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RATH Thermal Analysis Programs

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RATH Thermal Analysis Programs

by

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ABSTRACT

This report describes four computer codes for the computation of temperatures in solids of general geometry and the display of results. The codes permit temperature-dependent material properties; anisotropic conductivities; and convection, radiation, contact, and specified-flux boundary conditions.

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I. INTRODUCTION

This report describes certain features of a set of thermal analysis programs collectively called RATH (Reactor Analysis Thermal) comprising at present five programs: a mesher, which has been described in LAMS-2809; two heat-conduction codes called Mañana and Wanton; and two isotherm plotters which are described in this report. The heat-conduction codes are quite similar, their essential difference being that Mañana is an IBM 7030 (Stretch) code, while Wanton runs on the 7094. The Stretch code handles somewhat more complex boundary conditions and is more efficient for large problems, and consequently it is the one described in the body of this report. The 7094 code is described in Appendix A in terms of its differences with the Stretch code. The mesher, together with either of the heat codes, offers a highly automated system for solving fairly general two- and three-dimensional heat-conduction problems. An effort has been made to make the preparation of input for the system and the interpretation of results as simple and fast as possible for the user. In the following pages the heat-conduction and isotherm-plotting programs will be described. The usage of the mesher was described in the previously cited report, LAMS-2809.

II. GENERAL DESCRIPTION OF HEAT CODE

The heat-conduction code, Mañana, uses a lumped mass model of heat flow which permits a very general analysis in as many as three dimensions. Geometrical input, however, is via the mesher code, and consequently is restricted by the type of geometry which can be handled by the mesher. Either steady-state or transient solutions are available and may be

intermixed as desired. An implicit differencing scheme is used which allows any size of time step to be taken in a transient problem without danger of instability, and the extrapolated Liebmann method is used for the solution of the simultaneous equations resulting from either the transient or steady-state cases.

The program allows the following boundary conditions:

1. Convection, where the user supplies a boundary temperature and a film coefficient which may be functions of time, surface temperature, and material.
2. Contact coefficient between two solid regions.
3. Boundary flux. A boundary flux through a given surface may be specified in addition to any other fluxes arising from other boundary conditions applied at that surface.
4. Boundary radiation, i.e., radiation to a specified boundary temperature.
5. Internal radiation. Radiation among two or more surfaces in the problem can be handled in two dimensions only.

Any one or all of these conditions may be applied separately or together to a surface. No surface condition implies an adiabatic boundary.

A time and space dependent internal generation term is permitted, and provision is made for anisotropic thermal conductivity which may depend on space coordinates, direction of heat flow path, and temperature of the material. The program also permits a temperature-dependent specific heat.

III.. COMPUTATION FORMULAS

The computational model used by the code assumes that the material is divided into cells (or nodes) interconnected in any arbitrary manner by heat flow paths. No assumption is made about uniformity of size, shape, or material of the cells. Boundary conditions are represented

either as additional heat flow paths to other cells (internal radiation, surfaces in contact), as flow paths to reservoirs of fixed or given temperature (convection, boundary radiation), or as an additional source term (boundary flux). The interconnections among cells and boundary conditions, while arbitrary from the point of view of the formulas, are prescribed by the geometry of the problem and are defined by the code as a preliminary to the solution of the difference equations. This type of model has been used many times before, as the references listed at the end of this report demonstrate; however, there are differences in methods of solution and allowable nonlinearities so that it is desirable to set down the exact computational formulas used.

The equation from which the formulas are derived is the heat balance on cell i over the time interval t to $t + \Delta t$:

$$[T_i(t+\Delta t) - T_i(t)]C_i = \Delta t[Q_i + \sum_j K_{ij}(T_j - T_i)].$$

The symbols are defined as follows:

T_i is the temperature of cell i ,

C_i is the heat capacity of cell i ,

Q_i is the rate of heat generation in cell i ,

K_{ij} is the conductance of heat flow path ij ,

j is an index which ranges over all heat flow paths whether to other cells or to boundary conditions, and

T_j may be the temperature of another cell or a boundary temperature.

There is a question about the time at which quantities on the right should be evaluated. The choice determines the direction of the time differences and influences the numerical stability of the solution. In the present case it was decided to evaluate the temperatures T_i and T_j

at $t + \Delta t$ to gain numerical stability and to take Q_i at $t + \Delta t/2$ in order to get a good average value of the amount of heat generated during the time step.

The equation must then be solved for $T_i(t+\Delta t)$ yielding

$$T_i(t+\Delta t) = \frac{C_i T_i(t) + \Delta t [\sum_j K_{ij} T_j(t+\Delta t) + Q_i(t + \frac{\Delta t}{2})]}{C_i + \Delta t \sum_j K_{ij}}$$

Since $T(t+\Delta t)$ is unknown at every point i and since C_i , K_{ij} , and some boundary temperatures are allowed to depend on $T(t+\Delta t)$, we have a system of l nonlinear equations in l unknowns to solve at each time step, l being the number of cells. Although the authors know of no theoretical basis for solving such a general system, as a practical matter it yields to the popular iterative methods, and the one chosen in this case is extrapolated Liebmann. Successive values of the temperature $T_i(t+\Delta t)$ at each cell i at time $t + \Delta t$ are computed by means of the following formula:

$$T_i^{n+1}(t+\Delta t) = (1-\beta)T_i^n(t+\Delta t) + \beta \left\{ \frac{C_i T_i^n(t) + \Delta t [\sum_j K_{ij} T_j^m(t+\Delta t) + Q_i(t + \frac{\Delta t}{2})]}{C_i + \Delta t \sum_j K_{ij}} \right\},$$

where

n is the iteration number,

β is the relaxation extrapolation parameter,

$m = n + 1$ if $j < i$, and

$m = n$ if $j > i$.

