TRG

INC.

[redacted]

TECHNICAL RESEARCH GROUP
2 AERIAL WAY · SYOSSET, N. Y.

NYO-2675

HETEROGENEOUS REACTOR CALCULATION METHODS

Quarterly Progress Report No. 3
AEC Contract No. AT(30-1)-2375

Carl N. Klahr
Lawrence B. Mendelsohn
Jerome Heitner

TECHNICAL RESEARCH GROUP

NYO-2675
TRG-129-QTR-3

HETEROGENEOUS REACTOR CALCULATION METHODS

Carl N. Klahr
Lawrence B. Mendelsohn
Jerome Heitner

Quarterly Progress Report No. 3

October 1 - December 31, 1959
AEC Contract No. AT(30-1) - 2375

Submitted to:

U. S. Atomic Energy Commission
Washington, D. C.

Submitted by:

TRG, Incorporated
2 Aerial Way
Syosset, New York

Authors:

Carl N. Klahr
Carl N. Klahr

Lawrence B. Mendelsohn
Lawrence B. Mendelsohn

Jerome Heitner
Jerome Heitner

Department Head:

Raphael Aronson
Raphael Aronson

ABSTRACT

Three series of heterogeneous reactor physics calculations were carried out using HERESY 1, an IBM-704 code.

Significant results include:

(a) The variation in reactivity and power pattern as a large array of rods is gradually built up from a smaller array (Section 3).

(b) A study of power flattening in spiked cores, in which the average-to-maximum power ratio is varied considerably as the distribution pattern of enriched rods within an array is changed (Section 4).

(c) The sensitivity of the results obtained by self-consistent heterogeneous procedure is found to be only weakly dependent on errors in the kernels (Section 5).

A description of the HERESY 1 code is given in Section 2. This code treats an array of up to 6500 rods arranged in up to 50 rod types, with a typical computation time of less than one minute.

TABLE OF CONTENTS

Abstract

SECTION		PAGE
1.	Introduction	1
2.	Description of HERESY 1 Code	5
3.	Approach to Criticality of a Square Lattice in Graphite	18
4.	Study of Spiked Cores for Power Flattening	28
5.	The Self-consistent Procedure: Sensitivity to Kernel Errors	42
Appendix I - Third (Axial) Dimension in HERESY 1		53
References		55

Section 1. Introduction

The digital computer code for heterogeneous reactor calculations has been completed and debugged. This code, which has been dubbed HERESY 1, has been used for a number of calculations described in the present report. These calculations illustrate the scope and usefulness of heterogeneous reactor physics calculations, as opposed to the conventional homogenized calculations.

The HERESY 1 code treats an array of up to 6500 rods arranged in an infinite moderator in up to 50 rod types. The array is two dimensional when the rods are considered infinitely long in the axial dimension. If the rods are considered of finite axial extent, the third (axial) dimension of the core can be introduced into the calculations through the well known oversimplification of assuming an axial power profile proportional to a chopped-cff cosine. This assumption permits HERESY 1 to treat the axial dimension by simply using new parameter values. These recipes are given in Appendix I.

A description of HERESY 1, the input data required, and the output results obtained is given in Section 2. HERESY1 represents all resonance absorptions in U^{238} by one equivalent resonance. Resonance absorptions and fissions in U^{235} are ignored.

Work has begun on a new version of the heterogeneous code,

dubbed HERESY 2, which will include a number of resonance absorption levels in U^{238} and the effects of resonance fissions in U^{235}.

Three types of heterogeneous reactor calculations are treated in the present report. In Section 3 calculation results for a number of unenriched-rod configurations in a graphite moderator are presented. The core arrays range from a 3 by 3 lattice to a 9 by 9 lattice. Significant results include the variation in reactivity between configurations as a large array is gradually built up from a smaller array. More important, the relative absorptions in the individual rods are calculated, something that one cannot obtain from conventional homogeneous calculations. The variation of absorption patterns between configurations and within any one configuration are indicative of the variation of power between rods within a core as the core pattern is varied. Such calculations can be used to design cores of higher power density. To the reactor physicist it is important to be able to explain these variations in power density between rods in terms of the relative balance of moderation, flux depression, and the "shadowing" of some rods by other rods.

In Section 4 a study of spiked cores is made by heterogeneous calculation methods. An array of 81 rods in graphite is considered, of which 20 are enriched and the remainder are unenriched. By distributing the enriched rods in various ways within this array the reactivity and the average-to-maximum power

ratio can be varied considerably. A number of spiked configurations of this type have been calculated using the HERESY 1 code. The resulting pattern of absorptions indicates the spiking configurations that seem promising for increasing power density.

