 70
P(I)=1 $ M=1 $ GO TO 500
30 IF(C(2).LT.C(3))GO TO 40
IF(C(2).LT.C(4))GO TO 50
IF(C(2).LT.C(5))GO TO 60
IF(C(2).LT.C(6))GO TO 70
P(I)=2 $ M=2 $ GO TO 500
40 IF(C(3).LT.C(4))GO TO 50
IF(C(3).LT.C(5))GO TO 60
IF(C(3).LT.C(6))GO TO 70
P(I)=3 $ M=3 $ GO TO 500
50 IF(C(4).LT.C(5))GO TO 60
IF(C(4).LT.C(6))GO TO 70
P(I)=4 $ M=4 $ GO TO 500
60 IF(C(5).LT.C(6))GO TO 70
P(I)=5 $ M=5 $ GO TO 500
70 P(I)=6 $ M=6
500 C(M)=0.0
105 CONTINUE
C--SET FIRST PARAMETER TO OPTIMIZE
OP(1)=P(1)
C--CHECK OTHER 3 POSSIBILITIES TO SEE IF THEY

C--ARE SENSITIVE ENOUGH TO OPTIMIZE
DLIMIT=0.05
DO 110 K=2,4
N=P(K)
IF(SP(N).GE.DLIMIT)OP(K)=P(K)
110 CONTINUE
C--CHECK TO SEE IF PARAMETERS ARE CLOSE IN SENSITIVITY
N1=P(1) $ N2=P(2) $ NOTE=0
RATIO=SP(N1)/SP(N2)
IF(RATIO.LT.5.0)NOTE=2
RETURN
END

```

A.4 SUMSQ

SUMSQ gets the profiles constructed one at a time by calling SURF. If a profile is successfully built without any instabilities or other errors, SUMSQ finds its current error, then goes on to the next profile. This subroutine also calculates the SSQ for the parameter set.

A.4.1 SUMSQ Listing

```

SUBROUTINE SUMSQ(AREAL,ALTER,NPRD,SSQ,NP1,ERR)
  INTEGER ALTER
  DIMENSION ERR(12),AREAL(12)
  COMMON/B2/MELT,MLTA
  SSQ=0
  NEND=NP1+NPRD-1
  DO 20 NP=NP1,NEND
    CALL SURF(A,NP,MUN)
    IF(MUN.GT.0)RETURN
    IF(MELT.EQ.1)GO TO 40
10    ERR(NP)=A-AREAL(NP)
    IF(MLTA.EQ.1)GO TO 30
    SSQ=SSQ+ERR(NP)**2
20    CONTINUE
    RETURN
30    MLTA=NP
    RETURN
40    IF(NP.EQ.NEND)GO TO 10
    IF(ALTER.LT.1)GO TO 10
    ALTER=ALTER+1 $ MELT=0
    RETURN
  END

```

A.5 SURF

SURF calculates the pellet geometry by setting up the nodes. If there are "n" nodes specified, SURF builds up "n-1" equal nodal volumes. The next portion of this subroutine determines if there is some possible center temperature that will allow the calculated surface temperature (obtained from TEMP) to be greater than the observed (and corrected) surface temperature. If there is, then the center temperature can always be manipulated to match the correct surface temperature. If not, no center temperature for this parameter set will allow a matching surface temperature to be found. This is called the "MLTA" error (for max is less than actual) and when it occurs, SURF dumps right back to SUMSQ, then MANTRA for correction if possible.

The next major section of this subroutine iterates on center temperature until the corrected surface temperature is matched. SURF has the capability of determining whether a low or high power solution is necessary and for getting one or both of the profiles that go with the solutions. For all of the analyses done in this investigation, the normal high power solution is the only one used. The keying variable "OPT" is set to 2 so that the unnecessary low power solution is bypassed.

The profile is obtained when the calculated surface temperature gets within a set error range, "EMAX," of the actual surface temperature. "EMAX" need not be real small to yield good results, and a small value takes much more computer time. It was set to 0.5 for this report's analysis. When the profile is obtained, the power densities are calculated for each nodal volume from the power dissipated in that volume

found by TEMP. The center node is for a center temperature only and has no volume associated with it.

A.5.1 SURF Listing