The steady-state formula is obtained by setting $T_i(t) = T_i(t+\Delta t)$ in the basic equation, solving for $T_i(t)$, and then applying the extrapolated Liebmann method to the result. This process yields the following iteration formula:

$$T_i^{n+1} = (1-\beta)T_i^n + \beta \frac{\sum_j K_{ij} T_j^m + Q_i}{\sum_j K_{ij}}.$$

In order to take both boundary conditions and internal neighbors into account while using the same basic formula, the following set of rules for computing K_{ij} is used:

1. Internal Connections.

$$K_{ij} = \frac{k(x_i, y_i, z_i, x_j, y_j, z_j, T) A_{ij}}{\Delta x_{ij}}.$$

$k(x_i, y_i, z_i, x_j, y_j, z_j, T)$ is the thermal conductivity of the material as a function of position, direction of heat flow path, and temperature of the material. The two sets of coordinates give the positions of the centroids of the i th and j th cells so that anisotropic thermal conductivity may be used to a limited extent at least. An anisotropic conductivity in which the principal axes do not coincide with the coordinate axes introduces additional terms into the heat equation, which are not taken into account in this model. (See Carslaw and Jaeger, Conduction of Heat in Solids, p.41.) The temperature used to compute k is an average of the two node temperatures at the advanced time step.

A_{ij} is the interface area between the two nodes i and j .

Δx_{ij} is the distance between the centroids of two nodes i and j .

2. Convection.

$$K_{ij} = \frac{\alpha_c K_{is} h(t, T_s) A_s}{\alpha_c K_{is} + h(t, T_s) A_s}.$$

K_{is} is defined as in the internal connection case above except that the coordinates of the center of the surface face are used instead of the coordinates of point j , and the surface area A_s and centroid to center of face distance Δx_{is} are used.

$h(t, T_s)$ is the convection film coefficient [a function of time (t) and surface temperature (T_s)].

α_c is a proportionality factor which provides a rough estimate of the fraction of total heat flow through the face which is due to convection. It is equal to one unless there are radiation and convection conditions simultaneously at a boundary.

3. Contact Coefficient.

$$K_{ij} = \frac{K_{is} K_{sj} f A_s}{K_{is} K_{sj} + K_{is} f A_s + f A_s K_{sj}}$$

K_{is} and K_{js} are defined in analogy to those above. f is the contact coefficient between the materials in which nodes i and j lie.

4. Boundary Flux.

K_{is} as defined above is used. Boundary flux is actually equivalent to a line or surface source or sink lying along the boundary under consideration.

5. Boundary Radiation.

$$K_{ij} = \frac{\alpha_{rb} K_{is} K_{rad}}{\alpha_{rb} K_{is} + K_{rad}}$$

$$K_{\text{rad}} = \sigma \epsilon_i \epsilon_b V_{ib} A_s (T_s^2 + T_b^2) (T_s + T_b).$$

σ = the Stefan-Boltzmann constant. Unless the program is instructed differently, it will use 0.174×10^{-8} BTU/hr $\text{ft}^2(^{\circ}\text{F})^4$.

ϵ_i and ϵ_b are the emissivities of the material surface and the boundary surface, respectively.

V_{ib} is the view factor from the surface of node i to the boundary surface.

T_s is the surface temperature of the face of node i.

T_b is the boundary temperature, which is given.

α_{rb} is an estimate of the fraction of heat flow through the surface due to boundary radiation.

6. Internal Radiation.

$$K_{ij} = \frac{\alpha_{rij} K_{is} K_{\text{rad},ij} \alpha_{rji} K_{js}}{\alpha_{rij} K_{is} K_{\text{rad},ij} + \alpha_{rij} K_{is} \alpha_{rji} K_{js} + \alpha_{rji} K_{js} K_{\text{rad},ij}}.$$

$$K_{\text{rad},ij} = \sigma \epsilon_i \epsilon_j V_{ij} A_i (T_{si}^2 + T_{sj}^2) (T_{si} + T_{sj}).$$

σ , ϵ_i , ϵ_j , T_{bi} , and T_{bj} are the Stefan-Boltzmann constant, emissivities of the two surfaces, and the surface temperatures, respectively.

V_{ij} is the view factor from the surface of node i to the surface of node j. It is given by

$$V_{ij} = \frac{1}{2} \cos \varphi_i \cos \varphi_j \frac{A_j}{r}.$$

r is the distance between the two surfaces, and φ_i and φ_j are the angles the connecting line makes with their normals.

A_i and A_j are the areas of the two radiating faces.

T_{si} and T_{sj} are the surface temperatures of the faces of the two nodes.

$\alpha_{r_{ij}}$ is an estimate of the fraction of heat flow through the face of node i due to radiation to node j .

The test for convergence of the iterative procedure is handled in the following way. For a transient time step or a steady-state solution, successive iterations are carried on, constantly updating the nonlinear coefficients in the iteration formulas, until for all cells i the following relation is true:

$$\frac{|T_i^{n+1} - T_i^n|}{T_i^n} \leq \gamma.$$

γ is a convergence criterion specified by the user of the program for a particular time-step or steady-state solution.

The fractions α which appear in some of the formulas above deserve some further explanation. They are made necessary by the possibility of having multiple heat-flow paths meeting at a cell face. In this event the over-all conductances must be calculated in such a way that the conductance which lies within the cell is used just once. The procedure which we have adopted attempts to divide this internal conductance into a number of flow paths, one for each flow path through the cell face, the conductance of each part being proportional to the amount of heat which is to flow through it. No accurate scheme for calculating α has been developed. In the iterative scheme used, changing α at each iter-

ation seems to interfere with convergence rather seriously. Consequently an estimate is used based on the first 20 iterations. For the first three iterations α is set to one. Then for the next 17 iterations α is recomputed at each cycle by dividing the conductance of the heat-flow path exterior to the cell by the sum of all such conductances for that face. For example

$$\alpha_c = \frac{A_s h(t, T_s)}{A_s h(t, T_s) + K_{rad} + \sum_j K_{rad_{ij}}},$$

the summation index j ranging over all cells which exchange radiant energy with node i . The other α 's are computed in analogous fashion. After 20 iterations the α 's are not changed again until a new series of iterations is begun. Clearly the process provides only very rough estimates of the desired numbers, and the roughness of the radiation calculation should be kept in mind when using the code.

