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HERESY III COMPUTER CODE

D. R. FINCH

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Savannah River Laboratory

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HERESY III COMPUTER CODE

by

D. R. Finch

Approved by

P. L. Roggenkamp, Research Manager
Theoretical Physics Division

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E. I. DU PONT DE NEMOURS & COMPANY
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ABSTRACT

The HERESY III computer code is a general-purpose two-dimensional reactor code based on the diffusion theory source-sink formalism developed by S. M. Feinberg. The code is applicable to calculations of reactivity, control rod worth, power ratios, and other similar calculations for heavy-water- and graphite-moderated reactors. Options within the code permit a variety of criticality searches to be performed. This report contains a derivation of the theory on which the code is based, a description of the features of the code and their use, and finally, the input and output required for use of the code.

CONTENTS

1. INTRODUCTION

The HERESY III code is based on the source-sink theory developed concurrently by Feinberg[1] and Galanin[2] for two-dimensional, heterogeneous reactor calculations. It assumes that reactor assemblies can be represented by line sources and line sinks, and further that lattice components that absorb a significant number of neutrons are separated from each other by a few mean free paths of moderator, so that diffusion theory may be used in the moderator region to compute interactions between components. This assumption is well satisfied in heterogeneous reactor lattices moderated by heavy water or graphite. Codes employing the Feinberg-Galanin (heterogeneous or source-sink) approach have been developed by numerous groups interested in these reactor types.

The type of reactor calculation that must be considered as an alternative to heterogeneous calculations for heavy-water-moderated reactors is two-dimensional diffusion theory. The preference between the two depends on the problem, or the reactor, being considered. The heterogeneous theory seems clearly preferable for reactors characterized by a small number of fuel and control assemblies in a rather irregular arrangement, such as engineering test reactors like the Heavy Water Components Test Reactor (HWCTR).[3] Repeating "cells" required in diffusion theory calculations are impossible to define for such reactors.

Several computer codes have been developed to take advantage of the attractive features of heterogeneous theory in practical reactor calculations. The HERESY III code has evolved from some of these. The HERESY I[4] and HERESY II[5] codes were written by C. N. Klahr and associates. A rewritten version of HERESY I, called SRL - HERESY I,[6] was developed at the Savannah River Laboratory and contained a number of additional convenience features. HERESY II differed from the previous version primarily in permitting a more detailed treatment of epithermal events, including epithermal fission. HERESY III, developed at SRL, was based on the HERESY II equations, and added a number of features which increased its flexibility and ease of use. Furthermore, algorithms that convert the output of the HAMMER[7] cell code to HERESY III input have been incorporated. The resulting system has been useful for a variety of design and analysis purposes.

2. SUMMARY

The HERESY III code calculates two-dimensional reactor lattices by the use of the heterogeneous reactor theory developed by Feinberg[1] and Galanin.[2] The code will perform calculations on finite lattices, with or without reflector, or infinite lattices of repeating "supercells." The lattice size is limited to a maximum of 5000 lattice assemblies and to 50 types of lattice locations possessing unique geometrical or flux symmetry properties. The allowed number of physically different lattice assemblies is 20.

The code solves for thermal and epithermal neutron absorptions in each lattice assembly. Both epithermal absorption and fission are allowed in all assemblies for an arbitrary number of resonance levels up to a maximum of nine. The edit of the solved problem produces lattice-averaged values of the resonance escape probability p, heterogeneous thermal utilization f, fast fission factor ε, average heterogeneous thermal η, epithermal η^r, and the leakage-corrected static reactivity coefficient k.

Options are available to use output from the HAMMER[7] system as direct input to the heterogeneous lattice calculations.

Four criticality searches permit variation of selected parameters in the calculation until criticality is achieved in the lattice. The variation may be made in the heterogeneous thermal utilization, heterogeneous thermal η, or all values of the heterogeneous η parameter of a specified group of physically identical lattice assemblies. A criticality search may also be made on the axial buckling of the lattice.

3. THEORY

3.1 GENERAL

The heterogeneous theory in HERESY III is based on the source-sink method developed by Feinberg[1] and Galanin.[2] The notation used in this report is that of Feinberg.

The source-sink method separates the solution of the heterogeneous reactor critical equation into three logically distinct steps:

- Represent the reactor lattice as a set of axially infinite line sources and sinks of neutrons.
- Specify the interaction between each line source-sink and all other line source-sinks in the lattice.
- Assign suitable nuclear parameters to each line source-sink, combine these parameters with the specified interactions, and obtain from the heterogeneous critical equation the distribution of neutron absorptions in sinks and the static reactivity coefficient for the lattice.

The assemblies of a real reactor lattice are assumed to be adequately represented by the line source-sinks described above. This approximation is plausible providing a few mean free paths of moderator separate the surfaces of the assemblies. The lattice itself is described by providing the X and Y coordinates of each rod relative to an arbitrary origin.

The interactions between rods in the lattice are given by infinite medium, age-diffusion kernels. Corrections necessary to permit a reflector of finite thickness to be included will be discussed in Section 3.3.

Absorptions in rods are assumed to occur only at discrete neutron energies specified by a series of neutron ages τ^1, τ^2, τ^3, ..., τ from fission energy. Fission neutrons may be produced from an absorption at any of these discrete neutron energies (referred to as levels), and neutrons so produced appear at the source energy.

3.2 CRITICAL EQUATION

The heterogeneous source-sink critical equation is obtained from neutron conservation by summing the contribution of neutrons from all rods in the lattice to each individual rod at thermal energy. For the moment, an infinite reflector will be assumed, although this restriction will be removed later. Two assumptions are involved in this summation:

- The moderator and reflector properties are constant (independent of space).
- The interaction between rods may be adequately described by infinite medium kernels dependent only on the separation of the rod centers and the slowing down and diffusion parameters of the moderator.

First, a set of spatial distributions (or kernels) will be defined which depend only on moderator properties. These are understood to be age-diffusion expressions for both thermal flux and slowing down density in infinite media, although their explicit form will not be given until later. Sources for these distributions are all infinite line sources. These distributions have two subscripts, the second referring to the source positions and the first to the field or receptor position; each implies an X-Y coordinate. Superscripts represent epithermal energies. As implied by the dependence on moderator properties only, no absorption in "rods" is taken into account. Next a set of rod properties will be defined. From the above two sets, a set of derived spatial distributions will be obtained. Finally, the critical equation will be written in terms of the above quantities.

Moderator Distributions

q^{r}_{jk} $\equiv$ slowing down density, at energy denoted by r, at rod j due to a unit (1 neutron/cm-sec) source of fission neutrons at rod k

$q^{r\to s}_{jk}$ $\equiv$ slowing down density, at energy denoted by s, at rod j due to a unit source of neutrons of energy denoted by r at rod k

F_{jk} $\equiv$ thermal flux at rod j due to a unit source of fission neutrons at rod k

F^{r}_{jk} $\equiv$ thermal flux at rod j due to a unit source of neutrons of energy denoted by r at rod k

f_{jk} $\equiv$ thermal flux at rod j due to a unit source of thermal neutrons at rod k

Rod Properties

$$\gamma_n \equiv \phi_n(R_n)/i_n \tag{3.1}$$

where $\phi_n(R_n)$ is the total thermal flux at a distance R_n (the effective radius of the n^{th} rod) from the center of the n^{th} rod.† This is the flux that would be calculated at this location using source-sink distributions and taking all interactions into account. i_n is the number of thermal neutrons absorbed by the n^{th} rod per second.

$$A_n^r \equiv i_n^r/q_n^{*r} \tag{3.2}$$

where q_n^{*r} is the slowing down density, at energy denoted by r, at rod n. This is the value that would be calculated at this location using source-sink distributions and taking all interactions at higher energies into account.

$i_n^r \equiv$ number of neutrons absorbed at energy level r by the n^{th} rod per second

$\eta_n \equiv$ number of fission neutrons produced per thermal neutron absorbed in the n^{th} rod

$\eta_n^r \equiv$ number of fission neutrons produced per neutron absorbed at energy level r in the n^{th} rod

Methods of obtaining values for the above rod properties will be discussed in Section 3.4.

Derived Moderator Distributions

The intent here is to obtain expressions for both slowing down densities and the thermal fluxes which take into account absorptions in rods at all energies higher than the energy being considered. An expression for the slowing down density is obtained by assuming that the slowing down density at energy level r is a source contribution minus the sum of sink contributions from all levels higher in energy than r. Thus

$$q_{jk}^{*r} = q_{jk}^r - \sum_{s=1}^{r-1} \sum_{t=1}^{N} q_{jt}^{s\to r} A_t^s q_{tk}^{*s} \tag{3.3}$$

† This is the historical definition. It is shown in equation (3.19) that rod absorption properties may be cast into a form independent of the rod radius or the assembly radius.

where q^{*r}_{jk} is the desired corrected distribution, and N is the total number of rods in the lattice; and other quantities have already been defined. For the highest energy level (s = 1), $q^{*1}_{jk} = q^{1}_{jk}$. From q^{*1}_{jk}, the corrected distribution q^{*2}_{jk} can be obtained. By successively utilizing the corrected distributions for each of the higher levels, all corrected distributions can be obtained via equation (3.3). The $q^{s\to r}_{jt}$ term in equation (3.3) does not, and properly should not, account for interactions at levels between s and r, because the source term q^{r}_{jk} from which the corrections are being subtracted ignores all interactions at levels with $\tau < \tau^{r}$.

The second derived distribution that is required is an expression F^{*}_{jk} for the thermal flux which similarly accounts for all epithermal absorptions in rods. In analogy to equation (3.3).

$$F^{*}_{jk} = F_{jk} - \sum_{r=1}^{P} \sum_{t=1}^{N} F^{r}_{jt} A^{r}_{t} q^{*r}_{tk} \qquad (3.4)$$

where P is the total number of epithermal absorption levels. F^{r}_{jt} does not (as is clear from its definition) and should not account for rod absorptions between the r^{th} epithermal absorption and thermal levels.

Critical Equation

From the parameters and distributions defined and discussed above, the critical equation is

$$\gamma_n i_n = \frac{1}{k} \sum_{j=1}^{N} F^{*}_{nj} \left(\eta_j i_j + \sum_{r=1}^{P} \eta^{r}_{j} i^{r}_{j} \right) - \sum_{j=1}^{N} f_{nj} i_j \qquad (3.5)$$

where k is the eigenvalue or criticality factor, playing the same role in heterogeneous theory as it does in more conventional formulations. The left-hand side is the thermal flux at the radius of the n^{th} rod; the first summation over j on the right-hand side is the contribution of sources to the thermal flux at the n^{th} rod; the second summation is the contribution to depression of thermal flux at the n^{th} rod by thermal neutron absorptions in all rods.

Thus far no advantage has been taken of possible symmetry properties of the lattice. Many problems in practice have high degrees of symmetry, and the number of terms in the summations in equation (3.5) can be considerably reduced by taking advantage of that fact. Two terms applied to rods will be defined at this

point. Rods are of the same rod "kind" if they have identical physical properties. Rods are of the same rod "type" if they are of the same "kind" and have the same symmetry properties, such that it is known *a priori* that they will have the same reaction rates. Because all rods of the same type have the same i_j and i_j^r, a preliminary summation may be made over the source index j in equation (3.5) for each rod type. Thus, the summation limit N is reduced to the number of rod types rather than the number of rods; equation (3.5) is solved by the HERESY III code. The matrix formulation used is described in Section 3.7.

3.3 Moderator Spatial Distributions

Specific functional forms will now be assigned to the spatial distributions discussed symbolically in the previous section. Age-diffusion theory is the model used. The standard age solution for q_{jk}^r is

$$q_{jk}^r = \frac{1}{4\pi\tau^r} \exp - \frac{|\underline{r}_j - \underline{r}_k|^2}{4\tau^r} \tag{3.6}$$

where τ^r is the Fermi age from fission source energy ($\tau = 0$) to the r^{th} energy level (at age τ^r). The code, as discussed in Section 4, actually permits the flexibility of specifying a weighted sum of three such Gaussians. The remainder of the theory section will, however, ignore this because (a) it is a trivial extension of the single distributions, and (b) this flexibility has not proved particularly useful.

The next defined moderator distribution is given in a similar fashion

$$q_{jk}^{r\to s} = \frac{1}{4\pi(\tau^s - \tau^r)} \exp - \frac{|\underline{r}_j - \underline{r}_k|^2}{4(\tau^s - \tau^r)} \tag{3.7}$$

The next distribution, F_{jk}, was given by Galanin.[8] In infinite series form

$$F_{jk} = \frac{1}{2\pi D} e^{\tau/L^2} \left[K_0\left(\frac{|\underline{r}_j - \underline{r}_k|}{L}\right) - \frac{1}{2} \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left(\frac{\tau}{L^2}\right)^n E_{n+1}\left(\frac{|\underline{r}_j - \underline{r}_k|^2}{4\tau}\right) \right] \tag{3.8}$$

where D is the moderator thermal diffusion coefficient, τ is the Fermi age from source energy to thermal, L^2 is the moderator diffusion area corrected for transverse leakage, K_0 is the modified Bessel function of the second kind, and E_m is the exponential integral[9] function of order m. This series converges rapidly if τ/L^2 is small (a condition met in heavy water and graphite moderators). Truncating terms higher than n = 1 gives

$$F_{jk} = \frac{1}{2\pi D} e^{\tau/L^2} \left[K_0\left(\frac{|\underline{r}_j - \underline{r}_k|}{L}\right) + \frac{\tau}{2L^2} e^{-\frac{|\underline{r}_j - \underline{r}_k|^2}{4\tau}} - \frac{1}{2}\left(1 + \frac{|\underline{r}_j - \underline{r}_k|^2}{4L^2}\right) E_1\left(\frac{|\underline{r}_j - \underline{r}_k|^2}{4\tau}\right) + \cdots \right] \tag{3.9}$$

The F^r_{jk} distribution is identical to the above, with τ replaced by $(\tau - \tau^r)$, the age from the r^{th} energy level to thermal.

Finally, the f_{jk} distribution is the standard diffusion theory solution

$$f_{jk} = \frac{1}{2\pi D} K_0\left(\frac{|\underline{r}_j - \underline{r}_k|}{L}\right) \tag{3.10}$$

All of the above distributions are age-diffusion solutions for a line source in an infinite medium.

Transverse leakage (i.e., leakage in the direction parallel to the line sources) is taken into account in a straightforward fashion.[10] All distributions which involve fast leakage (i.e., all but equation 3.10) are multiplied by $\exp(-\Delta\tau B_Z^2)$, where B_Z^2 is the transverse buckling, and $\Delta\tau$ is the age difference appropriate to the particular distribution. The correction factor for equation (3.6) would have $\Delta\tau = \tau^r$; for equation (3.7), $\Delta\tau = \tau^s - \tau^r$; for equation (3.8), $\Delta\tau = \tau$; and for F^r_{jk}, $\Delta\tau = \tau - \tau^r$. In addition, in all expressions involving the moderator thermal diffusion area, L^2, the standard diffusion theory substitution is made

$$\Sigma_a' = \Sigma_a + DB_Z^2 \tag{3.11}$$

where Σ_a is the normal moderator macroscopic cross section, and Σ_a' is the value used to obtain the corrected diffusion area: i.e., $L^{2'} = L^2/(1 + L^2B_Z^2)$.

The procedures above correct for transverse leakage, but it has still been assumed that the moderator is infinite in the radial direction. This is adequate for treating infinitely repeating supercells, the central regions of large reactors, and reactors with very thick reflectors. In order to treat finite lattices with thin reflectors, the approximate method used by Klahr[4,5] in HERESY I and HERESY II has been used. This method employs an imaging technique in which each rod in the lattice is treated as having an image rod outside the reflector boundary. The image rod is located on a line passing through the center of the lattice and the real rod, and the image rod is located the same distance outside the reflector boundary as the real rod is inside the reflector boundary. The image rod is weighted by a negative source strength factor of $\sqrt{\rho_0/\rho_i}$, where ρ_i is the distance of the image rod from the reactor center and ρ_0 is the distance of the real rod from the reactor center. When the above technique is applied to one-region reactors with very thin reflectors, the flux does not extrapolate to zero at exactly the specified reflector boundary. This simply reflects the approximate nature of the image technique.

3.4 Rod Properties

The procedure to be described assumes that multigroup cell calculations are available for each of the rod kinds, although the cell area may be somewhat arbitrary. The rod properties are then related to cell-averaged properties (such as the cell-averaged thermal absorption cross section) and the cell area. Such an approach may seem contrary to the spirit of the source-sink method. However, a number of advantages accrue to it:

- Hundreds of man-years have gone into the development of sophisticated cell codes. It is only prudent to take advantage of this in the most natural fashion.

- Errors made in assigning values to the moderator properties discussed in the previous section tend to cancel out if this approach is taken.[4,11]

- The adequacy of the source-sink method for a given problem can be evaluated, to some extent, by examining the resulting variation in rod properties as a function of cell area. Ideally, they should be independent of this quantity.

