HEXEREI
A MULTI-CHANNEL HEAT CONDUCTION CONVECTION CODE
FOR USE IN TRANSIENT THERMAL HYDRAULIC ANALYSIS
OF HIGH-TEMPERATURE, GAS-COOLED REACTORS

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OAK RIDGE GASEOUS DIFFUSION PLANT
OAK RIDGE, TENNESSEE

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COMPUTER SCIENCES DIVISION

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Interim Report

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ABSTRACT

This interim report describes the development and verification of a generalized coupled conduction-convection, multichannel heat transfer computer program to analyze specific safety questions involving high-temperature gas-cooled reactors (HTGR). The HEXEREI code was designed to provide steady-state and transient heat transfer analysis of the HTGR active core using a basic hexagonal mesh and multichannel coolant flow. In addition, the core auxiliary cooling systems were included in the code to provide more complete analysis of the reactor system during accidents involving reactor trip and cooling down on the auxiliary systems.

Included in this report are brief descriptions of the components of the HEXEREI code and sample HEXEREI analyses compared with analytical solutions and other heat transfer codes. This report is intended to be interim documentation of the techniques and accuracy of the HEXEREI code.

I. INTRODUCTION

During the licensing process of high-temperature, gas-cooled reactors (HTGR), specific accidents involving reactor trip and core cooling down on auxiliary cooling systems were determined to be of prime importance to the overall safety of the reactors. The development of HEXEREI was initiated to provide the necessary analytical tool independent of those of the reactor manufacturers, General Atomic Corporation (GAC).

The HEXEREI code is a hexagonal and cylindrical mesh heat conduction code with axially flowing coolant in a large number of channels. HEXEREI consists of modified variable dimensioning, input, thermal properties and calculating routines from CCCM developed by W. D. Turner (Ref. 1) and new model generator, coolant temperature, flow redistribution, orifice sizing and output routines.

The flow redistribution and orifice sizing subroutines (FLODIS, ORFICE) are based on the developmental work of D. D. Paul (Ref. 2, Chapter 7). A series of subroutines (ACHERONS) to calculate the systems response of the Core Auxiliary Cooling System (CACS) are being added. ACHERONS represents an extension of the work done by J. R. Tallackson (Ref. 2, Chapter 4) and R. L. Reid (Ref. 2, Chapter 5).

The basic HEXEREI code will be partially described in this document along with several test cases designed to demonstrate the accuracy of the different options that can be exercised in HEXEREI.

HEXEREI is currently in a very fluid developmental stage and a complete description at this time will be outdated soon. However, accident analysis involving coolant flow can be performed at present on HTGR active cores. A completed version of HEXEREI capable of performing reactor trip accident analysis involving the whole primary cooling system will be in use by June 30, 1976.

II. THE HEXEREI COMPUTER CODE

Code development on HEXEREI was initiated in late summer of 1974 with the model generator, HPOINT. The subroutine that calculates the nonlinear properties (i.e., temperature-dependent effective conductance) was added and checked out together as much as possible. The variable-dimensioning and input subroutines were then added and further check-out progressed until the calculating package and other associated subroutines were added. After program debugging, the code was capable of calculating most of the heat transfer test cases described in Section III.

II.1 Variable Dimensioning and Input Subroutines

HEXEREI is a code (like CCCM and HEATING5) in which most of the variables are contained in arrays that can be easily increased or decreased in size to provide efficient utilization of computer core. The input reading subroutines HINPUT and HINPT1 are slightly modified versions of INPUT and INPUT1 from CCCM.

These routines enable the user to describe with ease models with very complex material properties, geometries, boundary conditions, and time histories of power generation and boundary conditions. Subroutines HINPUT and HINPT1 read data which describe the computing mesh as a collection of three-dimensional regions over which the material properties, boundary conditions, and power generation are described by functions. Only one function can describe a property over the region. The major modifications to HINPT1 involved the addition of the necessary common blocks and input reading section so that the HTGR and ACHERONS input could be from cards or previously generated data sets.