IV. FEATURES OF THE CODE

The Mañana code is capable of solving problems having very general geometries and a fairly large number of mesh points, and yet it requires only a modest amount of human labor for preparation of input. There may be as many as 32 solid regions of different materials and as many as 100 bounding surfaces having various boundary conditions. The number of points which may be handled in a problem varies from one problem to another because of the varying requirements for storage of heat-flow paths. A cell which is in the interior of a solid in a two-dimensional problem, for example, requires much less storage than a cell on a radiating boundary of a three-dimensional problem. Sixty thousand words of storage have been reserved for cell data, which should be sufficient for between three and four thousand points in an average problem.

Preparation of a problem for Mañana begins with meshing each separate region using the RATH mesher. A region need not be a contiguous figure, but it must all be of the same material. Once all regions have been meshed, the results are put together along with boundary conditions, material properties, specifications for extensions of the mesh in the third dimension, and a description of the type of solution desired (i.e., transient, steady-state, or a combination). This batch of data serves as input to Mañana.

A conventional set of axes has been adopted, using the xy-plane in terms of which the mesher input is described and then adding a z-axis perpendicular to it. Note that all input to the mesher for a given problem must be described relative to the same origin and in the same units if two or more regions are to run together successfully in Mañana. The mesh sizes, however, need not be the same.

Any consistent set of units may be used with the code, since no conversion factors have been used anywhere in the equations. All quantities which depend on units are input to the code. However, the assumption is made in the case of radiation that the temperatures are on an absolute scale; and the form of the convergence test, which is a ratio of change in temperature to temperature, makes it undesirable to have temperatures which range on both sides of zero.

It is possible to extend the geometry of the problem to the third dimension by what is basically a regeneration of the two-dimensional (xy) mesh at prescribed intervals in a perpendicular (z) direction. Some variations are allowed: Any region may be suppressed in any plane of points, and different boundary conditions and materials may be used in different planes. On the surfaces between planes all boundary conditions except internal radiation are permitted. Each plane of points is given a layer number, counting from the origin. Layer No. 1 has a surface at $z = 0$ and a surface at $z = \Delta z_1$. Its midpoint is at $z = \Delta z_1/2$. Layer No. 2 has a surface at $z = \Delta z_1 + \Delta z_2$ and its midpoint at $z = \Delta z_1 + \Delta z_2/2$. Each Δz is entered individually so that there is no

requirement for equal spacing along the z-axis.

Certain cylindrical and spherical problems can be done in two dimensions by allowing the thickness of the cells to vary. Consequently for two-dimensional problems the z-dimension of the cells is allowed to be any function of x and y.

V. INPUT

In order to achieve a high degree of generality, input to the code consists of three different kinds: FORTRAN subprograms, mesher output cards, and decimal data cards. Programs specifying material properties and their variations, initial conditions, and boundary conditions have been left to be supplied by the user of the system as FORTRAN subprograms so that they can be arbitrary functions tailored to the specific problem or to a specific class of problems. The mesher data supplies detailed information about the mesh or meshes which go into the problem, and the decimal data cards provide information which can be conveniently specified in a brief, generally order-independent way, such as types of boundary conditions to apply at each surface, specifications for regenerating the mesh in the third dimension, print controls, and running time. These three types of input are described in detail in the following four sections in their order of appearance in a deck.

A. FORTRAN Subprograms

Part of the problem description for the *Mañana* code is a set of 13 FORTRAN subprograms, 11 functions, and two subroutines. The routines can be divided into two logical groups; those which depend only upon space variables and material, and those which depend upon time or temperature. In general a physical property, for example, is assumed to be a separable function of the type $S(\vec{r},m)T(\theta,m)$, where S is a function only of space variables and material and T is a function only of temperature and material. S and T must be supplied as separate FORTRAN functions. The program multiplies them together at the appropriate time. Note that

there must be some kind of subroutine of each specified name supplied (even though it may be a dummy which does nothing) in order for the program to load properly. The first five programs described below are of the space-dependent type, and the rest are either time or temperature dependent. The subprogram titles given below show the type of program and the number of arguments in FORTRAN notation, and can be used as the first statement of each program.

1. FUNCTION TEMPER(X,Y,Z,M)
 TEMPER = initial temperature.
 X = x-coordinate of centroid of cell.
 Y = y-coordinate of centroid of cell.
 Z = z-coordinate of centroid of cell.
 M = material number.

2. FUNCTION GENER(X,Y,Z,M)
 GENER = heat generation rate in units of energy per unit volume
 per unit time.

 X,Y,Z,M are the same as in TEMPER.

3. FUNCTION CONDOC(X1,Y1,Z1,X2,Y2,Z2,M)
 CONDOC = thermal conductivity between points (X1,Y1,Z1) and
 (X2,Y2,Z2) in material M. The two sets of coordinates
 are given so that anisotropies in the thermal conductivity
 can be accounted for. In general they represent the cen-
 troids of two nodes or else the centroid of a node and
 center of its face.

4. FUNCTION HDRVF(NS,X,Y,Z,A,B,C)
 HDRVF = view factor for boundary radiation.
 NS = surface number.
 X,Y,Z = coordinates of a point on the surface.
 A = direction cosine of normal to the surface with x-axis.
 B = direction cosine of normal to the surface with y-axis.

C = direction cosine of normal to the surface with z-axis.

5. FUNCTION THICK(X,Y)

THICK = thickness of cells in the z-direction.

X,Y = coordinates of a point in the problem at which a thickness is needed.

6. FUNCTION FUN(M,T)

FUN = time-dependent part of the heat generation function. The final value of heat generation used is equal to GENER $\times$ FUN.