The general procedure is to write the source-sink equations being used, equation (3.5) in our case, for a uniform lattice infinite in all directions, evaluate the resulting equation, and make the proper identification of the result with the result of cell calculations.

3.5 Thermal Parameters γ and η

Klahr showed[4,12] that for purposes of relating γ to thermal cell parameters, epithermal events in equation (3.5) can be ignored, and the simpler equation used in the original papers[1,2] can be used without significant error. Physically this amounts to concluding that, for infinite uniform lattices, epithermal events do not significantly affect the source distribution entering the thermal group. Under these circumstances equation (3.5) reduces to[1]

$$\gamma = \frac{1}{f} \sum_{j}^{\infty} F_{nj} - \sum_{j}^{\infty} f_{nj} \tag{3.12}$$

where f is the heterogeneous thermal utilization factor, i.e., absorption in rod divided by absorption in cell. The infinite sums have been evaluated analytically.[1,13] For $L^2/V \gtrsim 3$, where V = cell area

$$\sum_{j}^{\infty} F_{nj} = \frac{1}{V\Sigma_a} \tag{3.13}$$

$$\sum_{j}^{\infty} f_{nj} = \frac{1}{V\Sigma_a}\left[1 + \frac{V}{4\pi L^2}\left(\ln \frac{V}{\pi R^2} - C\right)\right] \tag{3.14}$$

where

$$C = \begin{cases} 1.5 \text{ for a cylindrical cell} \\ 1.4975 \text{ for a hexagonal cell} \\ 1.4763 \text{ for a square cell} \end{cases}$$

R is the rod radius, and other symbols are as defined before. Substituting equations (3.13) and (3.14) into (3.12) yields

$$\gamma = \frac{1}{V\Sigma_a} \frac{(1-f)}{f} - \frac{1}{4\pi D}\left(\ln \frac{V}{\pi R^2} - C\right) \tag{3.15}$$

The above expression has been obtained previously.[2] The presence in this expression of the heterogeneous thermal utilization factor may seem ambiguous when the fuel assembly is complex, rather than a single rod. This ambiguity is removed by observing that in the reactor model, moderator fills the entire space and rod absorptions occur in a line. Hence

$$\frac{1-f}{f} = \frac{\Sigma_a}{\Sigma_a(\text{eff}) - \Sigma_a} \tag{3.16}$$

where $\Sigma_a(\text{eff})$ is the normally defined homogenized thermal absorption cross section of the cell, and Σ_a is the moderator absorption cross section. Thus

$$\gamma = \frac{1}{V(\Sigma_a(\text{eff}) - \Sigma_a)} - \frac{1}{4\pi D}\left(\ln \frac{V}{\pi R^2} - C\right) \tag{3.17}$$

The above expression is the desired one for relating the rod properties γ and R to the cell properties $\Sigma_a(\text{eff})$ and V (and moderator properties). However, one may go further and eliminate the radius R from the formalism altogether.

In equation (3.12), all terms on the right-hand side except f_{nn} may be evaluated using center-to-center distances (F_{nn} is quite flat near r = 0). However, the K_0 Bessel function is singular at r = 0. It is this fact which led to the introduction of the radius R in the first place. If this term is taken to the left,

$$\gamma + f\left(\frac{R}{L}\right) = \frac{1}{f}\sum_j^{\infty} F_{nj} - \sum_j^{\infty\,\prime} f_{nj} \tag{3.18}$$

where the prime denotes the absence of the j = n term. All of the equations for the general case, equation (3.5), can likewise be written this way, with all of the terms on the right-hand side being evaluated on the basis of center-to-center distances. Because $\gamma + f(R/L)$ always appears in this form, the combination may be regarded as a new rod parameter, δ, and evaluated accordingly. Adding and subtracting $(1/2\pi D)[K_0(R/L)]$ to both sides of equation (3.15) and passing the right-hand side to the limit $R \to 0$ yield

$$\delta = \frac{1}{V\Sigma_a} \cdot \frac{1-f}{f} + \frac{1}{4\pi D}\left[\ln\left(\frac{L^2}{V}\right) + C'\right] \tag{3.19}$$

where

$$C' = \begin{cases} 2.874 \text{ for a hexagonal lattice} \\ 2.853 \text{ for a square lattice} \end{cases}$$

If the transverse buckling is non-zero, Σ_a and L^2 should be the primed values, as in equation (3.11). In the first term of equation (3.19), however, it is merely necessary to be consistent; i.e., the uncorrected value of Σ_a may be used provided (1-f) also corresponds to zero transverse buckling.

The production term η is obtained from

$$\eta = \frac{(\eta f)_{cell}}{f} \tag{3.20}$$

where f is obtained from equation (3.16).

3.6 Epithermal Parameters A and η^r

Again it is assumed that cell calculations have been run for all rod kinds to be considered, and that the epithermal cell homogenized cross sections have been collapsed to a few group form. Specifically, values of $p_s = (\Sigma_r)^s/(\Sigma_r + \Sigma_a)^s$ and $\eta^s = (\nu\Sigma_f)^s/(\Sigma_a)^s$ are assumed available, where s indicates the energy group number. Then values of η^s may be used directly in equation (3.5). However, a relationship must be demonstrated between p_s (and the cell area V) and the heterogeneous parameters A^s.

Figure 3-1 illustrates the epithermal energy structure for an example of three epithermal groups.

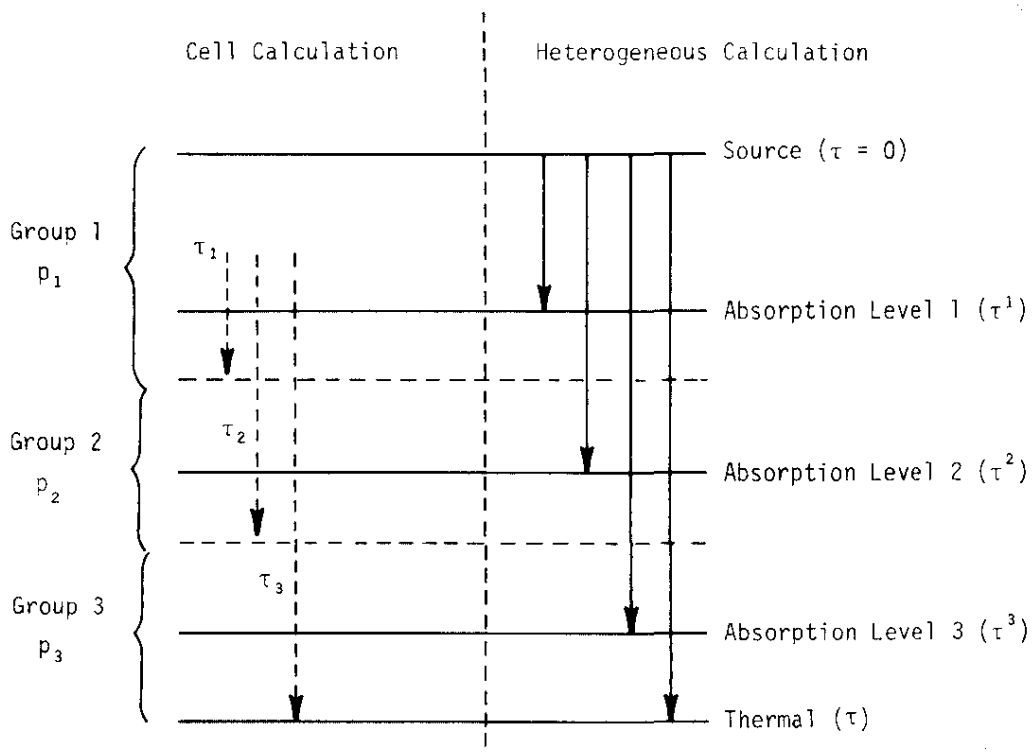

FIGURE 3-1 Epithermal Energy Structure

The absorption levels in the heterogeneous calculation are discrete, in the sense of each being characterized by a single effective value of τ^r. In the following discussion, it is assumed that single Gaussians with their associated τ^r characterize the slowing down distributions. (The code permits a more general specification, but the complication in notation is unwarranted here.) On physical grounds, it is required that $\tau^{n-1} < \tau^n < \tau^{n+1}$, but no more stringent condition on τ^n is required.

The heterogeneous case to be considered is an infinite uniform lattice. Hence no question of interaction between fast leakage and epithermal capture arises. For this condition, the cell calculated values of p_n are related to the following quantity in heterogeneous terms:

$$p_1\ p_2\ \cdots\ p_n = \frac{\text{Number of neutrons slowing down to level } n+1 \text{ with absorptions in levels 1 to } n}{\text{Number of neutrons slowing down to level } n+1 \text{ without absorptions in levels 1 to } n} \tag{3.21}$$

When n is the lowest epithermal absorption level, it is convenient to modify the above identification to

$$p_1\ p_2\ \cdots\ p_n = \frac{\text{Thermal flux with absorptions in levels 1 to } n}{\text{Thermal flux without absorptions in levels 1 to } n} \tag{3.22}$$

The one-epithermal group case will be considered first because of its simplicity. Later three-epithermal groups will be considered. For one-epithermal group, equations (3.4) and (3.22) yield

$$p = \frac{\sum_k^\infty F^*_{jk}}{\sum_k^\infty F_{jk}} = 1 - \frac{\sum_k^\infty \sum_t^\infty F^r_{jt}\ A_t\ q^r_{tk}}{\sum_k^\infty F_{jk}} \tag{3.23}$$

or

$$p = 1 - A\ \frac{\sum_t^\infty F^r_{jt} \sum_k^\infty q^r_{tk}}{\sum_k^\infty F_{jk}} \tag{3.24}$$

The infinite sum $\sum_k q_{tk}^r$ can be expressed conveniently in terms of a dimensionless function T defined by

$$T \equiv V \sum^{\infty} q^r \tag{3.25}$$

Since all rods are identical, equation (3.24) may be written using (3.25) as

$$p = 1 - \frac{AT}{V} \frac{\sum_t^{\infty} F_{jt}^r}{\sum_k^{\infty} F_{jk}} \tag{3.26}$$

From equation (3.13), the summations over t and k cancel even though different values of τ are used in the distributions, leaving

$$p = 1 - \frac{A}{V} T \tag{3.27}$$

or

$$A = (1 - p)V/T \tag{3.28}$$

This is the required connecting formula between cell properties and rod properties. The remaining problem is the evaluation of the infinite sum T. This is carried out by the use of the Poisson summation formula in the usual way. For rhombic cells with acute angle θ, the result is

$$T\left(\frac{\tau^r}{V}, \theta\right) = \sum_{\lambda=-\infty}^{\infty} \sum_{\nu=-\infty}^{\infty} \exp - \frac{4\pi^2\tau^r(\nu^2 + 2\nu\lambda \cos\theta + \lambda^2)}{V \sin\theta} \tag{3.29}$$

This function is tabulated in Appendix A for square lattices ($\theta = 90°$) and triangular lattices ($\theta = 60°$). The dependence on θ is weak, and this argument will be omitted as a notational convenience. For values of $\tau^r/V > 0.2$, T is essentially unity. For smaller values it is >1 and plays the role of a "resonance advantage factor," peaking the slowing down distribution at the source location. For a triangular lattice, the leading terms are

$$T\left(\frac{\tau^r}{V}\right) = 1 + 6\ \exp\left(-\frac{8\pi^2\tau^r}{\sqrt{3}\ V}\right) + 6\ \exp\left(-\frac{24\pi^2\tau^r}{\sqrt{3}\ V}\right) + \ldots \qquad (3.30)$$

For more than one epithermal energy group, capture at higher energies influences events at lower epithermal energies, and the equations become correspondingly more complex. For all but the lowest epithermal level, equation (3.21) gives

$$p_1\ p_2 \cdots p_r = \frac{\sum_k^\infty q_{jk}^{*r+1}}{\sum_k^\infty q_{jk}^{r+1}} \qquad (3.31)$$

And for the lowest level,

$$p_1\ p_2 \cdots p_r = \frac{\sum_k^\infty F_{jk}^*}{\sum_k^\infty F_{jk}} \qquad (3.32)$$

Substituting equations (3.3) and (3.4) into (3.31) and (3.32), respectively, yields

$$p_1\ p_2 \cdots p_r = 1 - \frac{\sum_k^\infty \sum_{s=1}^r \sum_t^\infty q_{jt}^{s\to r+1}\ A_t^s\ q_{tk}^{*s}}{\sum_k^\infty q_{jk}^{r+1}} \qquad (3.33)$$

where r is not the lowest epithermal level, and

$$p_1\ p_2 \cdots p_r = 1 - \frac{\sum_k^\infty \sum_{s=1}^r \sum_t^\infty F_{jt}^s\ A_t^s\ q_{tk}^{*r}}{\sum_k^\infty F_{jk}} \qquad (3.34)$$

where r is the lowest epithermal level. Following the same methods used previously leads to the following equations

$$p_1\ p_2\ \cdots\ p_r \;=\; 1 - \sum_{s=1}^{r} \frac{A^s g^s_{r+1}}{V} \tag{3.35}$$

$$g^s_{r+1} \;=\; \frac{T\left(\frac{\tau^{r+1}-\tau^s}{V}\right)\left[T\left(\frac{\tau^s}{V}\right) - \sum_{k=1}^{s-1} \frac{A^k}{V}\, T\left(\frac{\tau^s-\tau^k}{V}\right) T\left(\frac{\tau^k}{V}\right)\right]}{T\left(\frac{\tau^{r+1}}{V}\right)} \tag{3.36}$$

where r is not the lowest epithermal level, and

$$g^s_{r+1} \;=\; T\left(\frac{\tau^s}{V}\right) - \sum_{k=1}^{s-1} \frac{A^k}{V}\, T\left(\frac{\tau^s-\tau^k}{V}\right) T\left(\frac{\tau^k}{V}\right) \tag{3.37}$$

where r is the lowest epithermal level. The argument θ has been omitted in the T function, because it is assumed all cells are the same type.

For three epithermal groups, a common choice, the explicit results are

$$(1-p_1)V \;=\; A^1\, g^1_2$$

$$g^1_2 \;=\; \frac{T\left(\frac{\tau^2-\tau^1}{V}\right) T\left(\frac{\tau^1}{V}\right)}{T\left(\frac{\tau^2}{V}\right)} \tag{3.38}$$

$$(1-p_1p_2)V \;=\; A^1\, g^1_3 + A^2\, g^2_3$$

$$g^1_3 \;=\; \frac{T\left(\frac{\tau^3-\tau^1}{V}\right) T\left(\frac{\tau^1}{V}\right)}{T\left(\frac{\tau^3}{V}\right)}$$

$$g^2_3 \;=\; \frac{T\left(\frac{\tau^3-\tau^2}{V}\right)\left[T\left(\frac{\tau^2}{V}\right) - \frac{A^1}{V}\, T\left(\frac{\tau^2-\tau^1}{V}\right) T\left(\frac{\tau^1}{V}\right)\right]}{T\left(\frac{\tau^3}{V}\right)} \tag{3.39}$$

$$(1-p_1p_2p_3)V = A^1 g_4^1 + A^2 g_4^2 + A^3 g_4^3$$

$$g_4^1 = T\left(\frac{\tau^1}{V}\right)$$

$$g_4^2 = T\left(\frac{\tau^2}{V}\right) - \frac{A^1}{V} T\left(\frac{\tau^2-\tau^1}{V}\right) T\left(\frac{\tau^1}{V}\right)$$

$$g_4^3 = T\left(\frac{\tau^3}{V}\right) - \frac{A^1}{V} T\left(\frac{\tau^3-\tau^1}{V}\right) T\left(\frac{\tau^1}{V}\right) - \frac{A^2}{V} T\left(\frac{\tau^3-\tau^2}{V}\right) T\left(\frac{\tau^2}{V}\right) \qquad (3.40)$$

3.7 Method of Solving the Heterogeneous Critical Equation

Once moderator properties, rod properties, and geometry have been assigned, the problem is reduced to the solution of equation (3.5), a set of N linear equations in N unknowns, where N is the number of "rod types." The equations are cast in the form of a matrix eigenvalue problem for numerical solution. Equations (3.3) and (3.4) in matrix form are

$$\underline{\underline{Q}}^{*r} = \underline{\underline{Q}}^{r} - \sum_{s=1}^{r-1} \underline{\underline{Q}}^{s\to r} \underline{\underline{A}}^{s} \underline{\underline{Q}}^{*s} \qquad (3.41)$$

and

$$\underline{\underline{T}} = \underline{\underline{G}} - \sum_{r=1}^{P} \underline{\underline{G}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \qquad (3.42)$$

where

$$\underline{\underline{Q}}^{s\to r} \equiv \left\{q_{nj}^{s\to r}\right\},\ \underline{\underline{Q}}^{*s} \equiv \left\{q_{nj}^{*s}\right\},\ \underline{\underline{Q}}^{r} \equiv \left\{q_{nj}^{r}\right\},$$

$$\underline{\underline{G}} \equiv \left\{F_{nj}\right\},\ \underline{\underline{G}}^{r} \equiv \left\{F_{nj}^{r}\right\},\ \text{and}\ \underline{\underline{T}} \equiv \left\{F_{nj}^{*}\right\}$$

are all square matrices and $\underline{\underline{A}}^{r} \equiv \left\{A_{jj}^{r}\right\}$ is a diagonal matrix, all of order N. In terms of these the initial equation, (3.5), becomes

$$\underline{\underline{\Gamma}} \cdot \underline{i} = \frac{1}{k} \underline{\underline{T}} \cdot \left\{ \underline{\underline{\eta}} \cdot \underline{i} + \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{i}^{r} \right\} - \underline{\underline{D}} \cdot \underline{i} \qquad (3.43)$$

where

$\underline{\underline{D}} \equiv \left\{ f_{nj} \right\}$ is a square matrix; $\underline{\underline{\Gamma}} \equiv \left\{ \gamma_{jj} \right\}$,

$\underline{\underline{\eta}} \equiv \left\{ \eta_{jj} \right\}$ and $\underline{\underline{\eta}}^{r} \equiv \left\{ \eta_{jj}^{r} \right\}$ are diagonal matrices;

$\underline{i} \equiv \left\{ i_{j} \right\}$ and $\underline{i}^{r} \equiv \left\{ i_{j}^{r} \right\}$ are column vectors; and

k is a scalar (the eigenvalue).