The HTGR input block provides the capability for describing the radial power distribution, coolant channel, and orifice description in the inner hexagonal mesh region (active core and replacable side reflectors). The ACHERONS input block provides the capability of describing the CACS.

II.2 HPOINT Subroutine

Subroutine HPOINT is the model generator which generates the basic nodal locations in the R- θ plane. This basic grid is repeated in the axial direction by HTHRMP. The grid consists of nodes in a regular hexagonal mesh over an inner area and an optional outer area of cylindrical cells with nodes representing the centers of cells (Fig. II.1). Some cells are

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II.1 Typical node distribution for one axial plane of HTGR models

represented by half cells to allow nodes to be placed on boundaries (i.e., Outer Ring of Nodes, Fig. II.1). The interior active core node numbering technique follows the same pattern as evidenced in GAC's current designs. The nodes are numbered from the center out by completing the concentric hexagonal rings. At the border of the active core, in order to produce a core that approximates a right circular cylinder the outermost hexagonal rings of refueling regions are not completely filled with active refueling regions. Only the active core regions are used in the consecutive numbering sequence by GAC. HPOINT continues the full concentric hexagonal rings out to include the active core radius so that the replaceable side reflectors with coolant flow could be modelled with the same technique as the interior nodes and to minimize the number of irregular cells. Thus, HPOINT node numbers correspond to GAC's refueling region numbers in the interior region of the active core but not necessarily outside of this region. The meshing of the hexagonal cells with the cylindrical cells in the outer regions requires special cells on the outer hexagonal ring. These special cells were constructed to be connected to only one outer node and have the same cross sectional area as the regular hexagonal cells. If necessary, the outer ring of cylindrical nodes could be represented with fewer nodes than are in the outer hexagonal ring. Thus, the cylindrical nodes could be connected to more than one hexagonal node to reduce the number of nodes necessary to describe the reactor core, thermal barrier and PCRV.

Subroutine HPOINT also generates the effective conductance shape factor for the two-dimensional cells in Fig. II.1. This information is passed to subroutine HTHRMP to complete the effective conductance calculations. In HPOINT the effective conductance shape factor from one node to its neighbor consists of two components. Fig. II.2 presents a typical regular hexagonal cell with the connection to its neighbor shown. Since the material and the shape of the neighboring cell can be different, the shape factor is calculated for each cell. In all cases, the shape factor is the distance from the cell node to cell border in the direction of the neighboring node divided into the length of the common border.

II.2 Typical hexagonal cell with sample connector from node 1 to node 2

II.3 HTHRMP Subroutine

The extension of the nodal description in the axial planes is accomplished in this routine. The initial temperatures for these nodes are generated from input data describing the regions or from data for specified nodes. HTHRMP is a heavily modified version of CCCM's THRMPL.

The most important function of HTHRMP is exercised by the entry THRM1. THRM1 calculates the effective conductances, heat generation, and heat capacity of all the nodes. If any properties are temperature dependent, THRM1 reevaluates them when called by any of the calculating routines. THRM1 calls the appropriate routines to evaluate the temperature-dependent boundary conditions and coolant heat transfer coefficients.

Subroutine HTHRMP calculates the effective conductance in the R-0 plane with Equation (II.1)

$$C = \frac{Dz}{\frac{1}{k_1 S_1} + \frac{1}{k_2 S_2}} \quad (II.1)$$

where

Dz = axial length of cell

k = conductivity of material in cell
may be temperature dependent

S = shape factor component for cell as
calculated in subroutine HPOINT

Subscripts denote the cell to which
the property applies

Subroutine HTHRMP calculates the temperature-dependent material properties as a function of an average temperature for the material

between the cell center and cell border in the direction of the neighboring cell.

The major portion of the revisions to HTHRMP were required since HEXEREI uses the cell-centered nodal technique. Thus, HEXEREI's cells are homogeneous and all heat paths to neighboring nodes are series heat paths. CCCM and HEATING5 have cells that are not homogeneous and parallel heat paths.

II.4. HCALQT Subroutine

Subroutine HCALQT is a slightly modified version of CCCM's CALQLT. HCALQT performs the steady-state and explicit transient calculations and calls HTRANO which performs the implicit transient technique. These techniques are described in Refs. 1 and 2.