M = material number.

T = time.

7. FUNCTION CONCO(K,T1,T2)

CONCO = contact coefficient. The larger the coefficient, the better heat conduction. For the common case of perfect thermal contact between two regions, some arbitrary number large enough so that any other conductances in the problem will be insignificant when added to it should be supplied.

K = arbitrary identification number for boundary condition.

T1 = surface temperature at surface 1.

T2 = surface temperature at surface 2. The two temperatures can be distinguished if necessary by the fact that K is an arbitrary number associated with surface 1. Entering different values of K for the two surfaces will permit a test to determine which side the code is working from.

8. FUNCTION FUND(T,M)

FUND = temperature-dependent part of the conductivity. The value of the conductivity used in computation is equal to CONDOC $\times$ FUND.

T = temperature of the material.

M = material number.

9. FUNCTION FUR(M,T)
FUR = temperature-dependent part of the heat capacity. The value of heat capacity used in the calculation is equal to FUR × specific heat × volume of node. The specific heat is supplied on a "C" card which is described in a later section.
M = material number.
T = material temperature.
10. FUNCTION BFLUX(K,T)
BFLUX = rate of heat flow per unit area across a surface.
K = arbitrary number used for distinguishing among different conditions.
T = time.
11. FUNCTION EMMIS(K,T)
EMMIS = emissivity of a radiating surface for grey-body radiation.
K = arbitrary number for distinguishing surfaces or materials.
T = temperature at the radiating surface.
12. SUBROUTINE HDRAD(TI,K,TB,EP)
This subroutine describes the boundary radiation conditions. The output variables are the boundary temperature, TB, and the emissivity of the boundary surface, EP. The input variables are the time, TI, and the arbitrary number, K, used to connect the surface with the condition.
13. SUBROUTINE CONVEC(K,M,TS,H,TB,TI)
This subroutine describes the convection boundary conditions to the code. There are two output variables which the subroutine must supply:
TB = boundary temperature.
H = film coefficient.

These two quantities may be computed from any or all of the following input quantities:

K = arbitrary number used for connecting surface and condition.

M = material number of the solid which the surface bounds.

TS = surface temperature.

TI = time.

All of the foregoing subprograms must be supplied whether or not they are used, because the program loader requires them to be present before execution of the code is permitted. Depending on the complexity of a problem then, many of the subprograms may be simple, do-nothing routines which serve only to placate the loader but are never called upon for information. Whether or not they are called upon is controlled by the decimal data cards which are loaded later. These programs are made a part of the code deck; and if a series of problems has many of the same subprograms in common, the binary decks from the FORTRAN compilations can profitably replace the symbolic decks. These programs are customarily placed at the end of the Mañana code deck followed by the usual STRETCH "SUHTYPE, DATA" card, which introduces the program data.

B. Problem Identification

The first data card, problem identification, is a decimal punched card which is simply read and printed and does not affect the computation. This identification card is followed by the mesher data, described in the next section.

C. Mesh Data

Following the problem identification card is a set of cards which describes the geometry of the mesh. This set consists of a number of binary decks produced by the mesher. There is one deck of mesher data for each region in the problem, followed by two special cards, supplied with the binary deck, which designate the end of the mesh data. The mesher decks may appear in any order (although each one must be exactly as it came from the mesher), and there may be any number of them from

1 to 32 for Mañana. Each deck is assumed to describe a separate region which may or may not be of the same material as the others or have a surface or surfaces in common with the others. Of the identification and control numbers available from the mesher only the surface number and material number are used. It is important to note that surfaces which are in contact should coincide exactly for their entire lengths. This requirement may require the subdivision of real surfaces in an unnatural way. Although more than one region may have the same material number, the converse is not true. A single region need not be a contiguous single figure, but it must have the same material number throughout. The two cards which follow the last deck of mesher output are shown on the next page.

D. Decimal Input Cards

Following the collection of mesher decks is a group of cards which specify the boundary conditions, complete the description of the geometry of the problem, and supply miscellaneous information and controls such as print controls, values of heat capacities, convergence criteria, and so on. The cards have a decimal format with a blank in column 1 and a letter in column 2 identifying the data, if any, punched on the remainder of the card. The cards fall naturally into two groups, the first of which is concerned with initial set up of the problem, while the second tells how it should be run and what should be done during the running. The program reads the first group of cards until it encounters a card with "E" in column 2. It then stops and sets up the problem, printing a message when finished with that phase, and then reads the remaining cards one by one. These cards may, for example, request time steps of various lengths, steady-state solutions, or set the problem time to specific values. The action requested on each card is completed before the next one is read.

The cards in the problem-set-up group will be described first. The order in which these cards appear is immaterial, with the obvious exception

of the "E" card, which signals the end of the group. Each card is identified in this list by the letter which is punched in column 2 to identify it to the code; its format is given in standard FORTRAN notation, and the contents of the fields are explained in order.

- I. Format (A2,5I5). Define top and bottom surface numbers and/or a new material number for a given plane of points.

Field 1: "I" in column 2.

Field 2: Surface number. This number serves only to identify the region. The action specified on this card will apply to the whole region in which this surface occurs.

Field 3: Layer number. This number identifies the layer, or plane, of points to which this card applies. Layers are numbered consecutively from $z = 0$ upwards.

Field 4: Material number. The points occurring in this layer and region are given the material number specified in this field. The material number originally specified by the mesher cards is replaced by this number for this layer only.

Field 5: Top surface number. The surface which forms the top boundary of this region (larger z) in this layer of points is given the surface number which appears in this field.

Field 6: Bottom surface number. This number is assigned to the lower surface (smaller z) of the region and layer described in the first two fields of this card.

- M. Format (A2,I5,4E10.7). Define a mirror surface for use with radiation conditions at symmetry boundaries. A mirror surface must be a straight line defined by two points.

Field 1: "M" in column 2.

Field 2: Surface number. This surface is given the identifying number which appears in this field.