In solving equation (3.43), the following expression for the epithermal absorption in level r is used:

$$\underline{i}^{r} = \frac{1}{k} \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \cdot \left\{ \underline{\underline{\eta}} \cdot \underline{i} + \sum_{s=1}^{P} \underline{\underline{\eta}}^{s} \cdot \underline{i}^{s} \right\} \qquad (3.44)$$

Multiply equation (3.44) by $\underline{\underline{\eta}}^{r}$ and sum over r to yield

$$\sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{i}^{r} = \frac{1}{k} \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

$$+ \frac{1}{k} \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \cdot \left\{ \sum_{s=1}^{P} \underline{\underline{\eta}}^{s} \cdot \underline{i}^{s} \right\}$$

Solving this equation for $\sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{i}^{r}$ yields

$$\sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{i}^{r} = \left\{ \underline{\underline{I}} - \frac{1}{k} \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \right\}^{-1} \cdot \frac{1}{k} \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

where $\underline{\underline{I}}$ is the identity matrix.

Defining now the matrix $\underline{\underline{R}}$ as

$$\underline{\underline{R}} \equiv \frac{1}{k} \sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \tag{3.45}$$

so that

$$\sum_{r=1}^{P} \underline{\underline{\eta}}^{r} \cdot \underline{i}^{r} = \left\{\underline{\underline{I}} - \underline{\underline{R}}\right\}^{-1} \cdot \underline{\underline{R}} \cdot \underline{\underline{\eta}} \cdot \underline{i} \tag{3.46}$$

Substituting this sum into equation (3.43) gives

$$\underline{\underline{\Gamma}} \cdot \underline{i} = \frac{1}{k} \underline{\underline{T}} \cdot \left\{\underline{\underline{\eta}} \cdot \underline{i} + (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{R}} \cdot \underline{\underline{\eta}} \cdot \underline{i}\right\} - \underline{\underline{D}} \cdot \underline{i}$$

or

$$\left\{\underline{\underline{\Gamma}} + \underline{\underline{D}}\right\} \cdot \underline{i} = \frac{1}{k} \underline{\underline{T}} \cdot \left\{\underline{\underline{I}} + (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{R}}\right\} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

But

$$\underline{\underline{I}} + (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{R}} = (\underline{\underline{I}} - \underline{\underline{R}})^{-1}$$

so that

$$\left\{\underline{\underline{\Gamma}} + \underline{\underline{D}}\right\} \cdot \underline{i} = \frac{1}{k} T \cdot (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

Rewriting this gives

$$k \, \underline{i} = (\underline{\underline{\Gamma}} + \underline{\underline{D}})^{-1} \cdot \underline{\underline{T}} \cdot (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

Define a new matrix

$$\underline{\underline{A}} = (\underline{\underline{\Gamma}} + \underline{\underline{D}})^{-1} \cdot \underline{\underline{T}} \cdot (\underline{\underline{I}} - \underline{\underline{R}})^{-1} \cdot \underline{\underline{\eta}} \tag{3.47}$$

so that

$$k \, \underline{i} = \underline{\underline{A}} \cdot \underline{i} \tag{3.48}$$

Equation (3.48) is a standard eigenvalue problem from which the eigenvector $\underline{i}$ may be found to an arbitrary normalization, and k may be found as the largest eigenvalue of the matrix $\underline{\underline{A}}$. However, it may be noted that the definition of the matrix $\underline{\underline{R}}$ given in equation (3.45) contains k in each element of the matrix. To obtain the solution an iterative procedure is used. An initial guess is used for k and matrix $\underline{\underline{R}}$ is formed using it. The solution is then carried through equation (3.48) where a new k is obtained. The new k is used to re-form matrix $\underline{\underline{R}}$ and the process is repeated. An inner eigenvalue iteration is defined to be the iteration necessary to solve equation (3.48) for a given $\underline{\underline{R}}$ matrix. An outer eigenvalue iteration is defined to be the sequence of steps from the formation of matrix $\underline{\underline{R}}$ to the next formation of matrix $\underline{\underline{R}}$ for a new k.

The steps necessary to perform the solution are shown in the following list:

1. Form the $\underline{\underline{T}}$ matrix.
2. Initialize k and $\underline{i}$.
3. Form $(\underline{\underline{T}} + \underline{\underline{D}})$ matrix and invert.
4. Form $\underline{\underline{R}}$ matrix, $(\underline{\underline{I}} - \underline{\underline{R}})$ matrix, and invert to get $(\underline{\underline{I}} - \underline{\underline{R}})^{-1}$.
5. Form $\underline{\underline{A}}$ matrix.
6. Solve eigenvalue problem for k and $\underline{i}$.
7. Repeat steps 4, 5, and 6 until k and $\underline{i}$ have converged.

4. CODE DESCRIPTION

4.1 GENERAL

The HERESY III code is divided into three major parts. The first part contains an executive routine that

- Assigns parameter values where called for
- Performs rod parameter conversion
- Directs the code to the proper sequence of computation

The second part contains the lattice geometry and matrix generators that

- Generate lattice rod coordinates from simplified input
- Optionally plot, print, or punch cards containing the lattice rod coordinates
- Generate all necessary matrices

The third part contains the routines necessary to

- Solve the heterogeneous source-sink critical equation (3.43)
- Perform criticality searches on specified parameters
- Edit the results of the problem to provide lattice averaged parameters. The edit routine is discussed in Section 5.

In the operation of the code, data are read in the first part as described above. These data are stored in memory and are available for use by all parts of the code. If these data are altered in any part of the calculation (as would happen in a criticality search) the data are updated to reflect these changes. Because of this storage feature, it is only necessary to enter changes to the current data for problems after the initial problem. Information on how to enter data is given in Section 6.

The size limitations on problems that may be solved by HERESY III are the following:

Maximum number of "rod types"	=	50
Maximum number of "rod kinds"	=	20
Maximum number of rods in lattice	=	5000
Maximum number of epithermal levels	=	9

4.2 LATTICE GEOMETRY GENERATORS

The lattice rod coordinate generators in HERESY III contain provisions for both radially finite and radially infinite lattices. They are designed to accept a minimum amount of information about the desired lattice and to produce the X and Y coordinates (in centimeters) of each rod in the lattice.

Options are available to plot the rods on a rectangular grid, to list the rods by "rod type," and, for finite lattices, to punch out a set of cards containing the rod coordinates which may be reloaded with the normal input data.

4.2.1 Finite Lattices

Three generators are used to generate lattices of finite radial extent having respectively 60° rotational symmetry, 90° rotational symmetry, or patterns of rods equally spaced on circles about the center axis of the reactor. These will be described separately.

Hexagonal Lattices

A lattice having 60° rotational symmetry requires for input the X and Y coordinates of each rod with angles (with respect to the positive X axis) in the range $0 \leqslant \theta < 60°$. The generator then supplies the coordinates of the remaining five rods equally spaced at 60° angular intervals from the original rod. In large hexagonal lattices, however, 12 rods of the same "rod type" may occur at the same radius. To allow for this the hexagonal generator will optionally accept up to three rods in the range $0 \leqslant \theta < 60°$ as being of the same "rod type."

Square Lattices

A lattice having 90° rotational symmetry and reflection symmetry about 45° requires for input the X and Y coordinates of each rod with angles (with respect to the positive X axis) in the range $0 \leq \theta < 45°$. The generator then supplies the coordinates of the remaining rods at the same radius from the center of the reactor located at angles θ, $\pi/2 - \theta$, $\pi/2 + \theta$, $\pi - \theta$, $\pi + \theta$, $3\pi/2 - \theta$, $3\pi/2 + \theta$, and $2\pi - \theta$. (Rods falling at multiples of 45° are included only once.) A similar option is included for square lattices as for hexagonal lattices to allow up to three rods in the sector $0 \leq \theta < 45°$ to be of the same "rod type."

Patterns of Rods on Circles About Axis of Reactor

This generator allows a pattern of rods on circles about the axis of a cylindrical reactor to be produced. Three initial coordinates are required for each "rod type" in the lattice. These coordinates are the X and Y coordinates of the first rod encountered at a particular radius as one proceeds counterclockwise from the positive X axis, and the angular separation between rods at that radius. Coordinates of rods are generated from the initial position (at angle θ) to an angle equal to the initial angle plus 360 degrees. Single rods may be generated by making the angular separation between rods greater than 360 degrees. Up to three sets of initial X, Y, and $\Delta\theta$ coordinates may be input for a given "rod type" in the same manner as for hexagonal and square lattices.

4.2.2 Infinite Lattices

The infinite lattice generator in HERESY III generates a lattice that extends to a radially large distance such that the rods in the center of this large circle effectively "see" an infinite lattice.

The term "rod type" takes on a different meaning in this lattice than in the finite lattice considered above. The infinite lattice representation in HERESY III requires that a group of rods be found that are repeated over and over as the entire group is translated along a set of axes which may or may not be perpendicular. Each rod contained in this repeating group becomes a "rod type."

The data required for each "rod type" in the group are the distance in the X direction to the same rod in the next repeating group; the distance in the Y direction to the same rod in the next repeating group, the X and Y coordinates of the "rod type" relative to the coordinate origin; the outer radial limit of the "infinite" lattice; and the acute angle between the X and Y axes.

4.2.3 Plot, Print, Punch, and Scale Options

Four optional features are available for use with the geometry generators in HERESY III and are described in the paragraphs below.

Scaling

The option is available to input all coordinates in arbitrary units and to scale these coordinates by arbitrary scale factors. A scale factor is input for the X coordinates and for the Y coordinates separately. These factors scale the coordinates, and, for infinite lattices, also the distances between repeating groups of rods. If the scale factors are not entered, they are assumed unity.

Plotting

The plot option is available to obtain a visual display of the lattice used in the problem. It is made on a rectangular grid allowing up to 25 intervals along the positive and negative X and Y axes. The incremental distance between grid points is specified by scale factors along the X and Y axes. Rods are assigned to the closest grid point in the plot, and the "rod type" number appears at these positions.

Printing

The print option is available to list all of the coordinates of each "rod type." The list breaks the rods down by "rod type," and gives the X and Y coordinates (in centimeters) for each rod of that type.

Punching

The punch option is available for finite lattices only. The option will produce two decks of cards that may be reloaded directly back into another problem in the input data. The first deck contains the number of rods in the lattice for each "rod type," which is reloaded with fixed point data, and the second deck contains the X and Y coordinates for all rods in the lattice.

4.3 MODERATOR DISTRIBUTION GENERATORS

The interaction between two rods in the lattice depends only on the separation between the rod centers and the effective properties of the moderator material between the rods. Because the moderator properties are constant for a given problem, the distributions may be tabulated as a function of rod separation. A tabular procedure with interpolation has been found to be less

time consuming than calculating values for each rod separation.

The matrices are formed by summing up the contributions to a "rod type" in the lattice from all rods in the lattice (including itself).

A more general form is permitted for specifying the moderator distributions than the single distribution functions discussed in Section 3. Instead of the single Gaussian [equation (3.6)], the slowing down density may be given as

$$q^r_{jk} = \sum_{m=1}^{3} \frac{B_m}{4\pi\tau^r_m} \exp - \frac{|\underline{r}_j - \underline{r}_k|^2}{4\tau^r_m} \qquad (4.1)$$

where

$$\sum_{m=1}^{3} B_m = 1 \qquad (4.2)$$

The effective neutron age is then

$$\tau_{eff} = \sum_{m=1}^{3} B_m \tau^r_m \qquad (4.3)$$

All other distributions that depend on equation (4.1),(i.e., all but the diffusion solution, equation (3.10)), follow the three component weighting of equation (4.1). These reduce back to the standard solutions, when $B_1 = 1$ and $B_2 = B_3 = 0$.

4.4 AUTOMATIC PARAMETER CONVERSION

Although HERESY III may be used with all card input, it was designed to be used in connection with cell calculations performed by the HAMMER[7] system. The results of HAMMER cell calculations may be retained on tape (called a lattice library tape). This tape may then be mounted prior to HERESY III runs. A routine is included in the executive section of HERESY III, which may read this tape and automatically generate much of the input required. This may be done for either one epithermal group (level) or three epithermal groups (levels) corresponding to the two- or

four-group parameters provided by the HAMMER system. Moderator properties (thermal diffusion coefficient, thermal absorption cross section, and Fermi age(s)) are computed based on a weighted average of these properties, the weighting factors being the number of rods of each rod "kind" present. With these properties established, the "cell-rod" relations discussed in Section 3 are used to compute rod properties. Details are discussed below.

4.4.1 Moderator Properties

Thermal moderator properties are computed from the following:

$$\bar{\Sigma}_a = \frac{\sum^{\text{kinds}} N_i \, \Sigma_a^i}{\sum^{\text{kinds}} N_i} \tag{4.4}$$

$$\bar{D} = \frac{\sum^{\text{kinds}} N_i \, D^i}{\sum^{\text{kinds}} N_i} \tag{4.5}$$

$$L^2 = \frac{\bar{D}}{\bar{\Sigma}_a} \tag{4.6}$$

where N_i is the number of rods of each "rod kind." Equation (3.11) is used to modify these quantities to account for transverse leakage.

Several options are available for specifying the neutron ages for the resonance and thermal levels in a problem. Some of these options are historical in origin and are included in HERESY III only to maintain compatibility with previous versions of the code. A parameter (mnemonic NTAU) is used to specify six options.

- (NTAU = 1 or 5) Internally stored ages for one epithermal level are to be used. These ages are semi-empirical and are adequate for most survey problems, particularly if used with scale factors as described below. The first of these

two options (NTAU = 1) uses a one-term Gaussian distribution, and the second (NTAU = 5) uses a three-term Gaussian distribution. (Appendix B.)

- (NTAU = 2 and 6) Internally stored ages for three epithermal levels are to be used. All comments relating to the one resonance level set of ages apply also here (Appendix B).

- (NTAU = 3) Neutron ages will be computed from the HAMMER System output as part of the automatic conversion feature. These ages will be the average of the HAMMER ages for the different assemblies in the lattice weighted by the relative numbers of each assembly in the lattice. The number of epithermal levels (mnemonic NØTAU) must be specified for this option. The relations used to obtain these ages are shown in Appendix B.

- (NTAU = 4) Neutron ages will be entered by card input allowing any arbitrary set of ages to be available to the user. The number of epithermal levels (mnemonic NØTAU) must be specified for this option.

Any set of neutron ages specified by the options NTAU = 1, 2, 5, or 6 may be scaled by an arbitrary input constant (mnemonic CQ). For the option NTAU = 3, this scaling constant (mnemonic CQ) is used as an arbitrary multiplier on the lowest epithermal level above the thermal level (Appendix B).

If an external set of neutron ages is input (NTAU = 4), the parameter conversion uses this set for all assemblies, and no scaling is done for any assembly.

It is not required that all rod parameters be taken from a HAMMER system output. A sequence of numbers [mnemonics NCASE(I), $1 \leqslant I \leqslant$ NKIND] are entered, one for each "rod kind," when the conversion feature is desired. These numbers are the case Identification Numbers on the HAMMER lattice library. If a number is zero, the conversion is not performed for that "rod kind." It is important to note that if the moderator L^2 and Σ_a parameters are obtained from the conversion, then the process of not converting a "rod kind" by this feature will omit the effect of that "rod kind" on the moderator parameters.