II.5 HTRANO Subroutine

Subroutine HTRANO is a slightly modified version of CCM's TRANO and is close to the stage of debugging the subroutine coupled with HEXEREI. HTRANO will provide the capability of accurately using very large time steps for efficient and economic calculations by using the implicit transient technique described in Ref. 2.

II.6 EXPAME Subroutine

Subroutine EXPAME calculates the temperature-dependent coolant heat transfer coefficients to be used in HCALQT, HTRANO, and EXPAM. Coolant properties are provided by subroutine PRPHE (Ref. 3) and the heat transfer coefficients as described in correspondence from J. P. Sanders to W. D. Turner of August 22, 1973. This letter summarizes the available heat

transfer correlations applicable to the HTGR core and suggests a set of expressions to evaluate the heat transfer coefficient as a function of Reynolds number.

The coolant channels are represented by one channel for each axial column of solid nodes. Thus, each solid node is connected to its neighboring solid nodes and to one coolant node, which represents all of the coolant channels contained within the solid node's cell. Each coolant node is connected to one solid node and the coolant node above and below it in the same column. The heat transfer coefficient for each coolant node is calculated using the values of solid node and coolant node temperatures supplied by the calling routine, and coolant mass flow-rate in the channel supplied by the flow redistribution routines (FLODIS, FLOADJ). Subroutine EXPAME also calculates the variable array that is used in EXPAM to calculate the coolant temperature.

II.7 EXPAM Subroutine

Subroutine EXPAM utilizes the heat transfer coefficients provided by EXPAME, the solid node temperatures as provided by HCALQT or HTRANO and the coolant inlet temperature provided by either a time function or the ACHERONS routines.

The coolant temperature is calculated by assuming that the solid node temperature is constant along the axial length of the cell and that the transient heat capacity of the coolant is insignificant. By integrating the resultant differential equation, the coolant cell exit temperature can be expressed as Equation (II.2).

$$T_2 = T_s - (T_s - T_1)e^{-\left(\frac{h A_s}{G C_p A_f}\right)} \quad (\text{II.2})$$

where

A_s = channel heat transfer area,

A_f = channel flow area,

G = mass flux rate,

T_s = solid node temperature,

T_1 = inlet temperature,

T_2 = exit temperature, and

h = convective heat transfer coefficient.

In order to properly model reactors with coolant channels with different diameters, EXPAME calculates A_s and A_f as average areas per channel.

To insure that the same amount of heat is transferred to the solid from the coolant as is required by Equation (II.2), the effective cell coolant temperature is calculated from integrating the heat flux along the cell. This effective cell coolant temperature is used in the temperature-dependent properties for the heat transfer coefficients.

II.8 ACHERONS Subroutine

The series of subroutines used to calculate the performance of the CACS is the same as described in Ref. 2.

II.9. Flow Redistribution and Orifice Sizing Subroutines

The flow redistribution algorithm (subroutine FLODIS) distributes the flow between the refueling regions of the HTGR so that conservation of mass and momentum is achieved.

$$\frac{d(\rho Vz)}{dz} = 0$$

$$\rho Vz \frac{dv_z}{dz} = - \frac{dP}{dz} - \frac{\text{friction}}{\text{losses}} - \frac{\text{orifice}}{\text{losses}} - \frac{\text{entrance}}{\text{losses}} \\ - \frac{\text{contraction}}{\text{losses}} \pm \frac{\text{expansion}}{\text{losses or gains}}$$

where

ρ = density,

P = pressure, and

Vz = velocity z direction.

The algorithm is divided into two sections: one that calculates the initial orifice settings and flow distribution and another that redistributes the flow as the transient progresses.

The initial flows and orifice settings are calculated in subroutine ORFICE. The initial flows are determined from the power peaking factors which were calculated in a core physics analysis. It is assumed that the region with the highest flow rate at steady state will have the maximum orifice area available. This assumption enables the pressure drop from the top plenum to the lower plenum to be calculated. The orifice coefficients of the other refueling regions which yield the desired pressure drop may then be evaluated. The initial phase is now completed and the program is ready for transient calculations.