Field 3: x-coordinate of beginning point.

Field 4: y-coordinate of beginning point.

Field 5: x-coordinate of end point.

Field 6: y-coordinate of end point.

- R. Format (A2,3I5). Replace surface number from mesher data with new surface number given on this card.

Field 1: "R" in column 2.

Field 2: Original surface number.

Field 3: Layer number in which replacement is to take place.

Field 4: New surface number.

- B. Format (A2,8I5). State boundary conditions which apply to a given surface. A "B" card is used to relate a surface number as specified in mesher data or by an "I" or "R" card to boundary conditions.

There must be a "B" card for every surface which is not adiabatic.

Field 1: "B" in column 2.

Field 2: Identifying number of the surface to which the conditions on this card apply.

Field 3: Convection condition identification. If this field is neither zero nor blank, a convection boundary condition is attached to all nodes along the surface. The number in this field is used for the fixed point variable K in subroutine CONVEC.

Field 4: Boundary flux identification. A nonzero entry in this field attaches a boundary flux to this surface. The value of the flux is given by function BFLUX, and the identification number in this field becomes the argument K for BFLUX.

Field 5: Boundary radiation identification. A nonzero entry in this field indicates to the code that there is boundary radiation at this surface. The number in this field is sent to subroutine BDRAD in the guise of argument K so that BDRAD may, if necessary, use it to distinguish among several possibilities. Note that if boundary radiation exists, there should be an

entry in field 9, the emissivity identification.

Field 6: Contact coefficient identification. A nonzero entry in this field indicates to the code that this surface is in contact with another. The number of the other surface is stated in field 7, immediately following. When two surfaces are in contact, there must be a "B" card for each, listing the other as being in contact.

Field 7: Contact surface number. If field 6 is neither zero nor blank, this field contains the number of the neighboring surface which is in contact. Both surfaces should coincide exactly.

Field 8: Maximum number of node faces which each node face along this boundary is permitted to view in internal radiation. If this field is blank or contains zero, it will be assumed that there is no radiation to any other surface in the problem, although there may be radiation to a surface outside the problem, i.e., boundary radiation. Radiation among surfaces internal to the problem is treated by assuming that each cell face represents a small uniform radiating surface. Lists of the pairs of faces which can see each other and their view factors are made for subsequent use in the radiation calculations. Generally if all possible pairs were listed, the amount of storage required would be prohibitive. Consequently the number in this field is used to limit the number of pairs which will be retained. Those with the largest view factors are kept, and the view factors between pairs retained are increased to compensate for the discarded pairs.

Field 9: Emissivity identification. This number is argument K of function EMMIS and should be filled in if there is either boundary or internal radiation at this boundary, i.e., if either fields 5 or 8 are nonzero.

P. Format (A2,4I5). List a pair of surfaces which radiate to each

other and, as an option, a pair of surfaces which may obstruct their view of each other. The code figures out the smallest field of view defined by the obstructing surfaces if they are present, and restricts all radiation between the radiating surfaces accordingly. Each pair of radiating surfaces need be listed only once.

Field 1: "P" in column 2.

Fields 2 and 3: Surface number of radiating surfaces.

The order is immaterial; the fields are equivalent.

Fields 4 and 5: Surface numbers of obstructing surfaces. One or two surfaces which may obstruct the view between the two radiating surfaces may be listed in these fields. If the fields are left blank, then an open, unobstructed view is assumed.

D. Format (A2,I5). Number of dimensions of problem. If this card contains a three, the code will regenerate the mesh in the z-direction. If this card is omitted or if it contains a two, the problem will be assumed two-dimensional.

Z. Format (A2,4(I5,E10.7)). Delta z. In a three-dimensional problem it is necessary to enter the thickness of each plane of points, or layer. Each cell in a layer has the same dimension in the z-direction. The layer thicknesses are entered in an order-independent manner by means of as many "Z" cards as necessary. The integer fields contain the layer numbers, which may be entered out of order, but must, after reading all the "Z" cards, form a sequence of integers beginning with one and going without omissions to n, where n is the total number of layers of points. The maximum value of n allowed is 100. The floating point field following each layer number contains the corresponding layer thickness, Δz . The first blank integer field encountered on a card causes the remainder of the card to be skipped. In a two-dimensional problem there is no need for a "Z" card, and if any are read the information on them will be ignored.

- C. Format (A2,4(I5,E10.7)). Specific heat capacity. This card operates similarly to a "Z" card in that it contains four pairs of entries, each pair being a fixed-point number followed by a floating-point number; and the first blank, fixed-point field causes the remainder of the card to be skipped. The fixed-point numbers in this case are material numbers, corresponding to those read from mesher data or added by means of "I" cards. The floating-point number following each material number is the volumetric specific heat, i.e., the heat capacity per unit volume for the material. This number is the density times the specific heat as ordinarily defined.
- Q. Format (A2,3I1). Input print control. This card controls the printing of input data and descriptions of the cells generated. There are three options; in each a zero means do not print, and a one means print this option.
- Field 1: "Q" in column 2.
- Field 2: Print or do not print mesher input.
- Field 3: Print or do not print input from decimal cards.
- Field 4: Print or do not print a list of generated cells and their descriptions.
- G. Format (A2,14I5). Leave gaps in a three-dimensional problem.
- Field 1: "G" in column 2.
- Field 2: Surface number used to identify a region. The action taken by the card refers to the whole region which contains this surface number.
- Fields 3-15: Layer numbers. The region referred to in field 1 will be omitted from the problem in the layers listed in these fields. The first blank or zero field will cause the remainder of the card to be skipped.
- L. Format (A2,I5). Running time. This card enters the maximum running time in minutes. If the problem tries to run over this time, it will remove itself from the machine, giving a temperature print and

a tape dump from which the problem can be restarted. Since the print and the dump take place after the time is up, some allowance should be made for this in requesting computer time.