One can develop an iterative procedure to develop successive spiking configurations that progressively increase the average-to-maximum power ratio. This method has a number of advantages over methods previously proposed for power flattening based on homogeneous reactor physics calculations.

1. It calculates power density directly in each rod by obtaining the relative absorptions in the discrete rods.
2. A simple series of calculations is carried out on HERESY 1. No complicated differential equations need be solved.

In Section 5 a series of calculations is presented indicating the sensitivity of the self-consistent heterogeneous procedure. This procedure consists of using a set of kernel functions and a measurement of thermal utilization in a one-component infinite lattice to obtain the fuel element parameters. The parameters thus obtained are then used together with the original kernel functions to calculate reactivity and power distributions for configurations of interest. It has been shown[1] that this self-consistent procedure (using the same kernel functions to estimate the rod parameters and to make heterogeneous

calculations) leads to some cancellation of errors that may be present in the kernels and in the rod parameter estimation procedure. In particular it has been conjectured that the errors in the reactivity and the power pattern are much smaller than errors that may be present in the kernel functions and in the rod parameters. This conjecture, if substantiated, is quite important because it would attribute relatively high accuracy to heterogeneous calculations, e.g., those made using HERESY 1.

A series of calculations has been made to investigate this conjecture. In one series of calculations the kernels were varied. In another series of calculations the rod parameters were varied. In all the calculations the changes in reactivity and in power distribution consequent to the variations is relatively small. However, the evaluation of these results has not been completed.

Section 2. Description of HERESY 1 Code

HERESY, HEterogeneous REactor SYstem program, is an IBM 704 code for the calculation of reactivity and relative thermal neutron absorptions of representative rods within heterogeneous reactors. The code is capable of handling up to 50 types of rods which are defined by geometrical symmetry and composition. The maximum number of individual rods which may be used to map either a finite or infinite lattice reactor is 6500, though this may be increased. Typical computing time, including card reading, for a two-dimensional problem with 12 rod types, is less than one minute.

2.1 Mathematical Treatment

In matrix notation the HERESY 1 code solves the following problem:[2]

$$\underline{\underline{\gamma}}\ \underline{i} = \frac{1}{k}\ \underline{\underline{G}}\ \underline{i} - \underline{\underline{Z}}\ \underline{i} \qquad (2.1)$$

where $\underline{i}$ is the vector whose components are the relative absorptions in each rod type and $\underline{\underline{G}}$, $\underline{\underline{Z}}$, and $\underline{\underline{\gamma}}$ are matrices relating these absorptions to each other. k is the reactivity of the configuration. The HERESY 1 code solves for k and the vector $\underline{i}$ of relative rod absorptions in the various rod types.

All rods of identical composition, geometry, and spatial symmetry in the reactor are said to constitute a rod type. All rods belonging to the same type will be physically identical at all times during reactor burnup, and will experience identical neutron absorption (and fission) rates. The number of such different rod types determines the order of the matrices in (2.1).

Thus in an M type configuration the matrices $\underline{\underline{G}}$, $\underline{\underline{Z}}$ and $\underline{\underline{\gamma}}$ will be M by M and the vector i will be of order M. The elements of the matrices are as follows:

$\underline{\underline{\gamma}}$ is a diagonal matrix whose diagonal elements are the values γ_n for each of the rod types.

The $\underline{\underline{Z}}$ matrix is obtained from the thermal flux kernel f_{nm}. We shall designate rod types by a Roman letter subscript and a particular rod of that type by a Greek letter subscript. Thus f_{nm} will be written with four indices, $f_{n\alpha,m\beta}$, the two to the right of the comma referring to the source rod (the β rod of the m-th type), the two to the left of the comma referring to the receiver rod (the α rod of the n-th type). Then the element Z_{nm} of the matrix is defined as

$$Z_{nm} = \sum_{\beta} f_{n\alpha,m\beta} \tag{2.2}$$

the summation extending over all rods of the m-th type. Note that Z_{nm} is independent of α because of symmetry.