Distribution of the flow during a transient is not considered complete until the pressure drop across all regions and the total flow across the reactor are within specified limits of the new transient conditions. The iterative procedure to insure these criteria is as follows:

- (1) The flow is distributed initially to insure that all channels have the same pressure drop. The first two iterations of each channel utilize the Newton-Raphson method where

$$F(x) = \text{Pressure Target} - \text{Pressure Calculated}$$

$$\text{Flow}_{\text{new}} = \text{Flow}_{\text{old}} + \frac{F(x)}{F'(x)}$$

The subsequent iterations utilize linear fractional interpolation until convergence occurs.

- (2) The total flow is compared to the target flow and the pressure drop is adjusted and the program returns to Step 1. The adjusted value on the first pass is the ratio of target flow to total flow times the initial pressure; on the second pass, the adjusted value of the pressure drop is the midpoint of the initial and first adjustment. Subsequent adjustments utilize linear fractional interpolation until convergence occurs.

The parameters which drive the iterative procedure are the changes in flow rate and temperature. Since these two parameters are interactive, the flow rate cannot be considered converged until the temperature is also converged.

III. DESCRIPTION OF HEXEREI TEST CASES

All test cases use the same geometric model as shown in Fig. III.1. All test cases are compared with analogous HEATING5 or CCCM models and, when possible, with analytical results. The heat conduction portion of HEXEREI was checked out by using the first six test cases. The seventh test case was used to check out the coolant calculations.

Test case number 1 uses the model in Fig. III.1 with linear material properties as shown in Table III.1. A constant volumetric heat generation was applied throughout the model and a constant boundary temperature was maintained on the outer radius of the right circular cylinder. The steady-state radial temperature distribution is compared to analytical and HEATING5 results in Fig. III.2. The analytical results were produced by Equation III.1 from Ref. 4.

Test case number 2 is different from number 1 only by the nonlinear material properties shown in Table III.1. The comparison with HEATING5 is presented in Fig. III.3.

Test case number 3 applied a constant center line and outer radius boundaries of different values to the model in Fig. III.1 with the linear properties. The comparison with HEATING5 and analytical results are shown in Fig. III.4. The analytical results were produced by using Equation III.2 from Ref. 5 with the temperature at a radius of .393 assumed to be constant. The inner radius was used since both HEXEREI and HEATING5's nodal temperature represent the average temperature of the cell surrounding the node. Test case number 4 is the same as 3 but with the nonlinear properties the comparison with HEATING5 is shown in Fig. III.5.

III.1 Cylindrical model used in test cases

TABLE III.1

LINEAR MATERIAL PROPERTIES

Conductivity - 10 BT/LR-FT °F
Specific Heat - .45 BTU/lbm °F
Density - 10 lbm/FT³

NONLINEAR MATERIAL PROPERTIES

Conductivity - $100 e^{(-.00005)T}$
Specific Heat - $45 e^{(-.00005)T}$
Density - $100 e^{(-.00005)T}$

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III.2 Comparison of radial temperature distribution. Test case number 1 (uniform heat generation, constant properties, constant boundary temperature)

III.3 Comparison of radial temperature distribution. Test case number 2 (uniform heat generation, nonlinear properties, constant boundary temperature)

III.4 Comparison of radial temperature distribution. Test case number 3 (constant properties, constant boundary temperatures, no heat generation)

III.5 Comparison of radial temperature distribution. Test case number 4 (constant properties, constant boundary temperatures, no heat generation)

Test case number 5 uses the linear properties on the model assuming a constant initial temperature. The outer radius boundary temperature is changed and the radial temperature distribution is calculated at various times during a 100-hour transient. Figures III.6 through III.10 present the comparison with HEATING5 and analytical results from Ref. 6.

Test case number 6 is the same as number 5 with the exception of using the nonlinear properties. HEXEREI's results are compared with HEATING5's in Fig. III.11 through III.13.