```

SUBROUTINE SURF(AMPS,NP1,MUN1)
  INTEGER OPT
  COMMON/E1/T(12,50),R(12,50),O(12,50),N,VGLTS(12),CL(12),MUN
  COMMON/E2/MLT,MLTA,TSURF(12),IPRINT,RSURF(12),TM(12)
C
  101 FORMAT(///,5X,*DISSIPATED POWER*,4X,F12.4,* WATTS*,///,5X,*CURRENT*
    1,13X,F12.4,* AMPS*,///,5X,*VOLTAGE*,13X,F10.4,* VOLTS*,//)
  102 FORMAT(//,7X,*RADIUS (CM)*,4X,*TEMP. (K)*,4X,*POWER DENSITY (W/CM3)
    1*,//)
  104 FORMAT(* *,F15.5,F15.2,F15.4)
  200 FORMAT(* *,///,10X,*INFO ON RESULTS OF SURF, PART ONE. CONDITIONS
    1FOR MAX SURFACE TEMP.*)
  201   FORMAT(//,15X,*CENTER TEMP EXCEEDS MELTING.*)
  204   FORMAT(//,20X,*SPECIFIED VOLTAGE (V)*,F10.4,/,20X,*MAX SURFACE TE
    1MP. (K)*,F10.2,/,20X,*CORRESPONDING CENTER TEMP. (K)*,F10.2,/,
    2 20X,*RESULTING CURRENT (A)*,F10.4)
  206   FORMAT(///,5X,*TYPE ONE SOLUTION--*,//)
  207   FORMAT(///,5X,*TYPE TWO SOLUTION--*,//)
  208   FORMAT(//,20X,*MAX INCREMENTS EXCEEDED IN SURF, PART 2. PROFILE*,I2)
  299   FORMAT(//,20X,*MAX INCREMENTS EXCEEDED IN SURF, PART 1.*)
C--CALCULATE GEOMETRY OF NODES
  AN=N-1 $ MN=N-1 $ NP=NP1 $ MUN1=0
  Z=RSURF(NP)**2/AN
  VOL=3.141593*CL(NP)*Z
C--SOLVING FOR THE RADIAL POSITIONS OF THE NODES
  R(NP,1)=0.0 $ R(NP,N)=RSURF(NP)
  DO 11 I=2,MN
  11   R(NP,I)=SQRT(Z+R(NP,I-1)**2)
C*****
C**SURF PART 1, FIND MAX SURFACE TEMP FOR THIS PARAMETER SPACE
C****
  STEP=100.0 $ SMIN=1.0 $ TC=TM(NP)+400.0 $ TMELT=3137.0 $ NR=0
  ITER=0 $ MLTA=U $ UPI=2 $ MELI=U
C--GET INITIAL PROFILE
  CALL TEMP(A,ITER,TC,VOL,NP)
  IF(MUN.GT.0)GO TO 70
  TS1=T(NP,N)
  Z SIGN=1.0 $ IJ=0
C--STEP CENTER TEMP, INDICATE TO TEMP THIS IS NOT 1ST PROFILE
  TC=TC+STEP $ ITER=1
  CALL TEMP(A,ITER,TC,VOL,NP)
  IF(MUN.GT.0)GO TO 70
C--CHECK IF NEW SURFACE TEMP IS GREATER THAN OLD
  IF(T(NP,N).GT.TS1)GO TO 4
C--IF NOT, STEP CENTER TEMP OTHER DIRECTION
  SIGN=-1.0 $ TC=TC-2.0*STEP
  CALL TEMP(A,ITER,TC,VOL,NP)
  IF(MUN.GT.0)GO TO 70
  IF(T(NP,N).GT.TS1)GO TO 4
