MASTER

HEAT - A ONE-DIMENSIONAL HEAT TRANSFER EQUATION CODE FOR THE IBM-704

January 1959

CONTRACT AT-11-1-GEN-14

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C. M. King • R. F. Boyle

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This report describes an IBM-704 computer code which finds a one-dimensional solution to the general heat transfer equation. Specifically written for application in reactor fuel rod design, the code requires cylindrical geometry conditions and input parameters of surface temperature and power density. The maximum number of points for which temperature values may be obtained is 251, and the approximate running time for a typical problem varies from 1.0 to 2.0 minutes.

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INTRODUCTION

HEAT, a one-dimensional reactor fuel rod design code for the 8K IBM-704 computer, finds an approximate solution to the steady-state heat transfer equation. Although originally written to solve the heat transfer equation associated with research in the design of tubular fuel elements, HEAT may be applied to other types of problems, such as the design problem encountered in Joulean heating of electrical conductors where resistivity is a strong function of temperature.

The steady-state heat transfer equation solved by the code has the following form:

$$-P = K \left[T(r) \right] \frac{1}{r} \frac{1}{dr} \left[r \frac{dT(r)}{dr} \right] + \frac{dK[T(r)]}{dr} \cdot \frac{dT(r)}{dr} \quad (1)$$

where $K \neq f(\theta, z)$ and $T \neq f(\theta, z)$.

The physical interpretation of the above symbols is as follows:

- P = power density
- $K [T(r)]$ = thermal conductivity
- r = pellet radius
- $T(r)$ = absolute temperature

A description of the physical problem which raised the need for a heat transfer code and the details of the theory and use of this code follow.

PHYSICAL PROBLEM

Core I of the Shippingport Pressurized Water Reactor (PWR) consists of two parts: a seed assembly and a blanket assembly. The blanket assembly is comprised of 0.411 in. OD Zircaloy-2 tubes containing, as fuel material, 93-95% of theoretical density natural UO_2 pellets. Each of these fuel rods is 10.25-in. long and contains 26 UO_2 pellets of 0.3575-in. diam.

Sherman and Sherba (Ref 2) developed a heat transfer model for use in the design of these fuel rods. Certain discrepancies arose, however, between theory and experiment when proof tests of fuel rods were performed in test reactors under simulated PWR environments (Ref 3). As part of the effort to reconcile these differences, several additional series of tests were performed.

Although an analytic solution to the steady-state heat transfer equation exists, the code HEAT was designed to find a solution to Eq (1) in order to provide, for use in this thermal research program, a very fast method of calculating the temperature distributions of fuel pellets.

Two UO_2 thermal conductivity data sets are available. The first set, determined by Kingery and Vasilos, is a material property measure; whereas, the second set, determined by Hedge, gives an effective value for cracked UO_2 .^{*} So that the code will be general, three forms of the thermal conductivity law have been included and may be chosen in accordance with the particular data set used.

MATHEMATICAL THEORY OF THE HEAT CODE

Solution for the Temperature, T

In order to solve Eq (1) for the temperature values, $T(r)$, the WANDA solution of fluxes described in WAPD-TM-28 (Ref 1, pp. 6-11) was found to be applicable, for Eq (2) of WAPD-TM-28 can be reduced to Eq (1) of this report by the following modifications, substitutions, and specifications:

Set:

$\Sigma_T(r)$ equal to zero in all cases
 Σ_R equal to zero in all cases

Substitute:

K for D
 $T(r)$ for $\phi(r)$
P for $\chi S(r)$

Assume:

a one-group solution
cylindrical geometry
symmetry at the origin
a non-symmetric condition at the outer boundary with $\bar{T}$ at the outer boundary = a constant input surface temperature, T_s (this corresponds to the WANDA solution when $\phi = 0$ at the outer boundary)

The power density, P, and the surface temperature, T_s , are input values which are held constant throughout the solution. Initially, the conductivity is assumed to be equal to one at all points, and the initial temperature values are calculated by use of the technique described in Ref 1.