- A. Format (A2,E10.7). Stefan-Boltzmann constant. If there is any radiation present in the problem, a value of the Stefan-Boltzmann constant consistent with the units employed in the problem must be supplied. If none is supplied, the code uses 0.174×10^{-8} BTU/hr ft²(°F)⁴.
- E. Format (A2). End of problem set up. After all A, B, C, D, G, I, L, M, P, Q, R, and Z cards, there must be one card with "E" in column 2 to signal the end of this phase of the input.
- F. Format (A2). Change dump tapes. Immediately upon reading this card the current dump tape is rewound and unloaded, and a new tape is requested from the operator. An "F" card may appear either before or after the "E" card.

After the "E" card has been read, the geometry, material properties, and boundary conditions have been completely specified to the code. At this point all the cells are generated and stored in memory, which is equivalent to defining the complete set of difference equations and storing initial conditions. When this set-up process has been concluded, new cards are read describing what sort of computation is desired, and what activities are to be performed in the course of the computation. In general the cards are effective immediately when they are read, and a new card is read when the activity ordered by the previous one is completed. The only exception to this rule is the print-controlling "J" card which must wait for a succeeding "S" or "T" card to initiate a computation before it can take effect. Any sequence of steady-state and transient solutions can be obtained by supplying the proper cards in appropriate order.

- T. Format (A2,E10.7,3I5,E14.7). Transient time step description. As

soon as this card has been interpreted, a number of transient time steps, described on the card, are initiated.

Field 1: "T" in column 2.

Field 2: Size of time steps.

Field 3: Number of steps of this size and type to take before reading next card.

Field 4: Number of steps between print cycles. A one in this field means print the temperatures at the end of each time step.

Field 5: Maximum number of iterations per step. If the convergence criterion is not met when this number of iterations has been performed, a message is printed, a tape dump is taken, the temperatures are printed, and then the next step is taken as if convergence had been achieved.

Field 6: Convergence criterion. This field contains γ where convergence is defined as

$$\frac{|T_i^{n+1} - T_i^n|}{T_i^n} \leq \gamma \text{ for all cells } i.$$

S. Format (A2,E10.7,2I5). Steady-state solution. This card causes the code to obtain a steady-state solution of the problem at the current time.

Field 1: "S" in column 2.

Field 2: Convergence criterion. This is the same number, γ , which appears in field 5 of the "T" card.

Field 3: Print control. A zero means do not print temperatures at the end of the calculation. A one in this field causes the temperatures to be printed when the calculation is completed.

Field 4: Maximum number of iterations. This number has the same effect as field 4 of the "T" card.

- V. Format (A2,E10.7). Set problem time to the value on this card. The time is incremented automatically by the time steps during transient calculations. It is unchanged by a steady-state calculation. If no "V" card is read initially before a "T" or "S" card, the time is started at zero.
- X. Format (A2,E10.7). Extrapolation parameter. This card sets the extrapolation parameter β used in the extrapolated Liebmann iterative scheme for solving the difference equations. If no "X" card is present, a value of one is used. There is a test for suspected divergence which may reset β to one if it appears that the solution is diverging. Useful values of β all lie between one and two.
- J. Format (A2,4I5). Print details of iteration. This card causes printing of partial results while the iterative solution is in progress. It is intended only for the purpose of diagnosing difficulties and not for obtaining results. There are two types of print available:
- Type 1. Print all temperatures at specified iterations.
 - Type 2. Print all steps of every calculation at specified iterations.
- Field 1: "J" in column 2.
- Field 2: Iteration number at which to begin type 1 print.
- Field 3: Iteration number at which to end type 1 print.
- Field 4: Iteration number at which to begin type 2 print.
- Field 5: Iteration number at which to end type 2 print.
- N. Format (A2). Tape dump. A tape dump from which the problem may be restarted is obtained at the point where this card is read. The code then continues to read the next card, if any.

The program continues reading cards and performing the activities ordered until it runs out either of computer time (as specified on an "L" card) or of cards. In either event it then takes a last tape dump and stops.

VI. TAPE DUMPS

Whenever the program runs out of "S" or "T" cards, reads an "N" card, runs out of time, or fails to converge within the specified iteration limit, all information necessary for restarting from that point is written on a tape, a message is printed, and a card is punched. There exists a restart deck which will then start the problem over from any specified dump. The use of the restart deck is as follows: The message printed with each dump identifies it by number, and the same number is punched in columns 78, 79, and 80 of the card which is punched with the dump. The dump card bearing the appropriate number is the first card of the data deck which follows the binary restart deck. Following the dump card there should be a "Q" card containing zeroes, an "L" card giving the running time for the restart run, and an "E" card. Then there may be a collection of "S", "T", "V", "X", "J", "F", and "N" cards, just as in a normal run, which will be read according to the following rules:

1. If the dump was taken because the time was up, the current set of iterations will be completed before a new card is read. However, any remaining time steps specified on a "T" card which was being processed at the time of the dump will be ignored. That is, the program will complete the current time step, in the case of a "T" card and then skip to read a new card.
2. If the dump was caused by a failure to converge within the specified number of iterations, a new card is read immediately, but the problem time will not be advanced by the first card if it is a "T" card. Thus one has the option of increasing the iteration limit to try to obtain convergence.
3. If the dump was caused by either running out of cards or reading an "N" card, a new card is read immediately, and it causes the normal action for that card to be taken.

VII. OUTPUT

Output from the code consists of printed listings and cards. A "Q" card controls the listing of input and cell descriptions, which are divided into three parts:

1. Mesher data, consisting of boundary descriptions and detailed descriptions of boundary nodes, as entered on mesher cards, are printed as the first block of output.
2. A summary of the information contained on the decimal input cards is listed as a second block.
3. A detailed description of each cell with the material properties reduced to the form in which they enter the computation forms the last block. The cells are numbered in the sequence in which they are used in the computation (and stored in memory), boundary cells first and then internal cells. Neighboring cells having numbers greater than that of the current cell are also listed. The computation is done in such a way that neighboring cells with lower numbers need not be remembered.