The data necessary to perform the automatic parameter conversion include a signal (mnemonic NHAM), which specifies the number of resonance levels (1 or 3), series of case Identification Numbers [mnemonics NCASE(I), $1 \leqslant I \leqslant$ NKIND], a number giving the relative weight of this assembly in computing moderator properties [mnemonics NLB(I), $1 \leqslant I \leqslant$ NKIND], a library number for each "rod kind" telling the library from which the data are to be taken

[mnemonics NTAPE(I), $1 \leq I \leq$ NKIND], and a signal (mnemonic NTHER) indicating which option for the heterogeneous f parameter is to be used (see below).

HERESY III can use up to three lattice libraries in a single problem. These are referred to as libraries 17, 18, and 19. If no library is specified, 17 is assumed. The three libraries are assigned at execution time using suitable Data Definition (DD) control cards.

4.4.2 Rod Parameters

The relations used in the automatic parameter conversion to obtain the nuclear parameters for each "rod kind" are discussed in the following paragraphs.

Thermal Utilization

Four options are available for obtaining the heterogeneous thermal utilization for each "rod kind" from a HAMMER system cell calculation. A signal (mnemonic NTHER) specifies the options as follows.

- (NTHER=0, default case)

$$f_{het} = 1.0 - \frac{\bar{\Sigma}_a(\text{mod}) + \Sigma_a(\text{mod})}{2} \times \frac{1}{\Sigma_a(\text{cell})} \tag{4.7}$$

- (NTHER=1)

$$f_{het} = 1.0 - \frac{\bar{\Sigma}_a(\text{mod})}{\Sigma_a(\text{cell})} \tag{4.8}$$

- (NTHER=2)

$$f_{het} = 1.0 - \frac{\Sigma_a(\text{mod})}{\Sigma_a(\text{cell})} \tag{4.9}$$

- (NTHER=3)

$$f_{het} = 1.0 - M \tag{4.10}$$

where

$\bar{\Sigma}_a(\text{mod})$ = moderator thermal Σ_a based on the weighted average of all "rod kinds"

$\Sigma_a(\text{mod})$ = moderator thermal Σ_a for this "rod kind"

$\Sigma_a(\text{cell})$ = cell average thermal Σ_a for this "rod kind"

M = fraction of total thermal neutrons absorbed in the outermost material in the cell

Options 0, 1, and 2 give somewhat different results when thermal spectrum mismatch between cells is significant. Option 3 is included for historical reasons only. A discussion of the physical bases of these options is given in Appendix D.

Whichever choice of f is made is used together with the cell area in equation (3.19) to obtain the thermal absorption parameter δ.

η *Parameters*

The heterogeneous thermal eta parameter is computed using the (ηf) product from the THERMOS part of HAMMER and the heterogeneous f parameter computed by the algorithms in the previous section.

$$\eta_{\text{thermal}} = \frac{(\eta f)_{\text{HAMMER}}}{f_{\text{het}}} \tag{4.11}$$

The resonance η parameters are computed from the four-group macroscopic cross sections in the HAMLET part of HAMMER. For the three epithermal level conversion, they are given by

$$\eta^r = \frac{\nu\Sigma_f^r}{\Sigma_a^r} \tag{4.12}$$

where r indexes the resonance level. For the one epithermal level conversion, the groups are condensed by flux weighting and the resonance η parameter is given by

$$\eta^1 = \frac{\sum_{i=1}^{54} \phi_i \, \nu\Sigma_f^i}{\sum_{i=1}^{54} \phi_i \, \Sigma_a^i} \tag{4.13}$$

where the ϕ_i are the cell averaged fluxes for the fifty-four micro-groups in the HAMLET part of HAMMER.

Resonance Absorption Coefficients

For one epithermal level, the epithermal absorption coefficient is computed from equation (3.28). For three epithermal levels, the coefficients are computed from equations (3.38 to 3.40).

In the lists of input data in Section 6, the parameters that may be obtained from the automatic parameter conversion feature appear with an asterisk after the mnemonic.

4.5 CRITICALITY SEARCHES

Four criticality searches are available that enable the user to obtain a specified static reactivity coefficient (mnemonic EIGEN) as a function of the δ parameter, thermal η parameter, or all resonance η parameters for a specified "rod kind"; or as a function of the axial buckling B_Z^2.

Searches over the δ parameter, thermal η parameter, or all η parameters (specified by mnemonic LCRIT = 1, 2, or 3, respectively) require that a "rod kind" (mnemonic KSERCH) be specified for which the appropriate parameter will be varied. Searches over B_Z^2 (specified by mnemonic LCRIT = 4) do not require further specifications.

A short summary of the progress of the criticality search is output after each iteration of the search. A limit (mnemonic N5) is placed on the number of iterations that may take place in a search, since some cases may take an inordinate amount of time to achieve convergence.

At the completion of a δ parameter search the heterogeneous thermal utilization [mnemonic THERU(KSERCH)] is recomputed for the converged δ parameter for the "rod kind" searched over. This thermal utilization, as well as the η parameters or buckling in the other searches, is stored in the data array at the end of a solved problem. Thus the data will contain the results of the criticality search in all cases.

5. OUTPUT

5.1 GENERAL

Two output formats are available as user selected options from the HERESY III code. They are called "long form" or "short form" edits. The long form edit gives a detailed breakdown, level-by-level, of rod absorptions, average absorptions, and average eta parameter. The short form edit lumps all epithermal absorptions and production into single parameters averaged over all epithermal levels. Selection of the edit format is specified by the mnemonic variable NEDIT. If NEDIT is not specified, the long form edit will be output.

The information is divided into data summary, criticality search summary, and edit of solved problems.

5.1.1 Data Summary

This summary is the same for both edit forms. All data used in the solution to the problem are shown whether input from cards or by the automatic nuclear data conversion feature. The summary is output *before* the problem is solved and will not show changes to parameters that occur in criticality searches.

5.1.2 Criticality Search Summary

In the event a criticality search is performed, a section is output following data summary, which summarizes the progress of the search after each iteration. Contained in this summary are the current reactivity coefficient, the rod kind being searched over, and the current value of the parameter being varied.

5.1.3 Edit of Solved Problems

Solving the heterogeneous lattice problems yields the thermal absorptions normalized to the most highly absorbing rod in the lattice, and the static reactivity coefficient. From these and the input information, the resonance absorption and a variety of other parameters are obtained and output in the edit of solved problems. This edit is divided into the following parts:

Part 1

This part lists the last two successive inner and outer eigenvalues as a check of the convergence of the problem. If the problem does not coverge, a line is produced here stating the conditions under which the edit is being performed.

Part 2

Thermal and resonance absorptions for each "rod type" are summarized in a table. The long form edit lists resonance absorptions by individual resonance level and as a sum of all levels. The short form edit lists only the total resonance absorption for a given rod type.

Part 3

This part provides the lattice averaged resonance and thermal rod absorptions for each rod type. The long form edit provides averages for each resonance level, and the short form edit lists only the average total resonance absorptions for a rod type.

Part 4

This part provides the lattice averaged resonance and thermal eta parameters. The long form edit provides averages for each resonance level, and the short form edit lists only the averages over all resonance levels and lattice rods.

Part 5

This part gives the lattice averaged thermal eta parameter, resonance escape probability, thermal utilization, a nonleakage probability, total-to-thermal fission ratio, static reactivity coefficient, moderator absorptions, and total leakage. Under suitable conditions, the lattice material buckling is calculated.

Part 6

This part provides the lattice averaged resonances and thermal absorptions for each "rod kind." The long form edit provides averages for each resonance level, and the short form edit lists only the average total resonance absorptions for a rod kind.

Part 7

In the event a criticality search has been performed as part of the calculations, a line is printed out in this part giving the value of the parameter being varied when the search reached convergence.

5.2 EQUATIONS USED IN EDIT

The edit routine begins with a knowledge of the thermal absorptions, the static reactivity coefficient, and the input data. The following equations are used to obtain the remainder of the information in the output.

5.2.1 Epithermal Absorptions

From equations (3.44, 3.45, and 3.46),

$$\underline{i}^{r} = \frac{1}{k} \underline{\underline{A}}^{r} \cdot \underline{\underline{Q}}^{*r} \cdot \underline{\underline{I}} + \frac{1}{k}(\underline{\underline{I}}-\underline{\underline{R}})^{-1} \cdot \underline{\underline{R}} \cdot \underline{\underline{\eta}} \cdot \underline{i} \qquad (5.1)$$

where the matrices are defined at the end of Section 3. Equation (5.1) is used to compute epithermal absorption.

5.2.2 Average Absorptions

Average absorptions for any epithermal level, thermal level, or total epithermal absorption are obtained from

$$\bar{i}^{(r)} = \frac{\underline{\underline{W}} \cdot \underline{i}^{(r)}}{\omega} \qquad (5.2)$$

where $\underline{\underline{W}}$ = diagonal matrix of number of rods per rod type

ω = total number of rods

5.2.3 Lattice Parameters

Average lattice parameters are defined to satisfy the basic equation

$$k = \bar{\eta}\ \varepsilon\ p\ f\chi$$

where

k = static reactivity coefficient (k_{eff})

$\bar{\eta}$ = average thermal eta parameter

ϵ = ratio of total fissions to thermal fissions

p = resonance escape probability

f = thermal utilization

χ = nonleakage probability

The following terms are defined as

$P_t \equiv$ total neutron production from thermal sources

$$\equiv \frac{1}{k} \underline{W} \cdot \underline{\underline{\eta}} \cdot \underline{i}$$

$P_r \equiv$ total neutron production from epithermal sources

$$\equiv \frac{1}{k} \underline{W} \cdot \sum_{r=1}^{P} \underline{\underline{\eta}}^r \cdot \underline{i}^r$$

$T \equiv$ total thermal neutron absorptions in rods $\equiv \underline{W} \cdot \underline{i}$

$R \equiv$ total epithermal neutron absorptions in rods

$$\equiv \sum_{r=1}^{P} \underline{W} \cdot \underline{i}^r$$

$M \equiv$ total thermal neutron absorptions in moderator

$$\equiv \sum_{n=1}^{K} \frac{\overline{N_n i_n}(1-f_n)}{f_n}$$

$L \equiv$ total neutron leakage $\equiv P_t + P_r - T - R - M$

where

K = number of rod kinds in lattice

$\overline{N_n i_n}$ = total thermal neutron absorption in all rods of kind n

f_n = heterogeneous thermal utilization of rod kind n (input)

In terms of these quantities, the lattice parameters are:

$$\bar{\eta} = \frac{kP_t}{T} = \frac{\underline{W} \cdot \underline{\underline{\eta}} \cdot \underline{i}}{\underline{W} \cdot \underline{i}}$$

$$\bar{\eta}^r = \frac{kP_r}{R} = \frac{\underline{W} \cdot \sum_{r=1}^{P} \underline{\underline{\eta}}^r \cdot \underline{i}^r}{\underline{W} \cdot \sum_{r=1}^{P} i^r}$$

$$p = (T+M+L)/(P_t+P_r) \qquad (5.3)$$

$$f = T/(T+M)$$

$$\chi = (T+M)/(T+M+L)$$

$$\varepsilon = (P_t+P_r)/P_t$$

The separation between "moderator absorption" and "leakage" is somewhat arbitrary, and only the sum M+L or the product $f\chi$ is unambiguous.

5.2.4 Lattice Material Buckling

If the problem calls for the solution of an infinite lattice with zero axial buckling, then the static reactivity obtained in the solution of the problem is k_∞. The lattice averaged parameters are used in the two-group diffusion theory critical equation to obtain the material buckling of the lattice. This equation is

$$\chi = \frac{(1-p)\,\bar{\eta}^{res}}{1+\tau B_m^2} + \frac{pf\bar{\eta}}{(1+\tau B_m^2)(1+L^2 B_m^2)} \qquad (5.4)$$

where

τ = lattice effective thermal age

L^2 = lattice thermal diffusion area

B_m^2 = lattice material buckling

p, f, $\bar{\eta}^{res}$, $\bar{\eta}$, and χ defined in equation (5.3)

The material buckling is calculated using a common approximation for the thermal diffusion area. This approximation relates the moderator thermal diffusion area to the lattice thermal diffusion area by

$$L^2(\text{lattice}) = (1-\chi f)L^2(\text{mod}) \qquad (5.5)$$

For an infinite lattice, χ should be unity. The code computes a value different from unity due to the finite convergence criterion on fluxes and k_{eff}. The actual value computed is included in the equation (5.4) for numerical consistency.

6. INPUT

Data are broken into three types and input in the following order:

1. Alphanumeric data (1 card only)
2. Fixed point data
3. Floating point data

For each problem, there must be at least one card of each type in the input data deck. The three types of data are described separately in the following paragraphs.

6.1 ALPHANUMERIC DATA

These data consist of one card of alphanumeric symbols contained in columns 1-72 of the input card. This information is printed out as a page subheading in the output from the code.

6.2 FIXED POINT DATA

Fixed point data are entered in a fixed card format that allows any number of individual data up to five to be read from a single card. The card format is shown below:

Card Columns

1	5	6-12	13-24	25-36	37-48	49-60	61-72
Last card indicator	Number of data on this card (if blank or zero is assumed to be 5)	Relative location of Datum 1 on this card (see following list	Datum 1	Datum 2	Datum 3	Datum 4	Datum 5

All fixed point data are stored in a large singly indexed array JJ in core. Each datum is assigned a relative location in this array, and a list of these locations follows. The relative

location of datum 1 on the card is punched into columns 6-12. Data 2-5 are stored in sequential relative locations in the array.

If it is not desirable to input a full card of data (five data), it is only necessary to place the number of data actually appearing on the card in column 5 (a blank or a zero will cause five data to be read). For instance, if it is necessary to change one property of one rod type in a list of fifty rod types, the relative location of the datum may be determined from the list below and placed in columns 6-12, a number 1 placed in column 5, and the new datum placed in the datum 1 field as defined above.

All fixed point data are entered to the extreme right of the defined field, blank columns being read as zeros.

The last card of fixed point data must have a 1 punched in column 1 to indicate it is the last card.

Relative locations for fixed point data are contained in the following list.

Control and Geometry Data

1.	JJ(1) = KØØR		*Geometry Generator Control*
	= 0		Use the geometry of the previous problem.
	= 1		Generate a new lattice geometry.
	= 2		Read lattice geometry from cards.
2.	JJ(2) = KERN		*Kernel Generator Control*
	= 0		Use moderator spatial distributions from previous problem.
	= 1		Generate new moderator spatial distributions.
			NOTE: If either *the transverse buckling* or the moderator physical properties are changed, KERN = 1 should be used.
3.	JJ(3) = INF		*Problem Geometry Control*
	= 0		Finite lattice geometry.
	= 1		Infinite lattice geometry.
4.	JJ(4) = LAT		*Lattice Geometry Control*
	= 0		Hexagonal lattice.
	= 1		Square lattice.
	= 2		Pattern of rods on circles about axis of reactor.

5. JJ(5) ... = NICPRT(I) — Number of rotationally symmetric typical lattice locations to be used in geometry generator for each rod type. For example, in a hexagonal lattice in which some rod types contain 12 rods, NICPRT(I) would be set equal to 2 for those types: two sets of coordinates would (later) be specified which, by 60° rotation, would generate the full 12 rods. If any NICPRT(I) are zero, they are internally set equal to one (enter for finite lattices only; $1 \leqslant I \leqslant$ NTYPE).

6. JJ(55) ... = NRPRT(I) — Number of rods in lattice of each rod type (enter only if KØØR = 2; $1 \leqslant I \leqslant$ NTYPE).

7. JJ(105) = KPLØT — *Geometry Plot Option*

= 0	Do not plot geometry.
= 1	Plot geometry.

8. JJ(106) = KPRINT — *Geometry List Option*

= 0	Do not list lattice coordinates.
= 1	List lattice coordinates.

9. JJ(107) = KPUNCH — *Geometry Punch Option*

= 0	Do not punch lattice coordinate deck.
= 1	Punch lattice coordinate deck.

Moderator Control Data

10. JJ(109) = NTAU — *Resonance Level Scheme Option*

= 1	Single Gaussian stored 2-group levels.
= 2	Single Gaussian stored 4-group levels.
= 3	Single Gaussian levels are computed from HAMMER output (must supply value of NØTAU below) (recommend for automatic parameter conversion).
= 4	Arbitrary levels input from cards (must supply value of NØTAU below).
= 5	Triple Gaussian 2-group stored levels.
= 6	Triple Gaussian 4-group stored levels.

11. JJ(110) = NOTAU — Number of resonance levels (enter only if NTAU = 3 or 4).

Rod Specification Data

12. JJ(111) = NTYPE — Number of rod types in lattice (≤ 50).

13. JJ(112) = NKIND — Number of rod kinds in lattice (≤ 20).

14. JJ(113) = NHAM — *Automatic Parameter Conversion Control*

    = 0 — No parameters will be obtained from a HAMMER lattice library tape.

    = 1 — Some or all rod parameters will be obtained from a HAMMER lattice library tape in 2 groups.

    = 2 — Some or all rod parameters will be obtained from a HAMMER lattice library tape in 4 groups.