C--IF SURF TEMP STILL NOT INCREASING, GET CENTER TEMP BACK
  AND REDUCE STEP
  TC=TC+STEP $ GO TO 6
C--SAVE SURFACE TEMP AND INCREMENT CENTER TEMP AGAIN
  4 TS1=T(NP,N) $ IJ=IJ+1 $ TC=TC+SIGN*STEP
C--CHECK IF CENTER TEMP HAS GONE TOO HIGH
  IF(TC.GT.TMELT)GO TO 10
C--CHECK IF SURF TEMP IS ADEQUATELY ABOVE ACTUAL SURF TEMP

```

```

C--IF IT IS GO DIRECTLY ON TO SURF PART 2
  TCHK=TSURF(NP)+5.0
  IF(TS1.GT.TCHK)GO TO 8
  CALL TEMP(A,ITER,TC,VOL,NP)
  IF(MUN.GT.0)GO TO 70
  IF(IJ.GT.50)GO TO 99
  IF(T(NP,N).GT.TS1)GO TO 4
  TC=TC-SIGN*STEP
C--REDUCE CENTER TEMP STEP SIZE
  STEP=STEP/10.0
  IF(STEP.LT.SMIN)GO TO 8
  GO TO 2
99 PRINT 299 $ STOP
10 NP=1 $ TC=TMELT $ PRINT 201
  CALL TEMP(A,ITER,TC,VOL,NP)
  IF(MUN.GT.0)GO TO 70
C**T(NP,N) IS MAX SURFACE TEMP AVAILABLE
  TS=T(NP,N)
  IF(NR.NE.0)OPT=NR
C--CHECK IF PRINTING IS WANTED
  IF(IPRINT.NE.1)GO TO 14
  PRINT 200
  PRINT 204,VOLTS,T(NP,N),TC,A
C--IF MAX SURF TEMP AVAILABLE IS LESS THAN ACTUAL SURF TEMP,
C--NO SOLUTIONS CAN BE ACHIEVED, SET MLTA FLAG
  14 IF(T(NP,N).GE.TSURF(NP))GO TO 17
  MLTA=NP $ RETURN
  17 IF(OPT.NE.0)GO TO 26
  ACHK=A/2.0
C--CHECK FOR LOW OR HIGH POWER SOLUTION
  IF(AMPS.LE.ACHK)GO TO 30
  OPT=2 $ GO TO 26
  30 OPT=1
C--FIND CORRECT SURFACE TEMP BY ITERATING ON CENTER TEMP
  26 TC2=TC $ TS2=TS $ JJ=0 $ SIGN=1.0 $ EMAX=0.5
  IF(OPT.EQ.2)SIGN=-1.0
  32 TC1=TC2 $ TS1=TS2
  TC2=TC1*(TSURF(NP)/TS1)**SIGN
  CALL TEMP(A,ITER,TC2,VOL,NP)
  IF(MUN.GT.0)GO TO 70
  IF(JJ.GT.50)GO TO 35
  JJ=JJ+1 $ TS2=T(NP,N)
  ERR=ABS(TS1-TS2)
  IF(ERR.GE.EMAX)GO TO 32
C--HAVE PROFILE, FINISH ROUTINE
  IF(IPRINT.NE.1)GO TO 36
  IF(OPT.EQ.2)GO TO 38
  PRINT 206 $ GO TO 39
  38 PRINT 207
  39 CONTINUE
  DO 50 I=2,N
  50 Q(NP,I)=Q(NP,I)/VOL
  IF(IPRINT.NE.1)GO TO 36
  POWER=VOLTS(NP)*A
  PRINT 101,POWER,A,VOLTS
  PRINT 102
  PRINT 104,(R(NP,J),T(NP,J),Q(NP,J),J=1,N)
  36 IF(T(NP,1).LT.TMELT)GO TO 40
C--IF THERE ARE TEMPS>MELTING, SET ALL OF THEM TO TMELT
  NHALF=N/2
  DO 60 M=1,NHALF