Whenever output is requested on an "S" or "T" card, a block of printing which lists the central temperature of each node, the surface temperatures and fluxes, and a heat balance on the system is produced.

The cards produced by the program are of two types: decimal cards intended for input to the isotherm plotters and binary dump restart cards. The decimal cards produced are, in order, those described in subsections B, C, and F of Section VIII of this report, where input to the plotter is described. There will be one set of the cards described in VIII, F, for each time the temperatures are printed, and the binary dump cards may be intermingled with these sets. Some care is therefore necessary to sort out the card output.

VIII. ISOTHERM PLOTTERS: SMPLOT, SNPLOT.

Two isotherm plotters take the punched output from Mañana and Wanton and produce isotherms at temperatures requested by the user. The plots

are simply a series of dots at the interpolated values plotted on an outline of the figure. An off-line listing is also produced containing the coordinates of all values in the isotherms.

The two codes use identical input but differ in that SMPLOT (a FORTRAN IV 7094 code) can handle only two-dimensional problems while SNPLOT (a FORTRAN IV 7030 code) handles both two- and three-dimensional problems. (For the three-dimensional problems the isotherms in any plane of points can be plotted.)

The input to the codes is broken into four major categories: identification, boundary description, node storage descriptions, and temperatures. These are discussed below with both format and data requirements.

1. Identification card (format 12A6). This card must be the first card of the data deck. It contains 72 columns of identification which are reproduced on the output listing.
2. The boundary description is divided into two parts.
 - a. One card (format I5,F10.5) containing the total number of line segments, N, in the first field and a number, Δ , used in dividing circular arcs into straight line segments. The heat codes use $\min(\Delta X_i, \Delta Y_i)$ for all i (regions) for this value. (See IAMS-2809.)
 - b. The remainder of the boundary description cards (format 11,7E10.5) contain the description of each line segment. There must be N of these.*
Field 1, K: K = 1: Straight line, zero or finite slope.
K = 2: Vertical straight line.
K = 3: Circle.
Field 2, AORM: either a or m, depending on the value of K where a is the x-coordinate of the center of a circle and m is the slope of a straight line.
Field 3, B: the value of b where b is the y-coordinate of the center of a circle or the y-intercept of a

* A much more detailed description of these quantities is given in IAMS-2809.

straight line.

Field 4, RADIUS: the radius of the circle (for the sign of the radius see LAMS-2809, p.19).

Fields 5-8, XBEGIN, XEND, YBEGIN, YEND: the coordinates of the end points of the segment.

3. Node description cards (format 11,2I⁴,2I²,2F10.5,4(2I⁴,I²)) and (format 8(2I⁴,I²)) give the descriptions of every cell in the problem, the coordinates of its centroid, and a list of its neighbors. These node descriptions come in sets with one card of the first format above and as many as necessary of the second format to describe the node.

- a. First card (format 11,2I⁴,2I²,2F10.5,4(2I⁴,I²))

Field 1 (I¹) contains a count of the number of cards necessary to define this cell.

Field 2 (I⁴) contains the x-coordinate index describing the cell under consideration.

Field 3 (I⁴) contains the y-coordinate index of this cell.

Field 4 (I²) contains the region number of this cell.

Field 5 (I²) contains the layer number in which this cell lies.

Field 6 (F10.5) contains the coordinate of the x-centroid of the cell.

Field 7 (F10.5) contains the coordinate of the y-centroid of the cell.

Field 8 (I⁴) contains the x-coordinate index of a neighbor to this node.

Field 9 (I⁴) contains the y-coordinate index of the neighbor.

Field 10 (I²) contains the region number of the neighbor.

The remaining fields on this card are punched the same as fields 8, 9, and 10 and contain other neighbors of this node.

- b. Second card (format 8 (2I4,I2)). Cards of this type contain only neighbors of this node, and as many may be used as needed to complete the description. The fields in this card describe neighbors of the node and contain the same quantities punched in fields 8, 9, and 10 of the first card.
- 4. Following the descriptions of all the cells is a single card containing a minus punch (11 punch) in column one.
- 5. A card (format 20F4.0) must be supplied by the user for every set of temperatures he wishes to plot. This card contains those values at which he wishes to plot isotherms. There should be no blank fields between data fields on this card.
- 6. The temperatures are punched in sets with each being an individual problem to the plotter. Each set is composed of one layer of nodes and therefore has a card containing the layer number. The temperatures are punched in the same order as the node descriptions are punched. The temperature sets are punched on two types of cards.
 - a. The first card (format F6.0,I2) contains the problem time punched in the first field and the layer number punched in the second. This layer number instructs the codes to use that set of nodes which lie in this layer.
 - b. The second and succeeding cards (format 20I4) contain the temperatures of the nodes in this layer.

The user may plot any number of temperature sets simply by supplying a card containing the desired isotherms in front of each of the desired temperature sets. The code at the completion of one will read and process the next.

With each of the heat codes the user must supply a certain amount of input. With Manana he must supply the identification card, the minus card, and the card with the desired temperatures. The Wanton code requires that the user supply only the card with the desired isotherms.

The user must also decide what temperature sets he desires to plot and remove those which are not to be plotted. Also with Mañana he must be sure to remove any dump cards which have been punched in with the temperature sets.

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APPENDIX A

"WANTON"

The 7094 version of the heat-conduction code possesses most of the characteristics of the 7030 code. The code itself is broken into three chain links and therefore necessitates a particular arrangement of the FORTRAN subprograms. The subprograms, TEMPER, GENER, CONDUCT, and BDRVF, must appear in chain 1, and the remaining routines go in the third chain. The function, THICK, is not used at all and therefore need not be supplied. The code has no provision for internal radiation and therefore "P" and "M" cards must not be used. The tape change card, "F", must not be used, as dump tapes can readily be changed if necessary. A card (format I2) must precede the identification card in the data deck. This card contains the output tape number (at Los Alamos, tape 9 is output printed off-line and tape 12 is output on film). All input is via tape 10 (A2) and the program runs under the Version 2 Monitor.