Treatment of the Conductivity

After the spatial integration solution of initial temperature values has been completed, the thermal conductivity, K, is calculated for each point, using one of the three forms of the thermal conductivity law included in the code. They are defined as:

$$K[T(r)] = a T(r)^b, \quad (2)$$

* Kingery Data: $K = 1926T^{-0.9}$ Btu/hr-ft°F (Ref 4)

Hedge Data: $K = 434.3T^{-0.746}$ Btu/hr-ft°F [Thermal conductivity corrected to 94% theoretical density (Ref 5)]

$$K \left[T(r) \right] = a + \frac{b}{T(r)} , \quad (3)$$

$$K \left[T(r) \right] = \frac{a + b T(r)}{c + d T(r)} , \quad (4)$$

where

$T(r)$ = temperature values just obtained for each point

a, b, c, and d = input data constants

Test for Convergence

Now, the WANDA spatial integration solution of heat transfer Eq (1) is repeated, using the new values for the conductivity, K. The code then computes the sum of the differences between the temperature values just calculated and the temperature values resulting from the previous spatial integration. This iterative process is continued, K being recalculated after each iteration, until

$$\sum \left| T(r)_{n-1} - T(r)_n \right| \leq \epsilon , \quad (5)$$

where

$T(r)_n$ = temperature values just calculated

$T(r)_{n-1}$ = temperature values from the previous spatial integration

ϵ = an input convergence criterion

When Eq (5) has been satisfied, the final temperature values, $T(r)_n$, are printed out and the problem has been completed.

DETAILS OF CODE USE

Input Preparation

Certain quantities, such as surface temperature, the convergence criterion, the form of the thermal conductivity law desired, and the power density are necessary input to the HEAT code.

The requestor must also indicate the number of points for which the temperature should be calculated. It is possible either to divide the pellet radius into a number of mesh intervals of equal width or into a number of regions with the mesh intervals within a region being of equal width. A maximum of 250 mesh intervals distributed throughout a maximum of 25 regions is allowed, the boundaries necessarily lying on even numbered mesh points.

As specified in the description of the input form, several numbers are represented by the floating decimal form suitable for computer use, where the number 50 is increased by the power of ten to which the decimal fraction of the number being converted must be raised. The result is given as the first two digits of the floating decimal number and is succeeded by the decimal fraction. For example,

1/3 = 5033333333

-3 = -5130000000

0 = 0000000000

The input must be submitted on 704 coding sheets and should have the following format:

- 1) For all cards, columns 1-72 must be punched, each containing only one punch, and the code label HEAT must appear in columns 73-76. Columns 1-6 contain a plus and the sequence number of the card; for example, card number 1 would be labelled +00001.
- 2) The first input card should contain the following:
 - a) In columns 7-10, a plus and the number of mesh points including the origin (This should be an odd number.)
 - b) In columns 11-13, a plus and the number of regions

- c) In columns 14-24, a plus and the surface temperature, T_g , in floating decimal form
- d) In columns 25-35, a plus and the convergence criterion, ϵ , in floating decimal form
- e) In columns 36-37, a +1 (This indicates that the power density, P , will be considered to be constant throughout the rod. A +2 indicates that the power density is a function of the radius; but because this is an experimental solution and needs a different type of input on the power density input card, its description is not included in this report.)
- f) In columns 38-39, the form of the thermal conductivity law to be used is indicated by

$$a + 1 \text{ if } K \left[T(r) \right] = a T(r)^b, \quad (K1)$$

$$a + 2 \text{ if } K \left[T(r) \right] = a + \frac{b}{T(r)}, \quad (K2)$$

$$a + 3 \text{ if } K \left[T(r) \right] = \frac{a + b T(r)}{c + d T(r)}, \quad (K3)$$