60 IF(T(NP,M).GT.TMELT)T(NP,M)=TMELT
  MELT=1
40 AMPS=1 $ RETURN
  35 PRINT 208,NP $ MLTA=NP $ RETURN
70 MUN=NP $ MUN=NP
  RETURN
END

```

A.6 TEMP

This subroutine does the actual construction of the temperature profiles. The current center boundary condition causes the profile to be flat across node 1, or the center. If this profile has yet to be constructed for the first time, TEMP guesses values for each of the nodes in a determined manner. The center temperature is given to TEMP from SURF. TEMP therefore starts with the second node and works its way to the pellet surface. An average temperature for each node is found to be used when calling ELECT, for the electrical conductivity, or THERM for thermal conductivity. The values returned are used to find the power dissipated in the node and the temperature drop across the node.

TEMP recalculates this profile until a particular surface temperature is converged upon. This commonly takes a maximum of about 10 or 12 iterations. If too much of the profile is molten or the thermal conductivity parameters are not good, TEMP cannot converge on a final profile. This is the "nonconvergence error." If the calculated surface temperature suddenly starts getting too large or small, the present thermal conductivity parameter set is unacceptable. This is the "unstable solution error."

When a final temperature profile is achieved, the power dissipated in each node is summed and divided by voltage to get a calculated current for this profile and these thermal conductivity parameter values. It is this current that is compared to the actual measured current in SUMSQ to get the current error.

A.6.1 TEMP Listing

```

      SUBROUTINE TEMP(AMPS,ITER,TCENT,VOL,NP)
      DIMENSION X(50)
      COMMON/B1/T(12,50),R(12,50),O(12,50),N,VOLTS(12),CL(12),MUN
106  FORMAT(///,5X,* NONCONVERGENCE ERROR IN TEMP== ERROR STOP*,///)
      EMAX=0.1 $ MUN=0
      T(NP,1)=TCENT
      DO 10 I=2,N
10    X(I)=R(NP,I)
      C--CENTER BOUNDARY CONDITION
      X(1)=R(NP,2)/2.7182818
      C--GENERATED POWER MULTIPLIER
      Y=(VOLTS(NP)**2)*VOL/CL(NP)**2
      C--SET COUNTER AND START LOOP TO CONVERGE ON A TEMP PROFILE
      O(NP,1)=0.0
15    ITER=ITER+1
      OT=0.0
      C--FOR FIRST PROFILE GUESS TEMPS.
      IF(ITER.GT.1)GO TO 17
      REN=N
      DO 100 I=2,N
      REI=I
100    T(NP,I)=T(NP,I-1)-(18.0-10.0*(REI/REN))
17    TN=T(NP,N)
      CONTINUE
      C--GENERATE TEMP PROFILE
      DO 60 I=2,N
      C--AVERAGE NODE TEMPS FOR FINDING ELECT. COND.
      IF(I.GT.2)GO TO 20
      TA=(3*T(NP,1)+T(NP,2))/4 $ GO TO 50
20    IF(I.EQ.N)GO TO 40
      TA=(T(NP,I-2)+2*T(NP,I-1)+2*T(NP,I)+T(NP,I+1))/6.0
      GO TO 50
40    TA=(T(NP,N)+T(NP,N-1))/2.0
      C--GET ELECTRICAL CONDUCTIVITY, EC
50    CALL ELECT(TA,EC)
      C--FIND POWER GENERATED IN THIS NODE AND TOTAL POWER SO FAR
      Q(NP,1)=EC*Y
      OT=OT+Q(NP,I)
      C--GET THERMAL CONDUCTIVITY, TK
      CALL THERM(TA,TK)
      C--CALCULATE NEXT TEMP
      PHI=(6.2831853*CL(NP))/ALOG(X(I)/X(I-1))
60    T(NP,I)=T(NP,I-1)-OT/(PHI*TK)
      C--PRINT COMMANDS TO USE IN ERROR LOCATION
      C    PRINT 999,NP,T(NP,1),T(NP,N)
      C999  FORMAT(3X,I2,2F13.4)
      C--CHECK IF STABLE SOLUTION
      IF(T(NP,N).LT.1000.0.OR.T(NP,N).GT.3300.0)GO TO 80
      C--CHECK FOR CONVERGENCE
      ER=TN-T(NP,N)
      IF(ABS(ER).LE.EMAX)GO TO 70
      IF(ITER.GT.50)EMAX=1.0
      IF(ITER.LT.100)GO TO 15
      PRINT 106
      PRINT 187,(R(NP,K),T(NP,K),O(NP,K),K=1,N)
187  FORMAT(3X,F7.4,T18,F7.1,T34,F8.4)
      STOP