15. JJ(114) = NTHER — *Thermal Utilization Option Control*

    = 0 — Standard f computation (numerical average of options 1 and 2)

    = 1 — $f = 1 - \dfrac{\bar{\Sigma}_a(\text{mod})}{\Sigma_a(\text{cell})}$

    = 2 — $f = 1 - \dfrac{\Sigma_a(\text{mod})}{\Sigma_a(\text{cell})}$

    = 3 — f = 1 - absorption in outermost material region.

16. JJ(115) ... = NCASE(I) (omit if NHAM = 0) — HAMMER Case Identification number from which rod parameters are to be derived for each rod kind ($1 \leq I \leq$ NKIND) (enter zero if conversion is not to be performed for a rod kind I).

17. JJ(135) ... = NLB(I) (omit if NHAM = 0) — Relative number of rods of each rod kind in lattice ($1 \leq I \leq$ NKIND).

18. JJ(155) ... = NTAPE (I) (omit if NHAM = 0) — Library number of HAMMER lattice library for each rod kind (if zero, assumes library 17).

19. JJ(175) ... = KIND(I) — Rod kind associated with each rod type ($1 \leq I \leq$ NTYPE).

Criticality Search Control Data

20.	JJ(225)	=	LCRIT	*Criticality Search Control*
		=	0	No criticality search.
		=	1	Search for criticality over thermal η parameter.
		=	2	Search for criticality over thermal f parameter.
		=	3	Search for criticality over all η parameters.
		=	4	Search for criticality over axial buckling.
21.	JJ(226)	=	KSERCH	Rod kind to be searched over in criticality search.

Miscellaneous Control Data

22.	JJ(228)	=	NEDIT	*Edit Option Control*
		=	0	Long form edit.
		=	1	Short form edit.
23.	JJ(229)	=	LAST	*Last Problem Control*
		=	0	More problems follow.
		=	1	This is the last problem.
24.	JJ(231)	=	N2	Maximum number of iterations on eigenvalues and eigenvectors (set equal to 100 if left blank).
25.	JJ(232)	=	N3	Maximum number of iterations for outer eigenvalue iterations (set equal to 10 if left blank).
26.	JJ(233)	=	N5	Maximum number of iterations for criticality searches (set equal to 10 if left blank).

6.3 FLOATING POINT DATA

Floating point data are also input in a fixed card format that enables any number of individual datum up to five to be read from a single card. The card format is identical to that discussed for fixed point data; the only change made for floating point data is for the data to be read in FORTRAN FIXED DECIMAL FLOATING POINT notation (standard FORTRAN F type conversion). The number 10^{-6} would thus appear as .000001 on an input card.

A floating point datum may be entered anywhere within the defined field on the card so long as the decimal point is assigned the correct position in the number. If no decimal point is entered, it is automatically assigned as following the character appearing in the last column of the datum field. Blank columns are read as zeros.

All floating point data are stored in a singly indexed array BB in core, each datum being assigned a relative location in this array. A list of these relative locations follows.

The relative location of datum 1 on the card must be punched into columns 6-12, and provision for reading less than five data is identical to that for fixed point data.

The last card of floating point data must have a 1 punched in column 1 to indicate it is the last.

Relative locations for floating point data are given in the following list. Items with asterisks by the mnemonic may be omitted if automatic parameter conversion is used.

Data for Geometry Generators

(Items 1-5 refer to finite lattices only)

1.	BB(1) ... = XØ(I,1) BB(51) ... = XØ(I,2) BB(101) ... = XØ(I,3)	Initial values of X coordinates for rods in finite geometry generators ($1 \leq I \leq$ NTYPE). See Notes 1 and 2.
2.	BB(151) ... = YØ(I,1) BB(201) ... = YØ(I,2) BB(251) ... = YØ(I,3)	Initial values of Y coordinates for rods in finite geometry generators ($I \leq I \leq$ NTYPE). See Notes 1 and 2.
3.	BB(301) ... = THETA(I,1) BB(351) ... = THETA(I,2) BB(401) ... = THETA(I,3)	Angular separation between rods on same radius about axes of reactor (enter only if LAT = 2) ($1 \leq I \leq$ NTYPE). See Note 1.
4.	BB(452) = RØUT	Reflector outer radius (cm). If left blank, an ∞ reflector will be assumed.
5.	BB(453) = RIN	Radius within which image rod effects may be ignored (cm). If left blank, image contributions will be computed for all rods.

(Items 6-11 refer to infinite lattices only)

6.	BB(451) = ANGLE	Acute angle between X and Y axes (degrees). If left blank is set equal to 90 degrees.
7.	BB(454) = RADII	Practical outer radius of infinite lattice (cm). A suitable way to choose this parameter is to specify a radius within which the total number of rods is slightly less than 5000, the upper limit.
8.	BB(455) ... = XPITCH(I)	X pitch for I^{th} overlapping lattice ($1 \leq I \leq$ NTYPE). See Note 2.
9.	BB(505) ... = YPITCH(I)	Y pitch for I^{th} overlapping lattice ($1 \leq I \leq$ NTYPE). See Note 2.
10.	BB(555) ... = XI(I)	X coordinate of rod nearest origin in I^{th} overlapping lattice ($1 \leq I \leq$ NTYPE). See Note 2.

11.	BB(605) ... = YI(I)	Y coordinate of rod nearest origin in I^{th} overlapping lattice. ($I \leqslant I \leqslant NTYPE$). See Note 2.
12.	BB(655) = XCØR	Arbitrary scale factor on all X coordinates. See Note 2.
13.	BB(656) = YCØR	Arbitrary scale factor on all Y coordinates. See Note 2.
14.	BB(657) = XSCALE	Plotting interval along X axis in geometry plotter (if zero is set equal to XCØR).
15.	BB(658) = YSCALE	Plotting interval along Y axis in geometry plotter (if zero is set equal to YCØR).

(Items 16 and 17 refer to the KØØR = 2 option only)

16.	BB(1151) ... = X(I)	X coordinates for all rods (cm). $\sum_{I=1}^{NTYPE}$ NRPRT(I) values. See Note 3.
17.	BB(6151) ... = Y(I)	Y coordinates for all rods (cm). $\sum_{I-1}^{NTYPE}$ NRPRT(I) values. See Note 3.

Data for Moderator Spatial Distribution Generators

18.	BB(659) = XLSQ*	Moderator thermal diffusion area (cm^2).
19.	BB(660) = SIGA*	Moderator thermal macroscopic absorption cross section (1/cm).
20.	BB(661) = BSQ	Axial geometrical buckling ($1/cm^2$).

21.	BB(663) ... = B(I,J)*	Weighting factors for each component of triple Gaussian slowing down density. See Note 4. ($1 \leq I \leq$ NØTAU+1; $1 \leq J \leq 3$) (B(NØTAU+1,J) are thermal values) (enter only if NTAU = 4).
22.	BB(693) ... = TAU(I,J)*	Neutron age from fission to resonance energy for each resonance level and each component of triple Gaussian slowing down density. See Note 4. ($1 \leq I \leq$ NØTAU+1; $1 \leq J \leq 3$) (TAU(NØTAU+1, J) are thermal values) (enter only if NTAU = 4).
23.	BB(724) = CQ*	Arbitrary multiplicative factor for TAU(I,J) values. See Appendix B.
24.	BB(725) ... = AR(I,J)*	Resonance absorption parameter for each rod kind and each resonance level. See Note 4. ($1 \leq I \leq$ NKIND; $1 \leq J \leq$ NØTAU).

Nuclear Data for Individual Rods

25.	BB(905) ... = THERU(I)*	Thermal utilization for each rod kind ($1 \leq I \leq$ NKIND).
26.	BB(925) ... = ETAIN(I,J)*	Eta value for each rod kind and each resonance level. See Note 4 ($1 \leq I \leq$ NKIND; $1 \leq J \leq$ NØTAU+1). (ETAIN (I,NØTAU+1) values are thermal values).
27.	BB(1125) ... = VCELL(I)*	Cell volume for each rod kind ($1 \leq I \leq$ NKIND).

Data for Criticality Searches

28.	BB(1145) = EIGEN	Eigenvalue to be searched for (if zero is set equal to 1.0).
29.	BB(1146) = CR1	Convergence limit on matrix inversion (if zero is set equal to .000001).

30.	BB(1147) = CR2	Convergence limit on inner eigenvalue and eigenvector iterations (if zero is set equal to .001).
31.	BB(1148) = CR3	Convergence limit on outer eigenvalue iterations (if zero is set to .001).
32.	BB(1149) = CR4	Convergence limit on criticality searches (if zero is set equal to .001).

Note 1

Entering the initial coordinates XØ(I,J), YØ(I,J), and THETA(I,J) for the finite lattice generator must be done in the following order. The matrices for these quantities are 50 by 3 (50 rows and 3 columns). Data are entered column-wise, which implies that for each value of J the index I runs through its full range. Hence, using XØ as an example, the values would be entered as follows:

XØ(1,1) ..., XØ(I,1) ..., XØ(50,1), XØ(1,2) ..., XØ(I,2) ...,
XØ(50,2), XØ(1,3) ..., XØ(I,3) ..., XØ(50,3).

Relative locations associated with these coordinates are:

BB(1) = XØ(1,1)	BB(151) = YØ(1,1)	BB(301) = THETA(1,1)
BB(51) = XØ(1,2)	BB(201) = YØ(1,2)	BB(351) = THETA(1,2)
BB(101) = XØ(1,3)	BB(251) = YØ(1,3)	BB(401) = THETA(1,3)

Note 2

The scale factors XCØR and YCØR are used as arbitrary non-zero, non-negative multiplication factors to modify coordinate values input. These factors do not multiply all values, but only those indicated below:

XCØR multiplies the values of XØ(I,J), XPITCH(I), XI(I).

YCØR multiplies the values of YØ(I,J), YPITCH(I), YI(I).

If XCØR and/or YCØR is left blank or is entered negative, it is automatically set equal to 1.0.

Note 3

Coordinates are input in sequence starting with rod type 1 and running over all rods of that type. These are followed by rod types 2, 3, 4, ..., where, for each rod type, the coordinates of all rods of that type are successively entered.

Note 4

Entering the doubly indexed rod parameters and age parameters must be done in the correct order, else a programmed error message will occur. Matrices for these parameters are dimensioned at 10 rows and 3 columns for age parameters, and 20 rows and 10 columns for rod parameters. Data are always entered column-wise, which implies that the first index runs through its full range before the second index is incremented. If the ETAIN array is used as an example, the parameters are entered as follows:

ETAIN(1,1) ..., ETAIN(I,1) ..., ETAIN(20,1), ETAIN(1,2) ...,
ETAIN(I,2) ..., ETAIN(I,10) ..., ETAIN(20,10).

Relative locations for these parameters are shown below:

```
ETAIN(1,1) = BB(925)    AR(1,1) = BB(725)   TAU(1,1) = BB(693)
ETAIN(1,2) = BB(945)    AR(1,2) = BB(745)   TAU(1,2) = BB(603)
ETAIN(1,3) = BB(965)    AR(1,3) = BB(765)   TAU(1,3) = BB(713).
ETAIN(1,4) = BB(985)    AR(1,4) = BB(785)
ETAIN(1,5) = BB(1005)   AR(1,5) = BB(805)   B(1,1) = BB(663)
ETAIN(1,6) = BB(1025)   AR(1,6) = BB(825)   B(1,2) = BB(673)
ETAIN(1,7) = BB(1045)   AR(1,7) = BB(845)   B(1,3) = BB(683).
ETAIN(1,8) = BB(1065)   AR(1,8) = BB(865)
ETAIN(1,9) = BB(1085)   AR(1,9) = BB(885).
ETAIN(1,10) = BB(1105).
```

6.4 ERROR CONDITIONS

There are a number of tests built into the code to detect error conditions at different points in the computational sequence. These conditions may or may not produce a termination of the run depending on whether the condition is recoverable or not. At the occurrence of any such error condition, a number is printed out that indicates the condition and what action will be taken. The error condition codes are shown in the following list.

Error Condition Number	Reason for Error Condition	Action to be Taken by Code
100	HAMMER conversion is requested for a number of resonance levels not equal to 1 or 3.	Attempt next problem.
110	A HAMMER case is not in the designated library.	Attempt next problem.
210	The number of rods in the lattice exceeds 5000.	Exit machine
220	A machine branching error has occurred. Re-submit problem.	Exit machine.
230	The initial coordinates to the hexagonal lattice generator are in the wrong sector.	Exit machine.
240	The initial coordinates to the square lattice generator are in the wrong sector.	Exit machine
310	A negative radial distance was found in tabulating the slowing down kernel. Check geometry.	Exit machine.
320	An error condition was found in the Bessel's function subroutine in the epithermal slowing down kernel tabulation. Check geometry and/or moderator parameters.	Exit machine.
330	A negative radial distance was encountered in tabulating the epithermal slowing down kernel. Check geometry.	Exit machine.
340	An error condition was found in the Bessel's function subroutine in tabulating the thermal diffusion distribution. Check geometry and/or moderator parameters.	Exit machine.
350	A negative radial distance was encountered in tabulating the thermal diffusion distribution. Check geometry.	Exit machine.

Error Condition Number	Reason for Error Condition	Action to be Taken by Code
360	The mesh spacing is too large. Check geometry.	Exit machine.
370	The mesh spacing is too small. Check geometry.	Exit machine.
380	Argument of exponential is >174.0 in KERG2	Exit machine.
410	The $(\underline{\underline{\Gamma}}+\underline{\underline{D}})$ matrix failed to invert to the accuracy specified by CR1.	Attempt next problem.
420	The $(\underline{\underline{\Gamma}}+\underline{\underline{D}})$ matrix is singular.	Attempt next problem.
430	The $(\underline{\underline{I}}-\underline{\underline{R}})$ matrix failed to invert to the accuracy specified by CR1.	Attempt next problem.
440	The $(\underline{\underline{I}}-\underline{\underline{R}})$ matrix is singular.	Attempt next problem.
450	The inner eigenvalue iterations have exceeded N2 iterations	Attempt next problem.
460	The outer eigenvalue iterations have exceeded N3 iterations.	Attempt next problem.
510	The criticality search iterations have exceeded N5 iterations.	Attempt next problem
520	Criticality cannot be achieved with a positive axial buckling.	Attempt next problem.

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APPENDIX A

TABULATION OF $T(\tau/v,\theta)$ FUNCTIONS

The $T(\tau/v,\theta)$ functions defined in equation (3.29) and used to compute the resonance flux advantage factors are tabulated in the following list. Figure A-1 is a plot of these functions to obtain approximate values.