- g) In columns 40-48, a plus and the problem number
 - h) In columns 49-72, a plus followed by zeros
- 3) The next card, or cards, contains the boundary point numbers which must be even numbers. Usually, there will be only one point given, which would be the outer boundary point, unless the requestor wishes to divide the radius into regions with mesh intervals of different widths. Not more than 13 of these numbers are allowed to a card:
- a) In the columns following the card number, the boundary point number or numbers, each preceded by a plus
 - b) In the columns following the outer boundary, a plus and zero through column 72
- 4) The data constants (These are the constants of the data set which are applicable to the form of the thermal conductivity law being used.) For (K1) and (K2) there are only two data constants, a and b , but for (K3) there are four, a , b , c , and d given in that order. The first column specified for the constant contains the sign of that number, and the succeeding ten columns must contain the constant in floating decimal form:
- a) In columns 7-17, a
 - b) In columns 18-28, b
 - c) In columns 29-39, c
 - d) In columns 40-50, d
 - e) A plus sign followed by zeros through column 72 should follow last data constant whether b or d .
- 5) The mesh interval widths: If the radius is to be divided into intervals of equal mesh width, only one mesh width value is given. Otherwise, one must be given for each region in the order in which the regions occur (i.e., there must be the same number of mesh widths of input as the number of regions specified on the first card). Note that these are not values of the radius of the rod or of a whole region, but the width of each interval. There can be as many as six mesh widths to a card:
- a) In columns 7-17, a plus sign followed by the first, and possibly only, mesh interval width in floating decimal form; other mesh interval widths would follow in columns 18-28, 29-39, 40-50, 51-61, and 62-72.
 - b) The last mesh interval width must be followed by a plus and zeros through column 72.
- 6) The power density: The power value, which is constant throughout the rod (excluding the experimental solution mentioned earlier), is given in floating decimal form:
- a) In columns 7-17, the power density, P
 - b) In columns 18-72, a plus followed by zeros. This is the last input card for the particular problem.

Problem running time is reduced by running a group of problems in immediate succession. One and only one blank card must separate each problem input deck, and four blank cards must follow the last problem input deck.

A sample input form and a listing of the input appear in the Appendix.

Output

The code output is printed off-line and includes the following:

- 1) The initial temperature values calculated when thermal conductivity, K , equals 1 at all points
- 2) The value of $\sum |T(r)_{n-1} - T(r)_n|$ (the convergence criterion term) for each iteration
- 3) The final, converged temperature values

The temperature values are printed for each point in floating decimal form, where the power of ten is printed first, followed by the decimal fraction. The value of the radius at each point is printed in fixed point form and, if the radius is divided into separate regions, the regions are indicated on the printout. The number of each problem and the page number of the output for a set of problems run in succession are printed at the top of each page. "THE EDIT HAS BEEN COMPLETED" is printed after the completion of the output from a problem.

If an edit has been forced, either by use of sense switch 1 or upon completion of 200 iterations (the code allows a maximum of 200 iterations per problem), then "FORCED EDIT" is printed before the printout of the final temperature values which, in this case, have not converged.

A sample printout appears as Example 3 in the Appendix.

Operating Instructions

1) Starting

a) Tapes:

A blank tape must be mounted on logical tape 5.

b) Printer:

GLOUT2 printer board must be in the printer.

c) Sense Switches:

1	Up:	{ Normal
	Down:	{ Forced Edit at the end of the present iteration
		(mainly for experimental purposes)
2-6		Not used

d) Procedure:

Ready the input cards in the card reader, ready the printer, CLEAR, and LOAD CARDS.

2) Program Stops:

The normal end of program stop is (04447)₈.

For any other stops, note the reason. It is possible to try again by reloading the program and problem decks, but before doing so, remove the decks for those problems which have been completed successfully. (The list of these is printed on-line, and the problem number appears in columns 41-48 of the first card of each deck. A blank card separates each deck.) If it should fail again, write an EOF on Tape 5, and print up any output that might have been completed. If a requestor error occurs, and one or more problems have been completed, also write an EOF on Tape 5 and print up all complete output, leaving the rest of the problems to be run after correction.

List of Stops

Loc. (in octal)	Reason
03322	Blank card before end of input - Requestor error
03324	Card sequencing incorrect - Requestor error
03326	An odd boundary number - Requestor error
03330	A zero mesh width - Requestor error
04145	Overflow or underflow
04222	Input data constant, a, is less than or equal to zero - Requestor error
04231	A temperature is less than or equal to zero
04236	LogK is too large for exponential routine
04450	Zero mesh width encountered in calculation
04451	Zero conductivity encountered in calculation

3) Printing of output

Tape 5 is the output tape and should be printed with the Carriage Control Switch of the off-line Printer set to PROGRAM. An EOF follows the output of the last problem run and, therefore, defines the end of output from the tape.