      C--TEMP PROFILE ACHIEVED, CALCULATE AMPS
70    AMPS=OT/VOLTS(NP)
      ITER=1
      RETURN
      C--SET UNSTABLE FLAG AND RETURN
80    MUN=1
      RETURN
      END

```

A.7 ELECT and THERM

ELECT calculates the electrical conductivity from the equation described in Section 5.3 from a given input temperature. Since this equation does not hold for lower limits a check is made to see that the given temperature is above this, and if not, a constant electrical conductivity value is given. The maximum temperature allowed is also set to melting here.

THERM checks to see if the given input temperature is too high or low, then calculates the thermal conductivity from a given relationship. The comment lines marked with "CZZZ" locate the position where a new thermal conductivity equation can be put in. A temperature dependent porosity correction is also made before the final thermal conductivity value is returned. If the thermal conductivity of molten material is asked for, a factor of five jump is made on the final value. These equations and corrections are described in Section 5.2.

A.7.1 ELECT and THERM Listings

```

SUBROUTINE ELECT(TK,COND)
  COMMON/D3/CT(6),TD,CE(6)
  IF (TK.LT.1250)GO TO 10
  IF (TK.GT.3137.0)TK=3137.0
  A=EXP(CE(1)+CE(2)/TK+CE(3)/TK**2+CE(4)/TK**3)
  COND=A
  RETURN
10  COND=0.1
    RETURN
END
```

```

SUBROUTINE THERM(TK,TCON2)
COMMON/B3/CT(6),TD,CE(6)
BOLTZ=6.61612E-5
IF(TK.LT.1000.0)TK=1000.0
IF(TK.GT.3137.0)H=1
IF(TK.GT.3137.0)TK=3137.0
CZZZ3
A=1.0/(CT(1)+CT(2)*TK)
B1=(-CT(4)/(BOLTZ*TK))
B=CT(3)*TK*EXP(B1)
C1=(-CT(6)/(BOLTZ*TK))
C=CT(5)*EXP(C1)
CZZZ4
TCON1=A+B-C
IF(M.EQ.1)GO TO 10
C--THE POROSITY CORRECTION
ALPHA=2.6-0.5E-3*(TK-273.16)
POR=1.0-TD
TCON2=TCON1*(1.0-ALPHA*POR)
RETURN
10 TCON2=5.0*TCON1
RETURN
END

```

A.8 MANTRA-III Output

An example output from MANTRA-III is presented in the following listing. This was the interim run necessary in analyzing Run 13. The starting thermal conductivity values came from the single profile run as shown in Table 6.1.

A.8.1 Output Listing

 ---FROM DEH RUN #13---

STARTING AT OBSERVED TEMPERATURE OF 1100.0 AND ENDING AT 1550.0 CELSIUS
 THE TEMPERATURE INCREMENT USED IS 100.0

THE CUTOFF TEMPERATURE WHERE CURVE TWO STARTS IS: 1440.0
 THE CURRENT INCREMENT IS 5.0 AND THE MAX CURRENT ALLOWED IS 30.0

THE CONSTANTS GIVEN BY THE BMDX FIT FOR VOLTAGE FROM TEMPERATURE ARE:
 2.8821E+01 -1.6635E-02 0. 0.

CONSTANTS FOR CURVE TWO, VOLTAGE FROM AMPS:
 9.3222E+00 -2.3149E-01 1.9697E-03 1.9560E-08

THE CONSTANTS FOR THE CURRENT FIT, AMPS FROM TEMP:
 -9.0815E+01 2.9610E-01 -3.1943E-04 1.1747E-07

CONSTANTS FOR CURVE TWO, TEMP FROM AMPS:
 1.5235E+03 -4.3434E+00 1.8199E-02 6.6914E-04

THE SIX INITIAL THERMAL CONDUCTIVITY PARAMS ARE:
 4.452 2.7775E-02 1.1200E-03 1.575 4180. 3.323

THE INITIAL ELECTRICAL CONDUCTIVITY PARAMETERS ARE:
 9.646 -2.0870E+04 1.2310E+07 -6.4840E+09 0. 0.

SAMPLE CHARACTERISTICS:

RADIUS: .43220 CM.
 ACTIVE LENGTH: 1.21160 CM.
 CENTRAL VOID RADIUS: 0.00000 CM.
 INITIAL FRACTION OF THEORETICAL DENSITY: 90.70000 PERCENT

PROFILE INFO:

INITIAL NUMBER OF NODES: 25
 WORKING WITH 4 PROFILES AND 4 TEMP REGIONS
 THE PARAMETER OPTIMIZATION CODE: 0

INFORMATION ON THE SET OF 4 PROFILES

==PROFILE NUMBER 1==

MEASURED VALUES
 TEMPERATURE= 1100.0 C
 CURRENT= 4.74 AMPS
 VOLTAGE= 10.52 VOLTS
 PELLET AVERAGE VALUES:
 ELECTRICAL COND.= .92950 (1/OHM CM)
 TEMPERATURE= 1619.62 K
 EXPANSION CORRECTION= 1.01441
 CORRECTED VALUES
 RADIUS= .43843 CM
 LENGTH= 1.22906 CM
 SURF TEMP= 1388.49 K

==PROFILE NUMBER 2==

MEASURED VALUES
 TEMPERATURE= 1200.0 C
 CURRENT= 7.51 AMPS
 VOLTAGE= 8.86 VOLTS
 PELLET AVERAGE VALUES:
 ELECTRICAL COND.= 1.75115 (1/OHM CM)
 TEMPERATURE= 1757.07 K
 EXPANSION CORRECTION= 1.01648
 CORRECTED VALUES
 RADIUS= .43932 CM
 LENGTH= 1.23156 CM
 SURF TEMP= 1490.81 K

==PROFILE NUMBER 3==

MEASURED VALUES
 TEMPERATURE= 1300.0 C
 CURRENT= 12.36 AMPS
 VOLTAGE= 7.20 VOLTS
 PELLET AVERAGE VALUES:
 ELECTRICAL COND.= 3.54645 (1/OHM CM)
 TEMPERATURE= 1938.57 K
 EXPANSION CORRECTION= 1.01937
 CORRECTED VALUES
 RADIUS= .44057 CM
 LENGTH= 1.23507 CM
 SURF TEMP= 1593.31 K

==PROFILE NUMBER 4==

MEASURED VALUES
 TEMPERATURE= 1400.0 C
 CURRENT= 19.98 AMPS
 VOLTAGE= 5.53 VOLTS
 PELLET AVERAGE VALUES:
 ELECTRICAL COND.= 7.45677 (1/OHM CM)
 TEMPERATURE= 2170.34 K
 EXPANSION CORRECTION= 1.02334
 CORRECTED VALUES
 RADIUS= .44229 CM
 LENGTH= 1.23988 CM
 SURF TEMP= 1695.97 K

PARAMETER STARTING VALUES:
 4.452 2.7775E-02 1.1200E-03 1.575 4180. 3.323

INITIAL TEMP REGION BOUNDS FOR THE SET OF PROFILES:
 2473.1 2202.0 1930.9 1659.8 1388.7
 AVS 2337.6 2066.5 1795.4 1524.3

THE OPTIMIZING