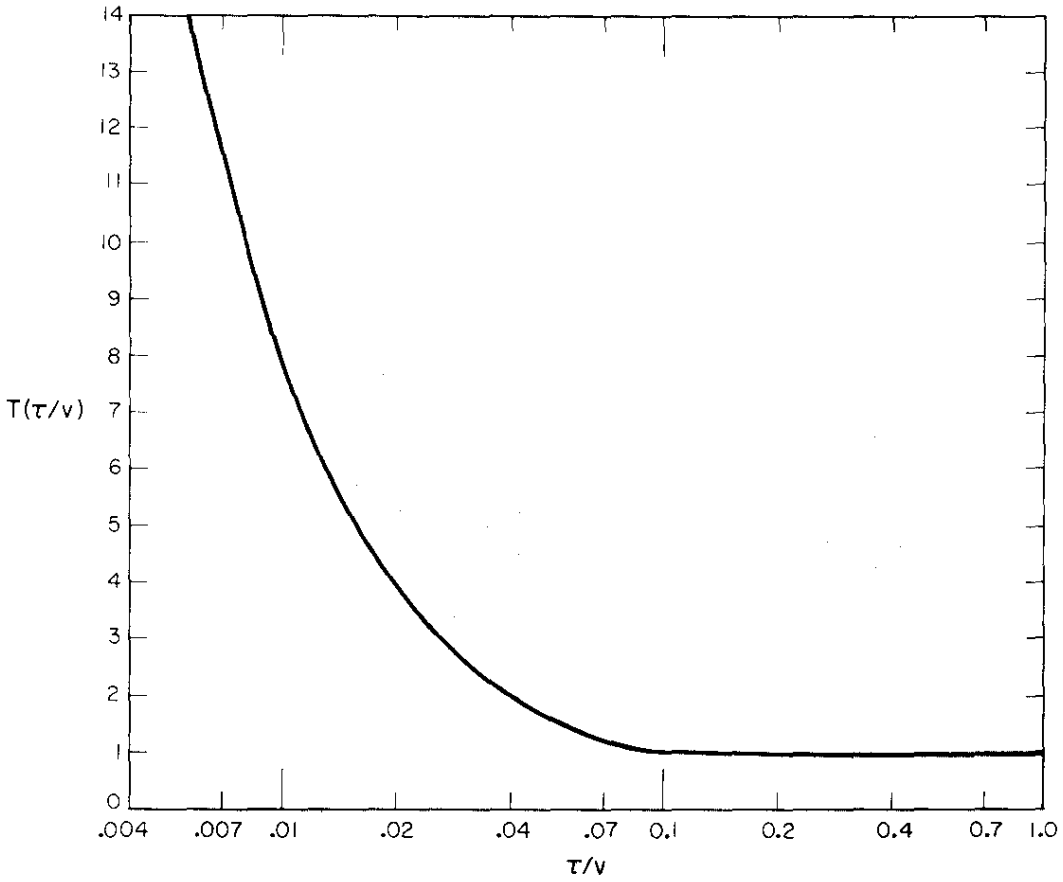


FIGURE A-1 $T(\tau/v)$ Versus τ/v for Square or Hex Lattices

TABULATION OF $T(\tau/V,\theta)$ FUNCTION FOR
ARGUMENTS BETWEEN 0.001 AND 0.050

No. of Terms in Function Sum = 2601

Argument (τ/V)	Square Lattice ($\theta = 90°$)	Hexagonal Lattice ($\theta = 60°$)
0.001	79.577184	79.574860
0.002	39.788655	39.787501
0.003	26.525795	26.525021
0.004	19.894349	19.893764
0.005	15.915486	15.915018
0.006	13.262906	13.262517
0.007	11.368205	11.367873
0.008	9.947179	9.946888
0.009	8.841938	8.841679
0.010	7.957745	7.957512
0.011	7.234314	7.234102
0.012	6.631455	6.631260
0.013	6.121342	6.121164
0.014	5.684104	5.683938
0.015	5.305165	5.305008
0.016	4.973595	4.973446
0.017	4.681035	4.680891
0.018	4.420987	4.420843
0.019	4.188320	4.188171
0.020	3.978933	3.978770
0.021	3.789506	3.789317
0.022	3.617325	3.617095
0.023	3.460153	3.459862
0.024	3.316125	3.315750
0.025	3.183677	3.183190
0.026	3.061488	3.060859
0.027	2.948436	2.947629
0.028	2.843559	2.842537
0.029	2.746030	2.744753
0.030	2.655133	2.653559
0.031	2.570246	2.568331
0.032	2.490823	2.488526
0.033	2.416387	2.413666
0.034	2.346516	2.343331
0.035	2.280837	2.277148
0.036	2.219017	2.214788
0.037	2.160759	2.155957
0.038	2.105798	2.100393
0.039	2.053893	2.047859
0.040	2.004829	1.998143
0.041	1.958409	1.951053
0.042	1.914455	1.906416
0.043	1.872806	1.864073
0.044	1.833313	1.823881
0.045	1.795840	1.785706
0.046	1.760262	1.749430
0.047	1.726465	1.714939
0.048	1.694342	1.682131
0.049	1.663795	1.650913
0.050	1.634734	1.621195

TABULATION OF $T(\tau/V,\theta)$ FUNCTION FOR
ARGUMENTS BETWEEN 0.050 AND 0.100

No. of Terms in Function Sum = 961

Argument (τ/V)	Square Lattice ($\theta = 90°$)	Hexagonal Lattice ($\theta = 60°$)
0.050	1.634734	1.621194
0.051	1.607073	1.592895
0.052	1.580735	1.565940
0.053	1.555647	1.540256
0.054	1.531740	1.515778
0.055	1.508951	1.492444
0.056	1.487220	1.470197
0.057	1.466492	1.448980
0.058	1.446715	1.428744
0.059	1.427838	1.409439
0.060	1.409817	1.391021
0.061	1.392608	1.273447
0.062	1.376171	1.356675
0.063	1.360467	1.340667
0.064	1.345459	1.325388
0.065	1.331115	1.310802
0.066	1.317401	1.296878
0.067	1.304287	1.283583
0.068	1.291745	1.270890
0.069	1.279747	1.258769
0.070	1.268269	1.247195
0.071	1.257284	1.236142
0.072	1.246771	1.225587
0.073	1.236707	1.215506
0.074	1.227072	1.205878
0.075	1.217847	1.196682
0.076	1.209012	1.187899
0.077	1.200549	1.179510
0.078	1.192443	1.171496
0.079	1.184677	1.163842
0.080	1.177235	1.156530
0.081	1.170104	1.149545
0.082	1.163270	1.142873
0.083	1.156719	1.136499
0.084	1.150439	1.130410
0.085	1.144419	1.124593
0.086	1.138647	1.119036
0.087	1.133112	1.113727
0.088	1.127804	1.108656
0.089	1.122714	1.103811
0.090	1.117831	1.099182
0.091	1.113147	1.094760
0.092	1.108655	1.090535
0.093	1.104344	1.086498
0.094	1.100209	1.082642
0.095	1.096240	1.078958
0.096	1.092433	1.075438
0.097	1.088778	1.072075
0.098	1.085272	1.068863
0.099	1.081906	1.065793
0.100	1.078675	1.062860

TABULATION OF $T(\tau/V,\theta)$ FUNCTION FOR
ARGUMENTS BETWEEN 0.100 AND 0.150

No. of Terms in Function Sum = 441

Argument (τ/V)	Square Lattice ($\theta = 90°$)	Hexagonal Lattice ($\theta = 60°$)
0.100	1.078675	1.062860
0.101	1.075574	1.060058
0.102	1.072597	1.057382
0.103	1.069740	1.054824
0.104	1.066997	1.052380
0.105	1.064363	1.050046
0.106	1.061834	1.047815
0.107	1.059406	1.045684
0.108	1.057074	1.043648
0.109	1.054836	1.041703
0.110	1.052686	1.039844
0.111	1.050621	1.038069
0.112	1.048638	1.036372
0.113	1.046734	1.034751
0.114	1.044905	1.033202
0.115	1.043149	1.031723
0.116	1.041461	1.030309
0.117	1.039841	1.028958
0.118	1.038284	1.027667
0.119	1.036789	1.026434
0.120	1.035352	1.025256
0.121	1.033972	1.024131
0.122	1.032647	1.023055
0.123	1.031373	1.022028
0.124	1.030150	1.021046
0.125	1.028974	1.020108
0.126	1.027845	1.019212
0.127	1.026760	1.018356
0.128	1.025718	1.017538
0.129	1.024716	1.016757
0.130	1.023754	1.016010
0.131	1.022829	1.015296
0.132	1.021941	1.014615
0.133	1.021087	1.013963
0.134	1.020267	1.013341
0.135	1.019478	1.012747
0.136	1.018721	1.012179
0.137	1.017993	1.011636
0.138	1.017293	1.011117
0.139	1.016621	1.010622
0.140	1.015975	1.010148
0.141	1.015355	1.009696
0.142	1.014758	1.009264
0.143	1.014185	1.008851
0.144	1.013634	1.008457
0.145	1.013104	1.008080
0.146	1.012595	1.007720
0.147	1.012106	1.007376
0.148	1.011636	1.007047
0.149	1.011185	1.006733
0.150	1.010751	1.006433

TABULATION OF $T(\tau/V,\theta)$ FUNCTION FOR
ARGUMENTS BETWEEN 0.150 AND 0.200

No. of Terms in Function Sum = 441

Argument (τ/V)	Square Lattice ($\theta = 90°$)	Hexagonal Lattice ($\theta = 60°$)
0.150	1.010751	1.006433
0.151	1.010333	1.006146
0.152	1.009932	1.005872
0.153	1.009547	1.005611
0.154	1.009177	1.005361
0.155	1.008821	1.005122
0.156	1.008478	1.004894
0.157	1.008150	1.004675
0.158	1.007833	1.004467
0.159	1.007530	1.004268
0.160	1.007238	1.004078
0.161	1.006957	1.003896
0.162	1.006687	1.003722
0.163	1.006428	1.003557
0.164	1.006179	1.003398
0.165	1.005939	1.003247
0.166	1.005709	1.003102
0.167	1.005488	1.002964
0.168	1.005275	1.002832
0.169	1.005071	1.002705
0.170	1.004874	1.002585
0.171	1.004685	1.002470
0.172	1.004504	1.002360
0.173	1.004329	1.002255
0.174	1.004161	1.002154
0.175	1.004000	1.002058
0.176	1.003845	1.001966
0.177	1.003696	1.001879
0.178	1.003553	1.001795
0.179	1.003415	1.001715
0.180	1.003283	1.001639
0.181	1.003156	1.001566
0.182	1.003034	1.001496
0.183	1.002916	1.001429
0.184	1.002803	1.001365
0.185	1.002694	1.001305
0.186	1.002590	1.001246
0.187	1.002490	1.001191
0.188	1.002393	1.001138
0.189	1.002301	1.001087
0.190	1.002212	1.001039
0.191	1.002126	1.000992
0.192	1.002044	1.000948
0.193	1.001964	1.000906
0.194	1.001888	1.000866
0.195	1.001815	1.000827
0.196	1.001745	1.000790
0.197	1.001677	1.000755
0.198	1.001612	1.000721
0.199	1.001550	1.000689
0.200	1.001490	1.000658

TABULATION OF $T(\tau/V,\theta)$ FUNCTION FOR
ARGUMENTS BETWEEN 0.200 AND 0.250

No. of Terms in Function Sum = 441

Argument (τ/V)	Square Lattice ($\theta = 90°$)	Hexagonal Lattice ($\theta = 60°$)
0.200	1.001490	1.000658
0.201	1.001432	1.000629
0.202	1.001377	1.000601
0.203	1.001323	1.000574
0.204	1.001272	1.000549
0.205	1.001223	1.000524
0.206	1.001176	1.000501
0.207	1.001130	1.000479
0.208	1.001086	1.000457
0.209	1.001044	1.000437
0.210	1.001004	1.000417
0.211	1.000965	1.000399
0.212	1.000928	1.000381
0.213	1.000892	1.000364
0.214	1.000857	1.000348
0.215	1.000824	1.000332
0.216	1.000792	1.000317
0.217	1.000761	1.000303
0.218	1.000732	1.000290
0.219	1.000704	1.000277
0.220	1.000676	1.000265
0.221	1.000650	1.000253
0.222	1.000625	1.000241
0.223	1.000601	1.000231
0.224	1.000578	1.000220
0.225	1.000555	1.000211
0.226	1.000534	1.000201
0.227	1.000513	1.000192
0.228	1.000493	1.000184
0.229	1.000474	1.000176
0.230	1.000456	1.000168
0.231	1.000438	1.000160
0.232	1.000421	1.000153
0.233	1.000405	1.000146
0.234	1.000389	1.000140
0.235	1.000374	1.000133
0.236	1.000360	1.000128
0.237	1.000346	1.000122
0.238	1.000332	1.000116
0.239	1.000319	1.000111
0.240	1.000307	1.000106
0.241	1.000295	1.000102
0.242	1.000284	1.000097
0.243	1.000273	1.000093
0.244	1.000262	1.000089
0.245	1.000252	1.000085
0.246	1.000242	1.000081
0.247	1.000233	1.000077
0.248	1.000224	1.000074
0.249	1.000215	1.000070
0.250	1.000207	1.000067

APPENDIX B

NEUTRON AGES AND WEIGHTING FACTORS

Two sets of neutron ages and weighting factors are stored internal to the HERESY III code. These sets are given below plus a third set suitable for a nine resonance level treatment of natural uranium systems. This latter set is from work by Nuclear Development Corporation of America* (now United Nuclear). In each set, the highest numbered level is the thermal level.

SET 1

2-Group HAMMER Conversion Set

(NTAU = 1 and 5)

Resonance Level	Fission Source 1		Fission Source 2		Fission Source 3		Effective Fission to Resonance Age
	B_1	τ_1	B_2	τ_2	B_3	τ_3	
1	0.726	61.53	0.002	536.70	0.272	166.00	90.896
2	0.654	82.70	0.003	543.00	0.343	184.50	118.998

SET 2

4-Group HAMMER Conversion Set

(NTAU = 2 and 6)

Resonance Level	Fission Source 1		Fission Source 2		Fission Source 3		Effective Fission to Resonance Age
	B_1	τ_1	B_2	τ_2	B_3	τ_3	
1	1.0	12.6	0.000	131.5	0.0	525.5	12.60
2	0.888	47.0	0.111	150.0	0.001	528.0	58.914
3	0.726	72.5	0.272	170.0	0.002	536.7	99.948
4	0.654	82.70	0.343	184.0	0.003	543.0	118.998

* W. L. Brooks and H. Soodak. *Resonance Absorption in D_2O Lattice Reactors.* USAEC Report NDA-2131-19, Nuclear Development Corp. of America, White Plains, N. Y. (1960).

SET 3

NDA 9-Level Resonance Scheme

Resonance Level	Effective Energy, ev	τ_1	B_1	τ_2	B_2	τ_3	B_3	$\sum_{i=1}^{3} \tau_i B_i$	Energy, ev		MUFT Groups
									Max	Min	
1	5.5×10^4	526.0	0.00125	23.5	0.860	131.5	0.150	22.4	10^6	10^4	1-23
2	2.7×10^3	527.5	0.00155	38.6	0.795	140.1	0.202	48.3	10^4	10^3	24-28
3	550	531.2	0.00175	47.3	0.765	148.2	0.230	71.2	10^3	245	29-31
4	190	534.0	0.00186	52.5	0.742	154.0	0.250	78.4	245	301	32-33
5	102.8	535.5	0.00193	55.8	0.730	157.5	0.262	83.0	130	86	34
6	66.3	536.6	0.00198	58.1	0.723	159.5	0.269	86.5	86	48	35-36
7	36.8	538.2	0.00205	61.4	0.714	162.5	0.279	90.3	48	29	37-39
8	21.0	539.5	0.00212	64.2	0.705	165.8	0.289	94.3	29	12	40-42
9	6.68	542.3	0.00225	70.4	0.690	172.5	0.315	104.1	12	5	47-54
Thermal	*	543.0	0.00253	82.7	0.654	184.5	0.343	118.7	0.625	0	

* Spectrum dependent.

APPENDIX C

NEUTRON AGES AND RESONANCE ESCAPE PROBABILITIES COMPUTED FROM THE HAMMER SYSTEM

One of the code options is to compute moderator ages directly from the data stored on a HAMMER[7] system lattice library. Problems arise from this procedure due to differences in the fission spectrum used in the HAMMER and HERESY III calculations for four groups. The methods used, which are in part empirical, are described in the following paragraphs.

The HAMLET section of the HAMMER system is a Fourier transform slowing down calculation for the homogenized lattice cell. Results are available for one or three epithermal groups. The fission spectrum for the HAMMER system has fission neutrons born in the three epithermal groups with the following groupwise spectrum.

$$\chi_1 = 0.7532 \qquad \chi_2 = 0.2466 \qquad \chi_3 = 0.0002 \qquad \chi_4 = 0.0$$

HERESY III assumes all neutrons are born at age $\tau = 0$.

For a HERESY III calculation with one resonance level, the HAMMER one epithermal group values may be utilized directly because there are no fission spectrum difficulties. Thus, the following definitions are used for the ages and resonance escape probability.

$p \equiv$ HAMMER one epithermal group resonance escape probability

$\tau_1 \equiv k \times \tau_{thermal}$ ($k < 1.0$ and set equal to 0.86 if not specified)

$\tau_2 \equiv \tau_{thermal}$

where $\tau_{thermal}$ is the thermal age or age to the top of the thermal energy group. The constant k that appears in the equation for τ_1 is in general lattice dependent, the default value being a number that has been found to be generally good for a large number of lattices.

For a HERESY III problem using three resonance levels, the difference in fission spectrums has an appreciable effect on the

input parameters. The methods used for the three resonance level conversion are designed to produce p's that reproduce the proper absorption ratios of each epithermal group (or resonance level) to the thermal group (or level) for an infinite lattice of identical rods. The ages are those necessary to produce the proper leakage in the same lattice.

Assume a fission source of 1 neutron in a homogenized cell. The absorption reaction rate in each group may be written as follows for the HAMMER homogenized cell and the HERESY III infinite lattice.