The 7094 code is designed primarily for small to medium two-dimensional problems (~1200 mesh points) and small three-dimensional problems. The code, however, provides for memory overflow on three-dimensional problems, but because of the time consumed the problems would be better run on the 7030.

The program will dump due to any one of the following three causes. First, the program dumps and exits when the time punched on an "L" card has run out. If there was no "L" card or one with time set to zero the program will run until otherwise interrupted. The code also dumps and exits if sense switch 3 is set by the operator. On dump restarts this is the only way to get off the machine unless all the data have been read and operated on. When an "N" card is read the program gives a

memory dump and proceeds to read the next data card. Whenever a dump is taken, a card is punched on-line containing the dump number in binary in the address portion of the first word (columns 1-36) of row 9. These cards may be used to restart the program.

Upon completion of the job in any normal manner tape A5 is unloaded by the code and will contain all dumps, if any, taken during the run. It should be saved for future restarts of the problem. Unlike the 7030 code the 7094 code will continue where it left off and completely satisfy all conditions of a "T" card. Thus it will complete the n time steps on a "T" card.

The code is restarted with a small binary deck loaded on-line. The dump tape should be remounted on unit A5. The card containing the dump number should be placed in the deck immediately following the card labeled TRANSFER. Thereafter may come any set of "S", "T", "V", "N", and "J" cards terminated by a card with an E in column 2 and two blank cards so the reader will not stop.

The code produces punched card output for the two plot programs described in Section VIII. This output is punched from logical tape 9 (at Los Alamos, the A3). The data contain an identification card, boundary descriptions, node descriptions, and temperatures. The temperature cards are punched every time the program prints output, i.e., when the time has run out, when sense switch 3 is depressed, or on completion of a condition on an "S" or "T" card. The temperatures are punched by layer number with the first card of each set of temperatures containing the time and layer number.

Sense switches used by the program.

1. Sense switch 1 need be set only on three-dimensional problems which overflow memory. If sense switch 1 is set on, the program will use tapes B1 and B2 for the overflow. Otherwise magnetic drums on channel C module 2 will be used.
2. Sense switch 2 not used.

3. Sense switch 3 can be set at any time and will cause the program to dump, print output, punch a dump restart card, unload tape A5, and exit.
4. Sense switch 4 can be set at any time and will cause the temperature print to be on the on-line printer when an "S" or "T" card condition is satisfied or when problem is stopped due to time up or sense switch 3 being set.
5. Sense switch 5 will cause the temperatures to be printed on-line at the completion of the current iteration. This feature should not be used frequently as it slows down the problem.
6. Sense switch 6 causes the total heat balance, the total heat generation, and the ratio of the two to be printed on-line. This can be helpful in determining when it becomes unprofitable to continue running a steady-state calculation.

The following tapes must be mounted at the beginning of a run and should not be changed during the run: A1 (Monitor systems), A2 (Monitor input (during a restart this tape is not needed)), A3 (Monitor printed and punched output), A4, A5, A6, B1, B2, B3, B5 (only if output listing is on film).

Rath Data Entry

Page ____ of ____

Programmer _____

Problem _____

Date _____

TYPE CODE	DATA FIELDS																																																																															
1 2	3 4 5 6 7	8 9 10 11 12	13 14 15 16 17	18 19 20 21 22	23 24 25 26 27	28 29 30 31 32	33 34 35 36 37	38 39 40 41 42	43 44 45 46 47	48 49 50 51 52	53 54 55 56 57	58 59 60 61 62	63 64 65 66 67	68 69 70 71 72	73 74 75 76 77 78 79 80																																																																	
B	SURFACE							CONVECTION COEFFICIENT							BOUNDARY FLUX COEF.							BOUNDARY RADIAT'N COEF.							CONTACT COEFFICIENT							CONTACT SURFACE							NODE TO NODE PAIRS							EMISSIVITY CONTROL																														
P	RADIATING SURFACE							RADIATING SURFACE							BOUNDING SURFACE							BOUNDING SURFACE																																																										
D	NUMBER OF DIMENSIONS																																																																															
Z	LAYER NUMBER							ΔZ							LAYER NUMBER							ΔZ							LAYER NUMBER							ΔZ							LAYER NUMBER							ΔZ																														
C	MATERIAL NUMBER							SPECIFIC HEAT							MATERIAL NUMBER							SPECIFIC HEAT							MATERIAL NUMBER							SPECIFIC HEAT							MATERIAL NUMBER							SPECIFIC HEAT																														
Q	PRINT NODE DESCRIPTIONS							PRINT DECIMAL INPUT							PRINT MESH INPUT																																																																	
G	SURFACE NUMBER							LAYER NUMBER							LAYER NUMBER																												LAYER NUMBER																																					
R	SURFACE NUMBER							LAYER NUMBER							NEW SURFACE NUMBER																																																																	
L	MINUTES																																																																															
I	SURFACE NUMBER							LAYER NUMBER							MATERIAL NUMBER							TOP SURFACE							BOTTOM SURFACE																																																			
A	STEFAN - BOLTZMANN CONSTANT																																																																															
M	SURFACE NUMBER							X - BEGIN							Y - BEGIN							X - END							Y - END																																																			
F	(CHANGE DUMP TAPE)																																																																															
E	(END OF DATA)																																																																															

APPENDIX B
CARD FORMATS

Rath Data Entry

Page ____ of ____

Programmer

Problem

Date _____

[illegible]

Rath Data Entry

Page ____ of ____

Programmer _____ **Problem** _____ **Date** _____

[illegible]

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APPENDIX C
DIAGRAMS OF DECKS

Order of Cards Input to Isotherm Plotters

Order of Cards Input to Wanton

Order of Cards Input to Mañana