```

*****
#--CURRENT ERRORS--#
REG PAR      VALUE      SSO      1 PROFILE      2 PROFILE      3 PROFILE      4 PROFILE
1 2 3.055E-02 39.09      3.052      1.657      -1.4924      -5.176
1 4* 1.73      33.27      2.112      .3470      -2.432      -4.773
1 4 1.42      34.02      2.071      2.0594E-02 -2.573      -4.807
2 2* 3.361E-02 15.32      2.215      .5004      -2.033      -2.455
2 2 3.361E-02 69.87      .8682      -.8264      -5.967      -5.730
2 2 2.750E-02 16.13      3.301      2.021      -2.050      1.052
#
#
STEP REDUCED TO .0100
1 4 1.40      14.01      2.230      .5232      -1.977      -2.202
1 6* 3.36      14.81      2.231      .5245      -1.973      -2.301
1 6 3.29      14.46      2.229      .5217      -1.903      -2.300
2 4 1.39      13.82      2.246      .5479      -1.917      -2.190
2 2 3.025E-02 11.39      2.347      .6909      -1.701      -1.585
2 2* 2.994E-02 11.67      2.448      .5299      -1.514      -1.764
3 2 3.055E-02 13.80      2.247      .5493      -1.915      -2.187
#
#
STEP REDUCED TO .0010
1 4 1.39      11.28      2.348      .6936      -1.694      -1.555
1 6* 3.32      11.32      2.348      .6934      -1.695      -1.565
1 6 3.33      11.25      2.348      .6937      -1.694      -1.545
2 2* 3.025E-02 11.37      2.330      .6895      -1.715      -1.574
2 2 3.022E-02 11.14      2.359      .7080      -1.672      -1.511
2 4 1.39      11.04      2.360      .7107      -1.665      -1.481
3 2 3.019E-02 10.94      2.370      .7250      -1.644      -1.446
3 4 1.39      10.84      2.372      .7277      -1.637      -1.416
4 2 3.016E-02 10.74      2.382      .7420      -1.616      -1.381
1 4 1.38      10.65      2.384      .7447      -1.609      -1.350
1 6 3.33      10.62      2.384      .7449      -1.608      -1.340
2 2 3.013E-02 10.53      2.394      .7592      -1.587      -1.306
2 4 1.38      10.44      2.396      .7620      -1.580      -1.274
3 2 3.010E-02 10.07      2.406      .4709      -1.588      -1.240
3 4 1.36      9.983      2.408      .4734      -1.582      -1.208
4 2 3.007E-02 9.894      2.418      .4876      -1.560      -1.173
1 4 1.38      9.809      2.420      .4901      -1.553      -1.141
1 6 3.33      9.785      2.420      .4902      -1.552      -1.131
2 4 1.38      9.702      2.422      .4927      -1.545      -1.098
2 2 3.004E-02 9.623      2.432      .5070      -1.524      -1.063
3 2 3.001E-02 9.547      2.442      .5212      -1.502      -1.028
3 4 1.38      9.472      2.444      .5238      -1.495      -0.9950
4 2 2.998E-02 9.403      2.454      .5380      -1.473      -0.9597
1 4 1.36      9.331      2.456      .5406      -1.466      -0.9265
1 6 3.34      9.311      2.456      .5408      -1.465      -0.9159
2 4 1.37      9.241      2.456      .5434      -1.458      -0.8823
2 2 2.995E-02 9.182      2.468      .5577      -1.436      -0.8467
3 2 2.992E-02 9.127      2.476      .5720      -1.414      -0.8111
3 4 1.37      9.065      2.480      .5747      -1.407      -0.7769
4 2 2.989E-02 9.017      2.491      .5890      -1.385      -0.7412
1 4 1.37      8.960      2.493      .5917      -1.377      -0.7066
1 6 3.34      8.943      2.493      .5918      -1.377      -0.6959
2 4 1.37      8.944      2.495      .5945      -1.369      -0.7017
3 2 2.986E-02 8.903      2.503      .6062      -1.355      -0.6599
3 4 1.37      8.851      2.505      .6089      -1.347      -0.6249
4 2 2.983E-02 8.817      2.515      .6233      -1.325      -0.5888
1 4 1.37      8.770      2.517      .6260      -1.318      -0.5534
1 6 3.34      8.803      2.517      .6261      -1.317      -0.5831
2 4 1.37      8.769      2.519      .6288      -1.310      -0.5582
2 2 2.980E-02 8.702      2.529      .6432      -1.288      -0.4813
3 2 2.977E-02 8.683      2.540      .6576      -1.266      -0.4450
3 4 1.37      8.681      2.542      .6605      -1.258      -0.4489
4 2 2.974E-02 8.635      2.552      .6749      -1.236      -0.3722
1 4 1.36      8.632      2.554      .6778      -1.226      -0.3756
1 6 3.34      8.623      2.554      .6779      -1.227      -0.3644
2 4 1.36      8.593      2.556      .6808      -1.220      -0.3273
2 2 2.971E-02 8.589      2.567      .6952      -1.197      -0.2903
3 2 2.968E-02 8.590      2.577      .7097      -1.175      -0.2533
#
#

```

* INDICATES DIRECTION WAS CHANGED
INDICATES REGION WAS SKIPPED

*****FINAL INFORMATION ON THE SET OF 4 PROFILES*****

SUM OF CURRENT ERRORS SQUARED= 8.59

PARAMETER VALUES

4.452 2.9707E-02 1.1200E-03 1.363 4180. 3.343

TEMP REGION BOUNDS FOR THE SET OF PROFILES:

2745.2 2405.9 2066.8 1727.8 1388.7
 AVS 2575.4 2236.4 1897.3 1558.3

PROFILE 1: TOBS= 1100.0C, VOLTAGE=10.52V, CURRENT= 4.74AMPS
 TSURF= 1388.5K, CURRENT ERROR= 2.57

RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	2188.1	0.0000
.0895	2036.6	15.9362
.1266	1951.4	10.2306
.1550	1888.1	7.6649
.1790	1835.9	6.1338
.2001	1791.0	5.0547
.2192	1751.5	4.2427
.2368	1716.1	3.6099