ACKNOWLEDGEMENT

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4. Kingery et al, "The Measurement of Thermal Conductivity of Refractory Materials," NYO-3647, 1953.
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CODING FORM FOR IBM TYPE 704 COMPUTER

DATE Aug. 7, 1958

SHEET 1 OF 1

[illegible]

HEAT1-THE EFFECT OF THERMAL CONDUCTIVITY UPON
THE TEMPERATURE OF PELLET FUEL
PROBLEM NUMBER-10000001

10000001 PAGE 1

REGION	POINT	RADIUS	TZERO-INITIAL TEMPERATURE VALUES
	1	.000000	4 42517995
	1	.000740	4 42442700
	2	.001480	4 42216816
	3	.002220	4 41840341
	4	.002960	4 41313276
	5	.003700	4 40635622
	6	.004440	4 39807377
	7	.005180	4 38828542
	8	.005920	4 37699118
	9	.006660	4 36419103
	10	.007400	4 34988498
	11	.008140	4 33407303
	12	.008880	4 31675518
	13	.009620	4 29793143
	14	.010360	4 27760179
	15	.011100	4 25576624
	15	.011840	4 23242479
	17	.012580	4 20757745
	18	.013320	4 18122420
	19	.014060	4 15336505
	20	.014800	4 12400000

ITERATION NO.	CONVERGENCE CRITERION TERM
1	4 95573013
2	4 37087034
3	3 89426180
4	3 16058630
5	2 23150421
6	1 28030853
7	29377747

REGION	POINT	RADIUS	TN-FINAL TEMPERATURE VALUES
	1	.000000	4 33657304
	1	.000740	4 33583142
	2	.001480	4 33361307
	3	.002220	4 32994005
	4	.002960	4 32484861
	5	.003700	4 31838894
	6	.004440	4 31062458
	7	.005180	4 30163181
	8	.005920	4 29149873
	9	.006660	4 28032432
	10	.007400	4 26821732
	11	.008140	4 25529501
	12	.008880	4 24168185
	13	.009620	4 22750804
	14	.010360	4 21290801
	15	.011100	4 19301878
	16	.011840	4 18297833
	17	.012580	4 16792333
	18	.013320	4 15298999
	19	.014060	4 13830723
	20	.014800	4 12400000

Example 3 - Output of Sample Problem
Running time for these two combined = 1.2 min.

THE EDIT HAS BEEN COMPLETED

10000001 PAGE 2

HEAT1-THE EFFECT OF THERMAL CONDUCTIVITY UPON
THE TEMPERATURE OF PELLET FUEL
PROBLEM NUMBER-10000002

10000002 PAGE 3

REGION	POINT	RADIUS	TZERO-INITIAL TEMPERATURE VALUES
1	1	.000000	4 42517995
	2	.000740	4 42442703
	3	.001480	4 42216816
	4	.002220	4 41840341
	5	.002960	4 41313276
	6	.003700	4 40635622
	7	.004440	4 39807377
	8	.005180	4 38828542
	9	.005920	4 37699118
	10	.006660	4 36419103
	11	.007400	4 34988498
	12	.008140	4 33407303
	13	.008880	4 31675518
	14	.009620	4 29793142
	15	.010360	4 27760179
	16	.011100	4 25576624
	17	.011840	4 23242479
	18	.012580	4 20757745
	19	.013320	4 18122420
	20	.014060	4 15336505
		.014800	4 12400000

ITERATION NO.	CONVERGENCE CRITERION TERM
1	5 17453652
2	4 53290814
3	4 10957721
4	3 17157141
5	2 21782059
6	1 23354034
7	21598816

REGION	POINT	RADIUS	TN-FINAL TEMPERATURE VALUES
1	1	.000000	4 25979361
	2	.000740	4 25933093
	3	.001480	4 25794685
	4	.002220	4 25565477
	5	.002960	4 25247666
	6	.003700	4 24844232
	7	.004440	4 24359147
	8	.005180	4 23796821
	9	.005920	4 23162536
	10	.006660	4 22462127
	11	.007400	4 21701947
	12	.008140	4 20888784
	13	.008880	4 20029769
	14	.009620	4 19132279
	15	.010360	4 18203842
	16	.011100	4 17252039
	17	.011840	4 16284411
	18	.012580	4 15308366
	19	.013320	4 14331090
	20	.014060	4 13359466
		.014800	4 12400000

THE EDIT HAS BEEN COMPLETED

10000002 PAGE 4