The $\underline{\underline{G}}$ matrix is obtained from the kernel F^*_{nm} which represents slowing down from fission followed by thermal diffusion, with corrections for the flux diminution due to resonance absorption.

$$G_{nm} = \sum_{\beta} F^*_{n\alpha,m\beta}\ \eta_m \tag{2.3}$$

It is convenient to define the following matrices:

$\underline{\underline{T}}$, with components $T_{nm} = \sum_{\beta} F_{n\alpha,m\beta}$

$\underline{\underline{T}}^r$, with components $T^r_{nm} = \sum_{\beta} F^r_{n\alpha,m\beta}$

$\underline{\underline{S}}^r$, with components $S^r_{nm} = \sum_\beta g^{(r-1)}_{n\alpha, m\beta}$

$\underline{\underline{A}}^r$, a diagonal matrix with components A_m

In terms of these matrices $\underline{\underline{G}}$ may be written as follows:

$$\underline{\underline{G}} = (\underline{\underline{T}} - \underline{\underline{T}}^r \underline{\underline{A}}^r \underline{\underline{S}}^r) \underline{\underline{\eta}} . \tag{2.4}$$

Equation (2.1) can be written as

$$\underline{\underline{L}}\ \underline{i} = \frac{1}{k} \underline{\underline{G}}\ \underline{i} , \tag{2.5}$$

where $\underline{\underline{L}} = \underline{\underline{Z}} \div \underline{\underline{\gamma}}$. This equation takes the conventional eigenvalue form as follows:

$$\underline{\underline{L}}^{-1} \underline{\underline{G}}\ \underline{i} = k\ \underline{i} . \tag{2.6}$$

The procedure in HERESY 1 is as follows: First one computes the type-to-type matrix elements Z_{nm}, G_{nm}, etc. by actual summation of the rod-to-rod kernels. One then adds $\underline{\underline{Z}} + \underline{\underline{\gamma}}$ to obtain $\underline{\underline{L}}$. $\underline{\underline{L}}^{-1}$ is then calculated by an iteration technique.

The next step is a matrix multiplication to obtain $\underline{\underline{L}}^{-1}\ \underline{\underline{G}}$. At this point one is ready to solve equation (2.6). The power method iteration technique[3] is used to obtain the maximum eigenvalue, which is equal to the reactivity of the configuration, and the eigenvector that corresponds to it. This eigenvector represents the relative absorptions in the various rod types.

2.2 Code Subprograms and Options

The code consists of four main-line subprograms with a number of additional options. The main-line subprograms are the following:

1. Calculation of type-to-type kernel matrices from the rod-to-rod kernels. The type-to-type kernel matrices which are calculated are $\underline{\underline{T}}$, $\underline{\underline{T}}^r$, $\underline{\underline{S}}^r$, $\underline{\underline{Z}}$.

2. Calculation of the matrix $\underline{\underline{L}}^{-1}\ \underline{\underline{G}}$.

3. Solution of the eigenvalue problem

$$\underline{\underline{L}}^{-1}\ \underline{\underline{G}}\ \underline{i} = k\ \underline{i} \tag{2.6}$$

for the reactivity k, which is the largest eigenvalue, and the associated eigenvector $\underline{i}$ which represents the relative thermal absorptions in the rod types.

4. Data processing to obtain p, f, and other lattice parameters.

The additional options available for selection by the problem organizer are the following:

A. Calculation of rod-to-rod kernels - either age-diffusion kernels, transport theory kernels, or a read in of an arbitrary table of kernel values.

B. Generation of many basic lattice geometries from minimum input.

C. High speed magnetic tape storage of data computed by options A and B.

D. Change of the convergence criteria for the matrix inversion and eigenvalue determination procedures.

E. Iteration on criticality. This includes comparison of the computed eigenvalue with unity, and forcing

HERESY through an iteration scheme (in exchangeable subroutine form) which computes successive values of γ, η and A, as enrichment is increased in specified rods, until criticality is attained.

2.3 Main-line Subprograms

The main-line subprograms will now be described in detail:

1. The T, Z, T^r, and S^r matrix elements are obtained using equations (2.2) and (2.3) by summing respectively, the F_{nm}, f_{nm}, F_{nm}^r, and $g_{nm}^{(r-1)}$ kernels from any rod of one type to all the rods of some other type. The F_{nm}, f_{nm}, F_{nm}^r, and g_{nm}^r kernels are tabulated at sixty values equally spaced Δh apart, as a function of the inter-rod distances, r_{nm}. The value of any of these kernels at a particular inter-rod distance is obtained from the tabulated values using Bessel's four point interpolation formula.[4] For the thermal sink kernel f_{nm}, a table of values of this kernel evaluated at the rod surface for each of the types is also provided. Thus a total of five kernel tables is used in the code. At present the problem organizer must check that the spacing between tabulated values Δh provides enough points for Bessel's interpolation formula to be applicable. However, a "trap" can be inserted to check for this.