.2531	1684.2	3.1048
.2685	1655.0	2.6944
.2830	1628.2	2.3560
.2968	1603.4	2.0738
.3100	1580.4	1.8360
.3227	1559.0	1.6339
.3349	1538.9	1.4608
.3466	1520.0	1.3115
.3580	1502.2	1.1820
.3690	1485.4	1.0689
.3797	1469.5	.9698
.3901	1454.4	.8824
.4002	1440.0	.8052
.4101	1426.3	.7365
.4198	1413.2	.6753
.4292	1400.7	.6205
.4384	1388.7	.5708

PROFILE 2: TOBS= 1200.0C, VOLTAGE= 8.86V, CURRENT= 7.51AMPS
 TSURF= 1490.8K, CURRENT ERROR= .695

RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	2159.9	0.0000
.0897	2058.8	10.6555
.1268	1998.7	7.7968
.1553	1951.7	6.4120
.1794	1911.5	5.4877
.2005	1875.7	4.7778
.2197	1843.3	4.2039
.2373	1813.6	3.7282
.2536	1786.2	3.3273
.2690	1760.7	2.9855
.2836	1736.8	2.6911
.2974	1714.4	2.4358
.3106	1693.4	2.2128
.3233	1673.5	2.0168
.3355	1654.6	1.8438
.3473	1636.7	1.6904
.3587	1619.7	1.5536
.3697	1603.5	1.4314
.3805	1588.0	1.3217
.3909	1573.2	1.2229
.4010	1559.1	1.1337
.4109	1545.5	1.0530
.4206	1532.4	.9796
.4301	1519.9	.9129
.4393	1507.6	.8510

PROFILE 3: TDES= 1300.0C, VOLTAGE= 7.20V, CURRENT= 12.36AMPS
 TSURF= 1593.3K, CURRENT ERROR= -1.20

RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	2332.5	0.0000
.0899	2225.3	11.4934
.1272	2159.4	8.6463
.1558	2107.0	7.1645
.1799	2061.6	6.1477
.2011	2020.9	5.3556
.2203	1983.9	4.7099
.2379	1949.8	4.1716
.2544	1918.2	3.7165
.2698	1888.8	3.3275
.2844	1861.2	2.9924
.2983	1835.3	2.7016
.3115	1810.9	2.4477
.3243	1787.9	2.2249
.3365	1766.1	2.0285
.3483	1745.4	1.8545
.3597	1725.7	1.6998
.3708	1706.9	1.5617
.3815	1689.0	1.4381
.3920	1671.9	1.3271
.4022	1655.5	1.2270
.4121	1639.8	1.1367
.4218	1624.8	1.0548
.4313	1610.3	.9804
.4406	1596.4	.9119

PROFILE 4: TDES= 1400.0C, VOLTAGE= 5.53V, CURRENT= 19.98AMPS
 TSURF= 1696.0K, CURRENT ERROR= -.290

RADII (CM)	TEMP (K)	POWER DENS (W/CM3)
0.0000	2745.2	0.0000
.0903	2606.5	17.0408
.1277	2517.8	12.8289
.1564	2445.4	10.5682
.1806	2381.1	8.9694
.2019	2322.5	7.7028
.2211	2268.4	6.6614
.2389	2218.2	5.7912
.2554	2171.2	5.0575
.2708	2127.4	4.4347
.2853	2086.3	3.9035
.2994	2047.7	3.4484
.3127	2011.3	3.0569
.3255	1977.0	2.7188
.3378	1944.7	2.4258
.3497	1914.1	2.1709
.3611	1885.1	1.9484
.3722	1857.7	1.7536
.3830	1831.6	1.5823
.3935	1806.7	1.4314
.4038	1783.1	1.2979
.4137	1760.6	1.1796
.4235	1739.0	1.0743
.4330	1718.4	.9804
.4423	1698.7	.8953

END VALUE REACHED===STOP

APPENDIX B

X-RAY DIFFRACTOMETER PROGRAM

The data collected for these measurements are from several sources. The diffraction angles are recorded on a synchronized linear chart recorder's spool of graph paper. The values are then taken from this paper. The Miller Indices come from the Selected Powder Diffraction Data for Metals and Alloys (1978). The copper k-alpha wavelength is from the basic text used in developing this method (Nuffield, 1966).

An example of a data input file for the program XRAY is given in Table B.1. The first number indicates the number of data points for this set. It is followed by a label for the data. The first column has the Miller Indices and the second the diffraction angles as read. The 999 indicates another data set remains to be read in.

A listing of the program XRAY follows this discussion. XRAY uses an extrapolation technique to find two lattice parameters for a given set of data. The lattice parameter and its error are obtained from a least squares analysis to find a best fit line (H. D. Young, 1962). The best fit line comes from two methods of determining precise lattice parameters, using the Nelson-Riley function or using the Cotangent function. The lattice parameter turns out to be the y-axis intercept of the best fit line through points given by one of the functions. The least squares analysis is carried out in the subroutine LSTSQR. An example output is given in Table B.2. (The output is from

Table B.1. XRAY Data Input

05	T5:unheated
35.	112.80
36.	115.35
40.	125.90
43.	143.85
44.	138.10
999	
05	T5: DEH Run 9
35.	112.80
36.	115.32
40.	125.90
43.	134.88
44.	138.15

Table B.2. An XRAY Output

I	TMI	DA	Y	B	A	COT	RF
B41H DEH Run 5							
1	35.	112.98	0.9859	.6952	5.46524	.438	.337
2	36.	115.44	1.0074	.7148	5.46633	.399	.310
3	40.	125.98	1.0994	.7938	5.46789	.260	.210
4	43.	135.00	1.1781	.8536	5.46702	.172	.141
5	44.	138.30	1.2069	.8733	5.46728	.145	.120

The lattice parameter from the NR method is $5.4685 \pm .72\text{E-}3$

The line's slope is $-.791\text{E-}2 \pm .300\text{E-}2$

For the CTN method $5.4684 \pm .667\text{E-}3$

diffraction data measured on the pellet that was Direct Electrically Heated with no argon flow.) "I" is a counter for the number of data points. "TMI" is the Miller Indices. "DA" is the diffraction angles as read. "Y" is the diffraction angle in radians. "B" is just an intermediate calculated value. "A" is for the individual lattice parameters. "COT" has the value of the Cotangent function. And finally, "RF" has the value of the Nelson-Riley function.

B.1 XRAY Listing