HAMMER	HERESY III
$\Sigma_{a_1}\psi_1 = \frac{\Sigma_{a_1}\chi_1}{\Sigma_{a_1}+\Sigma_{r_1}} = (1-p_1)\chi_1$	$\Sigma_{a_1}\psi_1 = \frac{\Sigma_{a_1}}{\Sigma_{a_1}+\Sigma^*_{r_1}}$
$\Sigma_{a_2}\psi_2 = \frac{\Sigma_{a_2}\chi_2 + \Sigma_{a_2}\Sigma_{r_1}\psi_1}{\Sigma_{a_2}+\Sigma_{r_2}}$	$\Sigma_{a_2}\psi_2 = \frac{\Sigma_{a_2}\Sigma^*_{r_1}\psi_1}{\Sigma_{a_2}+\Sigma^*_{r_2}}$
$= (1-p_2)(\chi_2 + p_1\chi_1)$	$= \frac{\Sigma_{a_2}p^*_1}{\Sigma_{a_2}+\Sigma^*_{r_2}}$
$\Sigma_{a_3}\psi_3 = \frac{\Sigma_{a_3}\chi_3 + \Sigma_{a_3}\Sigma_{r_2}\psi_2}{\Sigma_{a_3}\Sigma_{r_3}}$	$\Sigma_{a_3}\psi_3 = \frac{\Sigma_{a_3}\Sigma^*_{r_2}\psi_2}{\Sigma_{a_3}+\Sigma^*_{r_3}}$
$= (1-p_3)(\psi_3 + p_2(\psi_2 + p_1\chi_1))$	$= \frac{\Sigma_{a_3}p^*_1p^*_2}{\Sigma_{a_3}+\Sigma^*_{r_3}}$

where the $\Sigma^*_{r_i}$ and p^*_i are modified values of Σ_r and p to account for the spectrum differences. Equating each pair of equations yields the value for the Σ^*_r as

$$\Sigma^*_{r_1} = \left[\frac{1}{(1-p_1)\psi_1} - 1\right]\Sigma_{a_1}$$

$$\Sigma^*_{r_2} = \frac{p^*_1}{(1-p_2)(\chi_2+p_1\chi_1)}\Sigma_{a_2}$$

$$\Sigma^*_{r_3} = \left[\frac{p^*_1p^*_2}{(1-p_3)(\chi_3+p_2(\chi_2+p_1\chi_1))} - 1\right]\Sigma_{a_3}$$

These values for the modified cross sections then may be used to compute the modified resonance escape probabilities and ages in the HERESY III fission spectrum as follows:

$$\tau_1^* = \frac{D_1}{\Sigma_{a_1} + \Sigma_{r_1}^*} \qquad \tau_2^* = \frac{D_2}{\Sigma_{a_2} + \Sigma_{r_2}^*} \qquad \tau_3^* = \frac{D_3}{\Sigma_{a_3} + \Sigma_{r_3}^*}$$

$$p_1^* = \frac{\Sigma_{r_1}^*}{\Sigma_{a_1} + \Sigma_{r_1}^*} \qquad p_2^* = \frac{\Sigma_{r_2}^*}{\Sigma_{a_2} + \Sigma_{r_2}^*} \qquad p_3^* = \frac{\Sigma_{r_3}^*}{\Sigma_{a_3} + \Sigma_{r_3}^*}$$

The modified ages now are the ages from the highest to the lowest energy in each of the epithermal groups. The age to the effective resonance level within these groups, however, is less than this value. The level ages are assigned by an empirical algorithm based on studies of a range of lattices as follows:

$$\tau_1 = 0.5\ \tau_1^*$$

$$\tau_2 = \tau_1^* + 0.5(\tau_2^* - \tau_1^*)$$

$$\tau_3 = \tau_1^* + \tau_2^* + k(\tau_3^* - \tau_2^*) \qquad (k < 1.0 \text{ and is set equal to } 0.8 \text{ if not specified})$$

where τ_4 is the thermal age for the three resonance level problem.

APPENDIX D

THERMAL ABSORPTION PARAMETER OPTIONS

In Feinberg's initial paper,[1] it was shown that the heterogeneous thermal utilization satisfied the relationship

$$L^2(\text{lattice}) = (1-f)L^2(\text{mod}) \qquad \text{(D-1)}$$

Because thermal diffusion coefficients are assumed to be equal to that of the moderator throughout the reactor, this leads immediately to

$$1-f = \frac{\Sigma_a(\text{mod})}{\Sigma_a(\text{lattice})} \qquad \text{(D-2)}$$

where $\Sigma_a(\text{mod})$ is a constant throughout the reactor. If $\Sigma_a(\text{lattice})$ is identified with $\Sigma_a(\text{cell})$ obtained from some thermal cell calculation (such as THERMØS), then equation (D-1) may be taken to be the defining equation for f.

If the thermal spectra of the various cells representing components of the mixed lattice do not agree with each other, then some suitable weighted value of $\Sigma_a(\text{mod})$ must be obtained. The automatic conversion algorithm in HERESY III simply weights the moderator absorption cross sections by the number of such components (cells) in the lattice. One is then left with the problem of whether or not to accept the cell homogenized thermal cross sections for the various cells, based as they are on different thermal spectra, or whether to try to make some kind of "correction" for the thermal spectra mismatch. Option 1 corresponds to accepting the THERMØS computed cell-averaged cross sections directly, even when spectral mismatch is present. In Option 2, the THERMØS cell-averaged cross sections are combined with the moderator cross section from the same cell to produce f, thus largely "canceling" out the inconsistency. Only qualitative arguments can be summoned to support either of these choices.

Suich[14] has suggested that in order to avoid this difficulty, cell calculations can be rerun with altered cell boundaries for the various components until (in effect) a common thermal spectrum is obtained. Under this scheme, strongly absorbing components would be assigned large cell boundaries and weakly absorbing

components would be assigned small cell boundaries. He suggested a specific iterative scheme for achieving this. While some such approach seems justified for careful final design calculations, it would be somewhat laborious for survey calculations. His analysis emphasizes, however, the desirability of connecting the rod parameter δ with the THERMØS cell-averaged Σ_a and its corresponding cell size by means of an algorithm which is insensitive to the cell size.

Numerical examples are helpful in illustrating the sensitivity of results to the choice of the thermal absorption parameter option. THERMØS cell calculations were run for three different fuel assemblies slightly enriched uranium metal rods with (1-, 2- and 3-inch-diameters in heavy water at various pitches). The THERMØS results are shown in Table D-1. The corresponding rod parameters δ from equation (3.19) are plotted as a function of cell size in Figure D-1 for both Option 1 and Option 2. A constant value of Σ_a(mod) of 0.00007 cm^{-1} was used in equation (3.19), and in the case of Option 2 the spectrum in the 9-inch pitch lattice was chosen as "correct." In assessing the significance of dependence of δ on cell size, it should be kept in mind that a given percent change in δ will generally make a somewhat smaller percent change in absorption ratio in a mixed lattice. The shape of the curves in these examples suggests an obvious though inelegant algorithm for achieving insensitivity of the rod parameter δ to the cell area. Delta can be computed both ways and averaged. This is Option 0, the default option for the thermal absorption parameter. Plots of δ versus cell size using Option 0 are given in Figure D-1.

TABLE D-1

Cell Homogenized Absorption Cross Sections by THERMØS (cm^{-1})

Diameter of Fuel Rod, inches	1	2	3
Triangular Lattice Pitch, inches			
5	0.006836	0.018436	0.034443
7	0.003414	0.008695	0.015491
9	0.002033	0.004896	0.008290
11	0.001349	0.003090	0.005027
13	0.000967	0.002119	0.003319

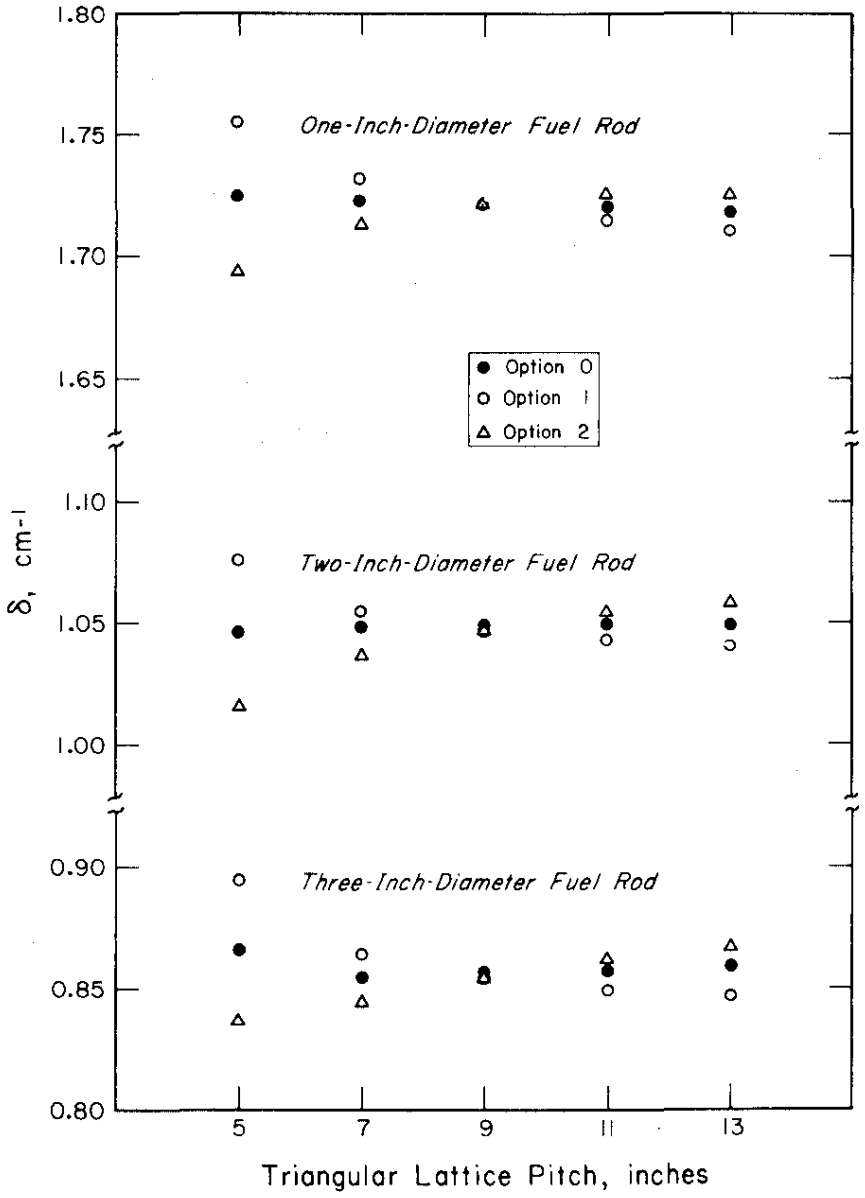


FIGURE D-1 Variation of Delta Versus Cell Size for Solid Rod Examples

The same shapes and lack of sensitivity are exhibited when the moderator absorption cross section is much larger (0.0005 cm^{-1}, corresponding e.g., to large transverse leakage) although the magnitudes are different. It would appear that if this option is used, and if the examples are at all typical, cell sizes can be chosen on the basis of intuition and the ensuing mixed lattice results will probably be satisfactory without the necessity of an iterative procedure.

As a check on the sensitivity of results to the choice of this option the experimental mixed-lattice results reported by Graves, et al.[15] were calculated using HAMMER cell calculations, automatic parameter conversion, and HERESY III with all three thermal absorption options. Results (buckling values only) are given in Table D-2. The differences in buckling are small enough so that there is little incentive to argue for a preference on the basis of these results.

TABLE D-2

Sensitivity of Buckling Results to Choice of Thermal Absorption Parameter Option

	Critical Vertical Buckling, M^{-2}			
Lattice Number[15]	Experimental[15]	HERESY III, with NTHER=		
		0	1	2
3	0.97	1.08	1.13	1.02
4	2.23	1.92	1.86	1.99
5	3.41	3.24	3.18	3.30

APPENDIX E

SAMPLE PROBLEMS

PROBLEM 1 - INFINITE LATTICE

A simple infinite lattice mixture (20-cm hexagonal cell) of two rod types is shown in Figure E-1. The lattice is generated by the internal generator using axes with an acute angle of 60° between them. Figure E-2 shows the input for this problem, and Figures E-3 and E-4 show the output from the code.

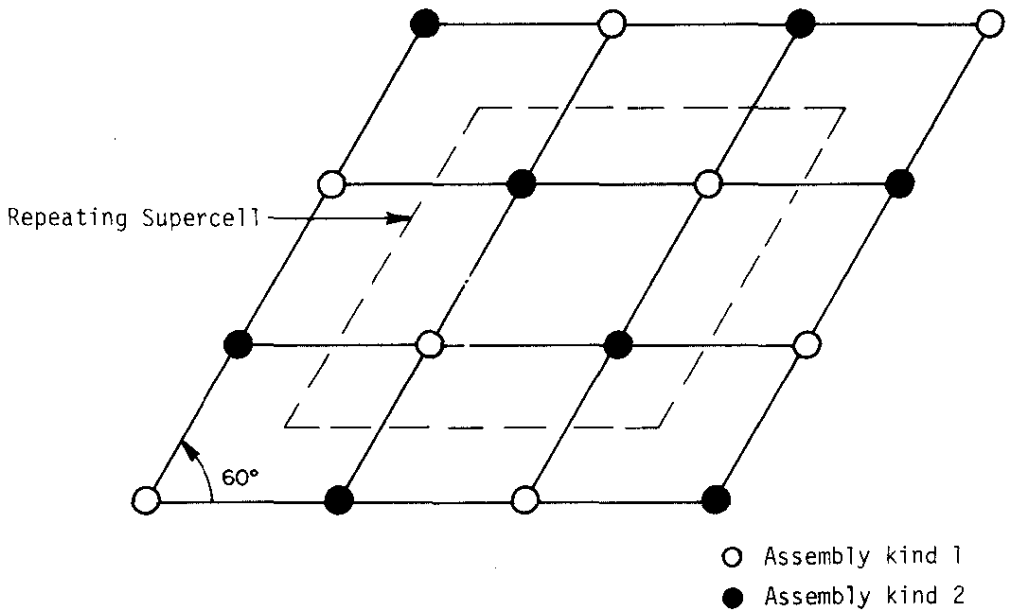


FIGURE E-1 Hexagonal Cell with 20-cm Pitch

FIGURE E-2

```
 HERESY III INFINITE LATTICE TEST PROBLEM - 20 CM PITCH HEX LATTICE
     4      1              1              1              1              0
     2    105              1              1
     4    109              1              1              4              2
     4    175              1              2              2              1
1    1    229              1
     4    451 60.0                                                  900.0
     4    455 40.0          40.0           40.0           40.0
     4    505 40.0          40.0           40.0           40.0
     4    555  0.0           0.0           20.0           20.0
     4    605  0.0          20.0            0.0           20.0
     2    657 4.0           4.0
     2    659 15000.        0.0001
     3    724 1.03          100.0          75.0
     2    905 0.995         0.985
     2    925 0.55          0.65
     2    945 1.65          1.35
1    2   1125 346.4         346.4
```

FIGURE E-3

SUMMARY OF SLOWING DOWN PARAMETERS AND LATTICE INPUT DATA FOR HERESY III

HERESY III INFINITE LATTICE TEST PROBLEM - 20 CM PITCH HEX LATTICE

THIS IS AN INFINITE LATTICE PROBLEM

NUMBER OF ROD TYPES = 4 NUMBER OF ROD KINDS = 2

****

ITERATION MAXIMUM LIMITS

INNER EIGENVALUE = 100 OUTER EIGENVALUE = 10 CRITICALITY SEARCH = 10

CONVERGENCE CRITERIA

INVERSION = 0.000001 INNER EIGENVALUE = 0.001000 OUTER EIGENVALUE = 0.001000 CRITICALITY = 0.001000

MODERATOR PARAMETERS

AXIAL BUCKLING = 0.0 DIFFUSION AREA = 15000.00 MODERATOR ABSORPTION XSECTION = 0.0001000000

RESONANCE LEVEL SCHEME

****

RESONANCE LEVEL	FISSION SOURCE 1 FISSION FRACTION	FISSION SOURCE 1 FISSION TO RESONANCE AGE	FISSION SOURCE 2 FISSION FRACTION	FISSION SOURCE 2 FISSION TO RESONANCE AGE	FISSION SOURCE 3 FISSION FRACTION	FISSION SOURCE 3 FISSION TO RESONANCE AGE	EFFECTIVE FISSION TO RESONANCE AGE
1	1.000	93.623	0.0	1.030	0.0	1.030	93.623
* 2	1.000	122.568	0.0	2.060	0.0	2.060	122.568

* - THERMAL LEVEL

PARAMETERS FOR EACH ROD KIND

****

ROD KIND 1 ** LATTICE CASE 0

THERMAL ETA = 1.6500 DELTA = 0.497455 THERMAL UTILIZATION = 0.995000 CELL VOLUME = 346.400

RESONANCE ETA 1) = 0.550

RESONANCE A 1) = 100.0

ROD KIND 2 ** LATTICE CASE 0

THERMAL ETA = 1.3500 DELTA = 0.792007 THERMAL UTILIZATION = 0.985000 CELL VOLUME = 346.400

RESONANCE ETA 1) = 0.650

RESONANCE A 1) = 75.0

PARAMETERS FOR EACH ROD TYPE

****

ROD TYPE	ROD KIND	NO. RODS	DELTA	ETA	F	1./DELTA
1	1	1207	0.49745	1.65000	0.99500	2.01023
2	2	1207	0.79201	1.35000	0.98500	1.26261
3	2	1207	0.79201	1.35000	0.98500	1.26261
4	1	1207	0.49745	1.65000	0.99500	2.01023