An infinite lattice is represented as a very large lattice with 500 or more inter-rod distances involved in calculating the type-to-type matrix elements for each rod type.

2. The matrices $\underline{\underline{L}}$ and $\underline{\underline{G}}$ are calculated from the type-to-type matrices above and from the input diagonal matrices $\underline{\underline{\gamma}}$ and $\underline{\underline{A}}^r$ as follows:

$$\underline{\underline{L}} = \underline{\underline{Z}} + \underline{\underline{\gamma}}$$

$$\underline{\underline{G}} = (\underline{\underline{T}} - \underline{\underline{T}}^r \, \underline{\underline{A}}^r \, \underline{\underline{S}}^r) \, \underline{\underline{\eta}} \qquad (2.4)$$

The first guess to $\underline{\underline{L}}^{-1}$ is obtained by the Gaussian elimination method,[5] which first triangularizes and then inverts the matrix. This is a standard IBM-704 program "Linear Equations Solution, LEQ-O-581009."[6]

Except in the cases of ill-conditioned or very large order matrices the first computation will pass reasonable convergence conditions. Where the first estimate to the inverse, $\underline{\underline{R}}_1$, fails to meet the criterion $\underline{\underline{R}}_1 \, \underline{\underline{L}} = \underline{\underline{I}}$, the program then uses the algorithm

$$\underline{\underline{R}}_{j+1} = \underline{\underline{R}}_j \, (2\underline{\underline{I}} - \underline{\underline{L}} \, \underline{\underline{R}}_j), \qquad (2.7)$$

where $\underline{\underline{R}}_j$ is the j-th estimate of the reciprocal matrix, $\underline{\underline{I}}$ is the identity matrix, and $\underline{\underline{R}}_{j+1}$ is the next estimate of the reciprocal matrix. Convergence criteria for the iteration essentially test the elements of the matrix product $\underline{\underline{R}} \, \underline{\underline{L}} = \underline{\underline{I}}$. These criteria determine the number of significant figures in each element of the reciprocal matrix and specify an outer limit to the number of iterations permitted for the subprograms.

3. At this point the eigenvalue subprogram is entered. This subprogram is a power method iteration[3] to obtain the maximum

positive eigenvalue of the matrix $\underline{\underline{L^{-1} \cdot G}}$, which is equal to the reactivity. A first guess to the corresponding eigenvector is stored as an input quantity. A good initial guess of this eigenvector reduces the number of iterations required. Essentially the relation

$$\underline{i}_{n+1} = (\underline{\underline{L^{-1} \cdot G}})\ \underline{i}_n \qquad (2.8)$$

is machine executed until agreement between elements of the vector of the n+1 iteration $\underline{i}_{n+1}$, and the elements of the vector $\underline{i}_n$ of the n-th iteration is obtained to within a scale factor (this scale factor is the reactivity, k), to a specified number of significant figures. Failure to obtain agreement after a restricted number of iterations will cause error routines to be executed.

With the eigenvector representing the relative absorption of the rod types determined, the program computes the eigenvalue as the scale factor

$$k = \frac{\text{maximum element of the vector } i_{n+1}}{\text{corresponding element of the vector } i_n} \,. \qquad (2.9)$$

4. The data processing subprogram includes calculation of the power distribution from the vector of absorptions; the calculation of the lattice parameters p, f, η, by the formulas given in the last quarterly report[7]; the calculation of the average to maximum power per rod. Additional input data required: A vector $\underline{W}$ giving the ratio of fissions to absorptions for each rod type; a vector $\underline{H}$ giving the relative number of rods of each type.

2.4 Available Options

The additional options available in HERESY 1 will now be described. These options are exercisable by either 1) the subprogram composition of the card decks or standard tapes, or 2) the setting of sense switches on the 704 console during machine operation.