```

PROGRAM XRAY(INPUT,OUTPUT,TAPE1=INPUT,TAPE2=OUTPUT)
DIMENSION DATA(10)
COMMON A(10),COT(10),RF(10),N,ADR,STDAOR,ADC,STDAOC
COMMON RM,STDRM,CM,STDCM
C COPPER K-ALPHA WAVELENGTH IS WL
WL=1.5405
C DATA FROM THE DIFFRACTOMETER OUTPUT, TMI IS THE MILLER INDICE NUMBER,
C DA IS THE DIFFRACTION ANGLE, N IS THE NUMBER OF DATA POINTS USED
C Y IS THE DIFF ANGLE IN RADIANS
100 IC=1
      WRITE(2,73)
      FORMAT(1H1)
20   READ (1,23)N,DATA
23   FORMAT(12,10A6)
      WRITE(2,63)DATA
63   FORMAT(///,3X,10A6,/,/,4X*1*,2X*TMI*,4X*DA*,6X*Y*,7X*B*,8X*A*,
16X*COT*,4X*RF*)
      DO 50 I=1,N
        READ(1,3)TMI,DA
        FORMAT(F8.2,F8.2)
3     Y=DA/(57.29578*2.0)
10    B=SIN(Y)**2
      C THE LATTICE PARAMETER IS 'A'
      A(I)=SORT((TMI*WL**2)/(4.0*B))
      C THE EXTRAPOLATION FUNCTIONS
      COT(I)=(COS(Y)/SIN(Y))**2
      RF(I)=0.5*(COS(Y)**2/SIN(Y)+COS(Y)**2/Y)
50    WRITE(2,53) I,TMI,DA,Y,B,A(I),COT(I),RF(I)
53    FORMAT(3X,12,2X,F3.0,2X,F7.3,2F8.4,2X,F7.5,2F7.3)
      CALL LSTSOR
      WRITE(2,13)ADR,STDAOR,RM,STDRM,ADC,STDAOC,CM,STDCM
13    FORMAT(3X,/,* THE LATTICE PARAMETER FROM THE NR METHOD IS*F7.4,
1* PLUS OR MINUS*E9.3,/,* THE LINE'S SLOPE IS*E10.3,3X,E9.3,
1/,* FOR THE CTN METHOD*F7.4,3X,E9.3,4X,*WITH SLOPE*
1E10.3,3X,E9.3)
      C CHECK TO SEE IF ANY MORE DATA IS PRESENT,
      C A 999 IN DATA FILE INDICATES ANOTHER SET REMAINS
      C***
      READ(1,33)LAST
22    FORMAT(13)
      IF(LAST.NE.999)STOP
      IC=IC+1
      IF(IC.GT.4)GO TO 100
      GO TO 20
      END

```

```

SUBROUTINE LSTSOR
  DIMENSION CSQ(10),AC(10),RSQ(10),AR(10),CMA(10),RMA(10)
  COMMON A(10),C(10),R(10),N
  COMMON ADR,STDADR,ADC,STDAQC,RH,STDRM,CH,STDCM
  C A IS THE LATTICE PARAMETER
  C C IS THE COT EXTRAPOLATION FUNCTION
  C R IS THE NELSON RILEY EXTRAPOLATION FUNCTION
  C N IS THE NUMBER OF DATA POINTS, M IS SLOPE, V IS VARIANCE
  SCSO=0
  SC=0
  SA=0
  SAC=0
  SRSO=0
  SR=0
  SAR=0
  U THE SUMMATION OF THE TERMS NEEDED IN THE LEAST SQUARES ANALYSIS
  DO 7 J=1,N
    CSQ(J)=C(J)**2
    SCSO=SCSQ+CSQ(J)
    SC=SC+C(J)
    SA=SA+A(J)
    AC(J)=A(J)*C(J)
    SAC=SAC+AC(J)
    RSQ(J)=R(J)**2
    SRSO=SRSO+RSQ(J)
    SR=SR+R(J)
    AR(J)=A(J)*R(J)
    SAR=SAR+AR(J)
  7  Z=N
  C FINDING THE LATTICE PARAMETER AND THE SLOPE OF THE LINE USING
  C THE TWO EXTRAPOLATION TECHNIQUES
  DELC=Z*SCSQ-SC**2
  ADC=(SA*SCSQ-SAC*SC)/DELC
  CM=(Z*SAC-SC*SA)/DELC
  DELR=Z*SRSO-SR**2
  ADR=(SA*SRSO-SAR*SR)/DELR
  PM=(Z*SAR-SR*SA)/DELR
  SCMA=U
  SRMA=0
  C FINDING THE STANDARD DEVIATION OF THE VALUES OBTAINED ABOVE
  DO 17 J=1,N
    CMA(J)=(CM*C(J)+ADC-A(J))**2
    SCMA=SCMA+CMA(J)
    RMA(J)=(RM*R(J)+ADR-A(J))**2
    SRMA=SRMA+RMA(J)
  17  VCAD=(SCMA/Z)*SCSQ/DELC
    VCM=SCMA/DELC
    STDADC=SQRT(VCAD)
    STDCM=SQRT(VCM)
    VRAD=(SRMA*SRSO)/(Z*DELR)
    VRM=SRMA/DELR
    STDADR=SQRT(VRAD)
    STDRM=SQRT(VRM)
    RETURN
  END

```

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