****

FIGURE E-4

HERESY III INFINITE LATTICE TEST PROBLEM - 20 CM PITCH HEX LATTICE

NO OUTER ITERATIONS = 3 CURRENT EIGENVALUE = 1.3009281 PREVIOUS EIGENVALUE = 1.3019133

NO INNER ITERATIONS = 1 CURRENT EIGENVALUE = 1.3009281 PREVIOUS EIGENVALUE = 1.3009291

ABSORPTIONS FOR EACH ROD TYPE

ROD TYPE	ROD KIND	NO RODS	RESONANCE ABS	THERMAL ABS
1	1	1207	0.295094	0.999988
2	2	1207	0.205026	0.456747
3	2	1207	0.205025	0.456719
4	1	1207	0.295094	1.000000

AVERAGE RESONANCE ABSORPTION = 0.250060 AVERAGE RESONANCE ETA = 0.590995

AVERAGE THERMAL ABSORPTION = 0.728364 AVERAGE THERMAL ETA = 1.555938

LATTICE AVERAGED PARAMETERS

AVERAGE THERMAL ETA = 1.555938 RESONANCE ESCAPE PROB = 0.746064 THERMAL UTILIZATION = 0.991843

NON-LEAKAGE PROB = 0.999560 TOTAL FISSION/SLOW FISSION RATIO = 1.130402 STATIC REACTIVITY (K) = 1.300928

APPROX MODERATOR ABSORPTIONS = 28.920898 TOTAL LEAKAGE = 1.560303

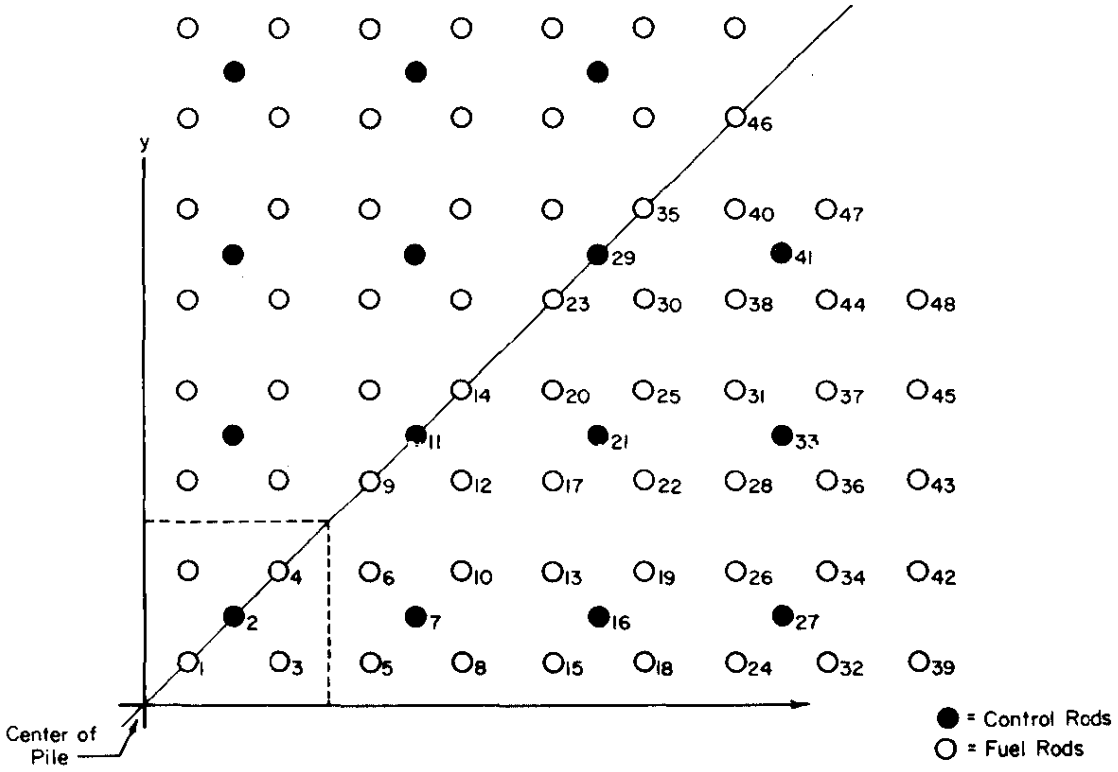
LATTICE MATERIAL BUCKLING = 1202.6 MICROBUCKS

AVERAGE ABSORPTIONS FOR EACH ROD KIND

ROD KIND	NO RODS	AVG THERMAL ABSORPTIONS	AVG RESONANCE ABSORPTIONS
1	2414	0.999994	0.295093
2	2414	0.456733	0.205026

PROBLEM 2 - FINITE LATTICE WITH CONTROL ROD SEARCH

A 10-inch pitch square cell finite lattice with interstitially located central rods is shown in Figure E-5. This lattice is generated by the internal square lattice generator. The input cards are shown in Figure E-6, and the code output is shown in Figure E-7 and E-8.



EXAMPLE PROBLEM

FIGURE E-5 Sector of Large Finite Lattice

FIGURE E-6

```
HERESY III FINITE LATTICE TEST PROBLEM - 10 INCH SQUARE PITCH
   4      1              1              1              0              1
   2    105              1              1
   4    109              1              0             48              2
        175              1              2              1              1              1
        180              1              2              1              1              1
        185              2              1              1              1              1
        190              2              1              1              1              1
        195              2              1              1              1              1
        200              1              2              1              2              1
        205              1              1              2              1              1
        210              1              1              1              1              1
        215              2              1              1              1              1
   3    220              1              1              1
1       225              2              2                                            1
          1 1.0          2.0            3.0            3.0            5.0
          6 5.0          6.0            7.0            5.0            7.0
         11 6.0          7.0            9.0            7.0            9.0
         16 10.0         9.0            11.0           11.0           9.0
         21 10.0         11.0           9.0            13.0           11.0
         26 13.0         14.0           13.0           10.0           11.0
         31 13.0         15.0           14.0           15.0           11.0
         36 15.0         15.0           13.0           17.0           13.0
         41 14.0         17.0           17.0           15.0           17.0
   3     46 13.0         15.0           17.0
        151 1.0          2.0            1.0            3.0            1.0
        156 3.0          2.0            1.0            5.0            3.0
        161 6.0          5.0            3.0            7.0            1.0
        166 2.0          5.0            1.0            3.0            7.0
        171 6.0          5.0            9.0            1.0            7.0
        176 3.0          2.0            5.0            10.0           9.0
        181 7.0          1.0            6.0            3.0            11.0
        186 5.0          7.0            9.0            1.0            11.0
        191 10.0         3.0            5.0            9.0            7.0
   3    196 13.0         11.0           9.0
   4    655 12.7         12.7           12.7           12.7
   3    659 12500.       0.00007        0.00015
   2    725 58.8         4.0
   2    905 0.986        0.93
   2    925 0.56         0.1
   2    945 1.25         0.0
1  2   1125 645.16       322.48
```

FIGURE E-7

SUMMARY OF SLOWING DOWN PARAMETERS AND LATTICE INPUT DATA FOR HERESY III

HERESY III FINITE LATTICE TEST PROBLEM - 10 INCH SQUARE PITCH

THIS IS A FINITE LATTICE PROBLEM IN AN INFINITE SEA OF MODERATOR

NUMBER OF ROD TYPES = 48 NUMBER OF ROD KINDS = 2

****

ITERATION MAXIMUM LIMITS

INNER EIGENVALUE = 100 OUTER EIGENVALUE = 10 CRITICALITY SEARCH = 10

CONVERGENCE CRITERIA

INVERSION = 0.000001 INNER EIGENVALUE = 0.001000 OUTER EIGENVALUE = 0.001000 CRITICALITY = 0.001000

MODERATOR PARAMETERS

AXIAL BUCKLING = 0.000150 DIFFUSION AREA = 12500.00 MODERATOR ABSORPTION XSECTION = 0.0000700000

RESONANCE LEVEL SCHEME

****

RESONANCE LEVEL	FISSION SOURCE 1 FISSION FRACTION	FISSION SOURCE 1 FISSION TO RESONANCE AGE	FISSION SOURCE 2 FISSION FRACTION	FISSION SOURCE 2 FISSION TO RESONANCE AGE	FISSION SOURCE 3 FISSION FRACTION	FISSION SOURCE 3 FISSION TO RESONANCE AGE	EFFECTIVE FISSION TO RESONANCE AGE
1	1.000	90.896	0.0	1.000	0.0	1.000	90.896
* 2	1.000	118.998	0.0	2.000	0.0	2.000	118.998

* = THERMAL LEVEL

PARAMETERS FOR EACH ROD KIND

****

ROD KIND 1 ** LATTICE CASE 0

THERMAL ETA = 1.2500 DELTA = 0.747381 THERMAL UTILIZATION = 0.986000 CELL VOLUME = 645.160

RESONANCE ETA 1) = 0.560

RESONANCE A 1) = 58.8

ROD KIND 2 ** LATTICE CASE 0

THERMAL ETA = 0.0 DELTA = 3.830420 THERMAL UTILIZATION = 0.930000 CELL VOLUME = 322.480

RESONANCE ETA 1) = 0.100

RESONANCE A 1) = 4.0

PARAMETERS FOR EACH ROD TYPE

****

ROD TYPE	ROD KIND	NO. RODS	DELTA	ETA	F	1./DELTA
1	1	4	0.74738	1.25000	0.98600	1.33801
2	2	4	3.83042	0.0	0.93000	0.26107
3	1	8	0.74738	1.25000	0.98600	1.33801
4	1	4	0.74738	1.25000	0.98600	1.33801
5	1	8	0.74738	1.25000	0.98600	1.33801
6	1	8	0.74738	1.25000	0.98600	1.33801
7	2	8	3.83042	0.0	0.93000	0.26107
8	1	8	0.74738	1.25000	0.98600	1.33801
9	1	4	0.74738	1.25000	0.98600	1.33801
10	1	8	0.74738	1.25000	0.98600	1.33801
11	2	4	3.83042	0.0	0.93000	0.26107
12	1	8	0.74738	1.25000	0.98600	1.33801
13	1	8	0.74738	1.25000	0.98600	1.33801
14	1	4	0.74738	1.25000	0.98600	1.33801
15	1	8	0.74738	1.25000	0.98600	1.33801
16	2	8	3.83042	0.0	0.93000	0.26107
17	1	8	0.74738	1.25000	0.98600	1.33801
18	1	8	0.74738	1.25000	0.98600	1.33801
19	1	8	0.74738	1.25000	0.98600	1.33801
20	1	8	0.74738	1.25000	0.98600	1.33801
21	2	8	3.83042	0.0	0.93000	0.26107
22	1	8	0.74738	1.25000	0.98600	1.33801
23	1	4	0.74738	1.25000	0.98600	1.33801
24	1	8	0.74738	1.25000	0.98600	1.33801
25	1	8	0.74738	1.25000	0.98600	1.33801
26	1	8	0.74738	1.25000	0.98600	1.33801
27	2	8	3.83042	0.0	0.93000	0.26107
28	1	8	0.74738	1.25000	0.98600	1.33801
29	2	4	3.83042	0.0	0.93000	0.26107
30	1	8	0.74738	1.25000	0.98600	1.33801
31	1	8	0.74738	1.25000	0.98600	1.33801
32	1	8	0.74738	1.25000	0.98600	1.33801
33	2	8	3.83042	0.0	0.93000	0.26107
34	1	8	0.74738	1.25000	0.98600	1.33801
35	1	4	0.74738	1.25000	0.98600	1.33801
36	1	8	0.74738	1.25000	0.98600	1.33801
37	1	8	0.74738	1.25000	0.98600	1.33801
38	1	8	0.74738	1.25000	0.98600	1.33801
39	1	8	0.74738	1.25000	0.98600	1.33801
40	1	8	0.74738	1.25000	0.98600	1.33801
41	2	8	3.83042	0.0	0.93000	0.26107
42	1	8	0.74738	1.25000	0.98600	1.33801
43	1	8	0.74738	1.25000	0.98600	1.33801
44	1	8	0.74738	1.25000	0.98600	1.33801
45	1	8	0.74738	1.25000	0.98600	1.33801
46	1	4	0.74738	1.25000	0.98600	1.33801
47	1	8	0.74738	1.25000	0.98600	1.33801
48	1	8	0.74738	1.25000	0.98600	1.33801

****

SUMMARY OF CRITICALITY SEARCH OVER THERMAL UTILIZATION PARAMETER

EIGENVALUE BEING SEARCHED FOR = 1.000

ITERATION NO	CURRENT EIGENVALUE	PREVIOUS EIGENVALUE	CURRENT F VALUE	ROD KIND BEING SEARCHED
1	1.0998993	1.0762491	0.367900	2
2	0.9805847	1.0998993	0.990017	2
3	1.0042658	0.9805847	0.986038	2
4	0.9997435	1.0042658	0.986861	2

FIGURE E-8

HERESY III FINITE LATTICE TEST PROBLEM - 10 INCH SQUARE PITCH

NO OUTER ITERATIONS = 2 CURRENT EIGENVALUE = 0.9997435 PREVIOUS EIGENVALUE = 0.9997827

NO INNER ITERATIONS = 1 CURRENT EIGENVALUE = 0.9997435 PREVIOUS EIGENVALUE = 0.9997556

ABSORPTIONS FOR EACH ROD TYPE

ROD TYPE	ROD KIND	NO RODS	RESONANCE ABS	THERMAL ABS
1	1	4	0.119871	1.000000
2	2	4	0.007824	0.475322
3	1	8	0.118292	0.986381
4	1	4	0.116688	0.972536
5	1	8	0.115400	0.963161
6	1	8	0.113747	0.948904
7	2	8	0.007429	0.451318
8	1	8	0.110912	0.924439
9	1	4	0.110721	0.924630
10	1	8	0.109187	0.909554
11	2	4	0.007009	0.425821
12	1	8	0.106020	0.884065
13	1	8	0.103760	0.866072
14	1	4	0.101101	0.841623
15	1	8	0.105597	0.881749
16	2	8	0.006703	0.407205
17	1	8	0.100444	0.839342
18	1	8	0.098957	0.824423
19	1	8	0.097027	0.807774
20	1	8	0.095250	0.794524
21	2	8	0.006235	0.378789
22	1	8	0.093464	0.779084
23	1	4	0.089079	0.745075
24	1	8	0.092145	0.769715
25	1	8	0.087905	0.731123
26	1	8	0.090108	0.752130
27	2	8	0.005775	0.350865
28	1	8	0.086313	0.721738
29	2	4	0.005370	0.326222
30	1	8	0.081300	0.677929
31	1	8	0.080310	0.669907
32	1	8	0.084693	0.703680
33	2	8	0.005241	0.318440
34	1	8	0.082578	0.685468
35	1	4	0.073122	0.607028
36	1	8	0.078534	0.653064
37	1	8	0.072061	0.597126
38	1	8	0.073137	0.612196
39	1	8	0.069820	0.665245
40	1	8	0.064082	0.537279
41	2	8	0.004197	0.255079
42	1	8	0.067964	0.647485
43	1	8	0.064236	0.611724
44	1	8	0.063332	0.530536
45	1	8	0.058433	0.555480
46	1	4	0.048603	0.504300
47	1	8	0.045777	0.459931
48	1	8	0.046560	0.485778

AVERAGE RESONANCE ABSORPTION = 0.072852 AVERAGE RESONANCE ETA = 0.553295

AVERAGE THERMAL ABSORPTION = 0.675580 AVERAGE THERMAL ETA = 1.130577

LATTICE AVERAGED PARAMETERS

AVERAGE THERMAL ETA = 1.130577 RESONANCE ESCAPE PROB = 0.909423 THERMAL UTILIZATION = 0.986082

NON-LEAKAGE PROB = 0.936644 TOTAL FISSION/SLOW FISSION RATIO = 1.052773 STATIC REACTIVITY (K) = 0.999743

APPROX MODERATOR ABSORPTIONS = 3.280142 TOTAL LEAKAGE = 15.941782

AVERAGE ABSORPTIONS FOR EACH ROD KIND

ROD KIND	NO RODS	AVG THERMAL ABSORPTIONS	AVG RESONANCE ABSORPTIONS
1	284	0.740129	0.086556
2	60	0.370050	0.006091

THE VALUE OF THE THERMAL UTILIZATION PARAMETER FOR ROD KIND 2 AT CRITICAL IS 0.986862

APPENDIX F

COMPUTER ENVIRONMENT INFORMATION

The HERESY III code was written in FORTRAN IV for operation on the IBM System/360-65 computer. It requires 180,000 bytes (45,000 single precision words) of high speed care, and up to 420,000 bytes (105,000 single precision words) of disk or drum storage. The user may optionally call for up to three tapes to be mounted.

The amount of disk or drum storage necessary will depend on the problem defined by the user. The following is a list of data set reference numbers, usage, device types, and volumes of data required for the maximum size problem that HERESY III will solve.

Data Set Number	Use	Device	Volume of Data
5	Data input	System imput	20 to 100 cards
6	Data output	System output	100 to 1000 lines
17,18,19	Lattice libraries	Tape	
20	Temporary storage	Disk or drum	10,000 single precision words
21 to 58	Temporary storage	Disk or drum	2,500 single precision words per data set