A. Kernel Functions

Currently two kinds of input are available to HERESY 1 for obtaining kernel functions. They may be obtained by machine computation of the functions or by directly reading kernel tables obtained elsewhere. With the use of a subprogram deck placed before input data, the following kernel functions based on the age-diffusion kernels given by Galinin[8] can be computed. The kernel function $g^r(d)$ is taken as a linear superposition of three Gaussian kernels. This allows us to compile not only age theory slowing down kernels (2 of the A_i's are set equal to 0) but any empirical slowing down distribution which can be fitted by two or three Gaussians. The kernels are expressed as the following functions of d, the inter-rod distance.

$$f(d) = \frac{1}{2\pi L^2 \sigma_a} K_o\left(\frac{d}{L}\right)$$

$$f(R_o) = \frac{1}{2\pi L^2 \sigma_a} K_o\left(\frac{R_o}{L}\right)$$

where R_o = radius of the fuel rod

$$g^r(d) = \sum_{i=1}^{3} \frac{A_i}{4\pi\tau_i^r} e^{-\frac{d^2}{4\tau_i^r}}$$

$$F(d) = \sum_{i=1}^{3} A_i \frac{e^{\tau_i/L^2}}{2\pi L^2 \sigma_a} \left[K_o\left(\frac{d}{L}\right) + \frac{\tau_i}{2L^2} e^{-d^2/4\tau_i} - 1/2\left(1 + \frac{d^2}{4L^2}\right) E_1\left(\frac{d^2}{4\tau_i}\right) \right].$$

To calculate $F^r(d)$ replace τ_i by $\tau_i - \tau_i^r$ in the equation for $F(d)$. Here

$f(d)$ = thermal diffusion kernel

$g^r(d)$ = empirical or age theory slowing down kernels to resonance energy

$F(d)$ = slowing down-diffusion kernel from fast energies

$F^r(d)$ = slowing down-diffusion kernel from resonance energies

L = diffusion length of thermal neutrons in the moderator

σ_a = macroscopic thermal absorption cross section

τ = neutron age to thermal energies

τ_r = neutron age to resonance energy

A_i = linear weighting coefficients which are usually obtained in an empirical fit to the slowing down density. The input to the code using this option consists of values of L^2, A_i, τ_i, τ_i^r, σ_a and Δh, the spacing interval in the kernel tables. It will be straightforward to code a subprogram which will compute the transport theory kernels given in the previous quarterly report.

B. Rod Geometry

Three kinds of input of the coordinates of individual rods in the reactor under study are available. This option is determined by use of a sense switch (to permit a change while running a series of different reactor problems), and by subprogram composition.

1) Direct input of cartesian coordinates grouped by rod type can be made which allows any configuration to be utilized. In this option the x and y coordinates of all the rods of each type are read in successively. The maximum number of individual rods and rod types are respectively 6500 and 50.

2) Infinite lattices consisting of geometries that can be regarded as a maximum of 50 intersecting rectangular simple lattices with sides parallel to the rectangular coordinate axes can be computed. The geometrical input data required are the coordinates of a representative rod position for each simple lattice and the corresponding lattice dimensions. In addition the radius of a circle, centered at the origin, which determines the number of contributing rods is left as an input quantity.

3) A hexagonal lattice subroutine applies to certain configurations of rods arranged on a simple hexagonal mesh. The rod types are distinguished by their spatial symmetry relative to a central rod which is designated the first type. Thus, the second type consists of the three nearest neighbor rods, the third type of the six next nearest neighbors, and so on.

Accordingly the central rod, or any other ring or partial ring constituting a spatial type may be removed or further distinguished by composition changes in the reactor under study. Again the hexagonal lattice may be regarded as either a finite or infinite array depending on how many rod types are used. The distance between adjacent points on the primitive hexagon is required as input. The only other input quantity is the number of types.

C. High Speed Magnetic Tape Storage of Kernel Data

By depressing a sense switch the kernel functions within the machine will be saved on tape. Since the kernel tables are short relative to the capacity of the tape the HERESY program (excluding whatever options are not being used for the problem) will be written on tape enabling production runs at a later time with only rod information required as input.

D. Change of Convergence Criteria

The three major iterations within the code are the matrix inversion, the eigenvector determination, and the iteration to criticality. By depressing certain sense switches convergence criteria for each or any of the iterations may be relaxed one significant figure per switch depression. Printouts on the on-line printer at the 704 will indicate such needs and give in addition a record of three iteration results. An option will be included to restore original convergence criteria and convert the arithmetic steps used to double precision, if too many significant figures are lost when the convergence criteria are relaxed.

E. Iteration to Criticality

Upon insertion of the appropriate subprogram card deck HERESY 1 will compare the eigenvalue k to unity and when sufficiently different, will compute new values of ν_n, η_n and A_n for some rod types, corresponding to a change in enrichment in these rod types. Tables of ν, η, and A for these rod types as functions of enrichment will be input quantities. The new enrichment in the selected rod types will be proportional to 1-k with prescribed proportionality factors. After the new enrichment is computed the tabulated values of ν, η, and A will be used to compute, by a simple interpolation between the tabulated enrichments, the new values of ν, η, and A for the iteration step. HERESY will then recompute the matrix $\underline{\underline{L}}$ and pass once more through the major subprograms of the system to obtain the next k. The iteration will stop when either 1) k is sufficiently close to 1, or 2) a maximum number of iterations have been made.