The above test cases exercise most of the different options available in HEXEREI and verify the validity of the code. In the steady-state test cases (1 through 4), the maximum temperature different from the analytical or HEATING5 results was 1.45%. Test case number 5 demonstrates a maximum temperature difference from the analytical of 3%. This larger error is due to the accumulated error along the transient. Test case number 6 demonstrates a maximum temperature difference with HEATING5 of $\sim 2\%$. In general, HEXEREI overestimates the conductivity by about 1-1/2%.

Test case number 7 exercises the coolant flow capability of HEXEREI without flow redistribution. The basic geometric model is the same as used in the above test cases (Fig. III.1). Only a portion of the hexagonal mesh cells have volumetric heat generation and these same cells have coolant flow. The heat generation and coolant flow are the same for each of the cells. Since the model is uniform, intercell conductances can be neglected because the thermal gradients will be small. Thus, an analogous test case for CCCM would be a model that has the same graphite heat capacity, heat generated, coolant mass flow rate, channel diameter, and inlet conditions as HEXEREI. Since HEXEREI lumps all of the channels in

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III.6 Comparison of radial temperature distribution. Test case number 5 (Transient, constant properties and boundary temperature, no heat generation)

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III.7 Comparison of radial temperature distribution. Test case number 5 (Transient, constant properties and boundary temperature, no heat generation)

III.8 Comparison of radial temperature distribution. Test case number 5 (Transient, constant properties and boundary temperature, no heat generation)

III.9 Comparison of radial temperature distribution. Test case number 5 (Transient, constant properties and boundary temperature, no heat generation)

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III.10 Comparison of radial temperature distribution. Test case number 5 (Transient, constant properties and boundary temperature, no heat generation)

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III.11 Comparison of radial temperature distribution. Test case number 6 (Transient, nonlinear properties, constant boundary temperature, no heat generation)

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III.12 Comparison of radial temperature distribution. Test case number 6 (Transient, nonlinear properties, constant boundary temperature, no heat generation)

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III.13 Comparison of radial temperature distribution. Test case number 6 (Transient, nonlinear properties, constant boundary temperature, no heat generation)

the same cell into one, the heat capacity, heat generation and mass flow rate must be developed from the HEXEREI model using the input number and size of coolant channels.

Figure III.14 compares axial coolant temperature distribution from CCCM with those from HEXEREI for a steady-state analysis. Figures III.15 through III.18 present the same type of comparison for a transient analysis. The steady-state results agree very well; however, the transient results show a maximum error of 3-1/2% for the coolant exit temperature.

Figure III.19 compares the volume average temperature from CCCM with HEXEREI's solid temperatures for the steady-state analysis and Figs. III.20 through III.23 present the same type of comparison for the transient analysis. Since HEXEREI neglects the possible temperature gradients in the graphite, the maximum difference of 6% indicates an area of possible reduced accuracy and improvement. Further investigation of this difference is necessary since it is uncertain if the difference is due to the coolant calculation technique differences or graphite temperature gradient treatment differences of the two codes.

In general, the good agreement of HEXEREI demonstrates the validity of the code in HTGR analysis.

III.14 Comparison of axial coolant temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation and coolant flow rate)

III.15 Comparison of axial coolant temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation and coolant flow rate)

III.16 Comparison of axial coolant temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation and coolant flow rate)

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III.17 Comparison of axial coolant temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation and coolant flow rate)

III.18 Comparison of axial coolant temperature distribution. Test case number 7 (transient, uniform and constant properties, heat generation and coolant flow rate)

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III.19 Comparison of axial solid temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation, and coolant flow rate). CCCM points are volume average temperatures

III.20 Comparison of axial solid temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation, and coolant flow rate). CCCM points are volume average temperatures

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III.21 Comparison of axial solid temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation, and coolant flow rate). CCCM points are volume average temperatures

III.22 Comparison of axial solid temperature distribution. Test case number 7 (Transient, uniform and constant properties, heat generation, and coolant flow rate). CCCM points are volume average temperatures

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III.23 Comparison of axial solid temperature distribution. Test case number 7 (transient, uniform and constant properties, heat generation, and coolant flow rate). CCCM points are volume average temperatures.

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