2.3 Accuracy and Timing Tests of HERESY 1

A number of problems designed to estimate the generated error and iteration times of the code have been completed. Actual results confirm that single precision* arithmetic and storage are sufficient to maintain an accuracy of at least five figures where the matrix order is ≤ 12 and the matrices and eigenvector guess are derived from reasonable physical systems.

*Single precision operations on the IBM 704 are carried out with 8 decimal figures.

The time for such a 12 rod type problem is, with card reading, less than one minute.

In one case the reactivity and relative absorptions of a reactor composed of 12 rods was computed by desk machine. The 12 rod system was divided into 3, 6, and 12 rod types arbitrarily and a HERESY production run made. In the three cases the values of k and i_n obtained by the machine code agreed to five significant figures with the hand calculated results.

The following test of rapidity of convergence of the eigenvector subprogram was made for the 12 rod problem treated as 12 types. In computation I a fairly good initial guess of the eigenvector was made in which all elements of the eigenvector were taken to be unity. In computation II a poor initial guess was used in which one element was taken to be 3.0 while all the others were unity. Both computations eventually converged to the same eigenvector, none of whose components differed substantially from unity. The problem running times and number of iterations required in the eigenvector subprogram were as follows

Computation	Running Time	Number of Iterations
I	50 sec	17
II	75	81

Section 3. Approach to Criticality of a Square Lattice in Graphite

Calculations of the reactivity and the relative power distribution have been made using HERESY 1 for a number of configurations representing progressively larger cores in an infinite graphite reflector. In these calculations the rods are physically identical; the rod parameters are identical with those used previously[9] for unenriched uranium metal rods in graphite. These parameters are:

η = 1.34 (including fast fission factor)

γ = 0.255 cm^{-1}

R_o = 2 cm

A = 51 cm^2

τ = 350 cm^2 to thermal energy

$\tau_r = 3\tau/4 = 262.5$ cm^2 to the energy of the single equivalent resonance

L^2 = 2800 cm^2.

τ and L^2 are properties of the pure graphite moderator. τ_r, the age to the single equivalent resonance which is assumed in HERESY 1, is a property of both the moderator and the U^{238} in the rod.

Six configurations of this single physical rod type (of natural uranium) have been studied in an infinite graphite moderator. (The use of an infinite graphite moderator is no real

limitation, since a reflector two or three diffusion lengths thick is practically equivalent to an infinite reflector as far as power distribution in the core is concerned.) These configurations were chosen to describe the approach to criticality of a square lattice as the number of rods per side of square increases. The interesting effects which heterogeneous calculations show are first of all, the relative reactivity changes between configurations, and secondly, the individual peculiarities of the power distribution. The configurations are the following:

Configuration 1A: 3 by 3 array with lattice spacing of 20 cm. Central rod absent. The geometry is shown in Figure 1 where the central rod is shown as present. The numbers of the various rods distinguish different rod symmetries. All rods with the same number have the same spatial symmetry. This notation will be used throughout this report.

Results for Configuration 1A.

$$k = 0.649$$

$$p = 0.9461$$

$$f = 0.512$$

$$i_1 = 1$$

$$i_2 = 0.9735$$

The flux depression at the corner rods lowers the power in them. It should be noted that the maximum value of any eigenvector component (i_j) has been normalized to 1 in all HERESY 1 results.

Configuration 1B: 3 by 3 array with lattice spacing of 20 cm. Central rod present. The geometry is shown in Fig. 1.

Results for Configuration 1B:

$$k = 0.663$$

$$p = 0.930$$

$$f = 0.529$$

$$i_1 = 0.977$$

$$i_2 = 1$$

$$i_3 = 0.931$$

Note that insertion of the central rod depresses the flux sufficiently at its nearest neighbors to give the corner rods the highest power density. The central rod has the lowest power.

Configuration 1B - enlarged. This is a 3 by 3 array with a pitch of 40 cm. The enlarged pitch changes the power distribution significantly. The geometry is given in Fig. 1.

Results for configuration 1B - enlarged:

$$k = 0.6387$$

$$p = 0.9738$$

$$f = 0.4894$$

$$i_1 = 0.833$$

$$i_2 = 0.698$$

$$i_3 = 1$$

Note that the central rod has the largest power with this enlarged pitch.

Configuration 2B: 5 by 5 array with central rod present. The pitch is 20 cm. The geometry is shown in Figure 2. There are six rod symmetries.

Results for Configuration 2B:

$$k = 0.8428$$

$$p = 0.9117$$

$$f = 0.6899$$

$$i_1 = 0.954$$

$$i_2 = 0.910$$

$$i_3 = 0.934$$

$$i_4 = 0.856$$

$$i_5 = 0.893$$

$$i_6 = 1.0$$

The central rod has the highest power. Rods 3 on the periphery have a larger power density than rods 2 in the interior, a rather surprising result. The corner rods have the lowest power density.

Configuration 4: 7 by 7 array with pitch of 20 cm. The geometry is shown in Figure 3. There are ten rod symmetries.

Results for Configuration 4:

$$k = 0.9279$$

$$p = 0.8998$$

$$f = 0.7696$$

$i_1 = 0.965$

$i_2 = 0.931$

$i_3 = 0.871$

$i_4 = 0.760$

$i_5 = 0.841$

$i_6 = 1.000$

$i_7 = 0.683$

$i_8 = 0.729$

$i_9 = 0.805$

$i_{10} = 0.832$

Configuration 5: 9 by 9 array with pitch of 20 cm. The geometry is shown in Figure 4. There are 15 rod symmetries.

Results for Configuration 5:

$k = 0.9772$

$p = 0.8927$

$f = 0.8167$

$i_1 = 0.9781$

$i_2 = 0.9584$

$i_3 = 0.9023$

$i_4 = 0.8209$

$i_5 = 0.8900$

$i_6 = 1.0000$

$i_7 = 0.6367$

$i_8 = 0.7236$

$i_9 = 0.7824$

$i_{10} = 0.8058$

$i_{11} = 0.5598$

$i_{12} = 0.6052$

$i_{13} = 0.6858$

$i_{14} = 0.7394$

$i_{15} = 0.7596$

The results of these calculations are summarized in Table 1. As the lattice size increases-p decreases, f increases, and k increases. It is significant that the average-to-maximum power within the lattice decreases as k increases, and that the quantity $(1-k)n^2$ is constant to within a factor of 2 or so as the lattice is built up, where n is the number of rods per lattice side.

TABLE 1

Approach to Criticality of a Square Lattice

n Rods per Lattice Side	a Rod Spacing	k	p	f	Average to Maximum Power	Minimum to Maximum Power	$-(k-1)n^2$
3	20 cm	.663	.930	.529	.982	.93	3.03
3*	20 cm	.649	.946	.512	.986	.97	
3	40 cm	.6387	.9738	.4894	.792	.70	3.25
5	20 cm	.8428	.9117	.6899	.910	.86	3.93
7	20 cm	.9272	.8998	.7696	.820	.68	3.57
9	20 cm	.9772	.8927	.8167	.767	.5598	1.85

*Central rod missing

Fig. 1 Rod Symmetries in Configuration 1A and 1B

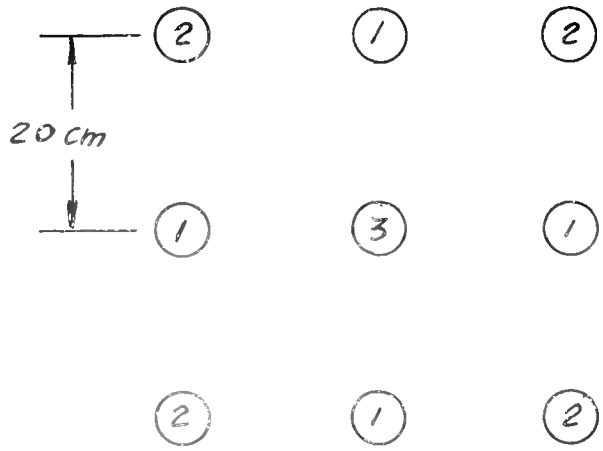


Fig. 2 Rod Symmetries in Configuration 2B

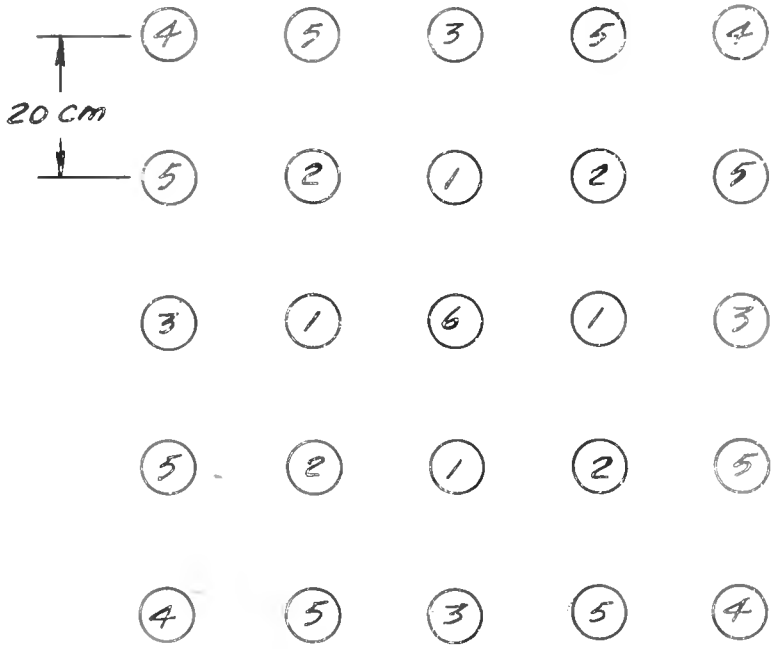


Fig. 3 Rod Symmetries in Configuration 4

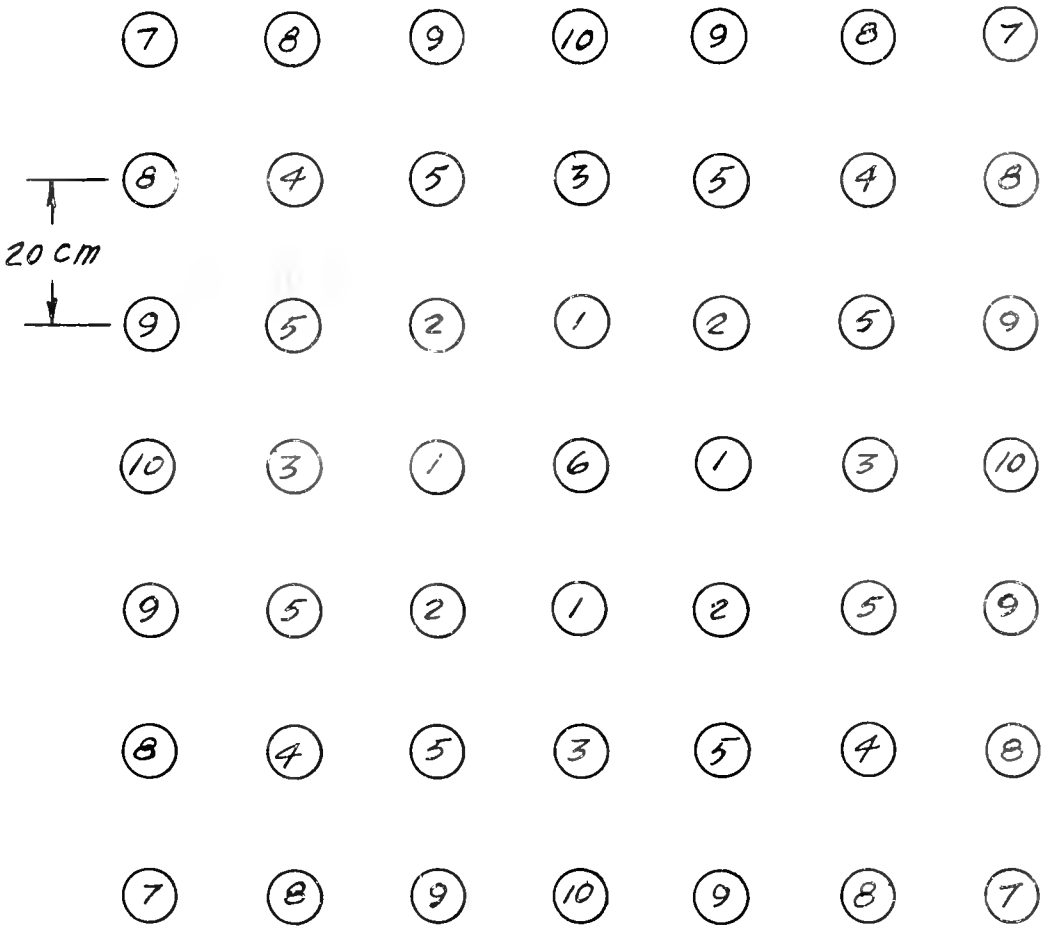
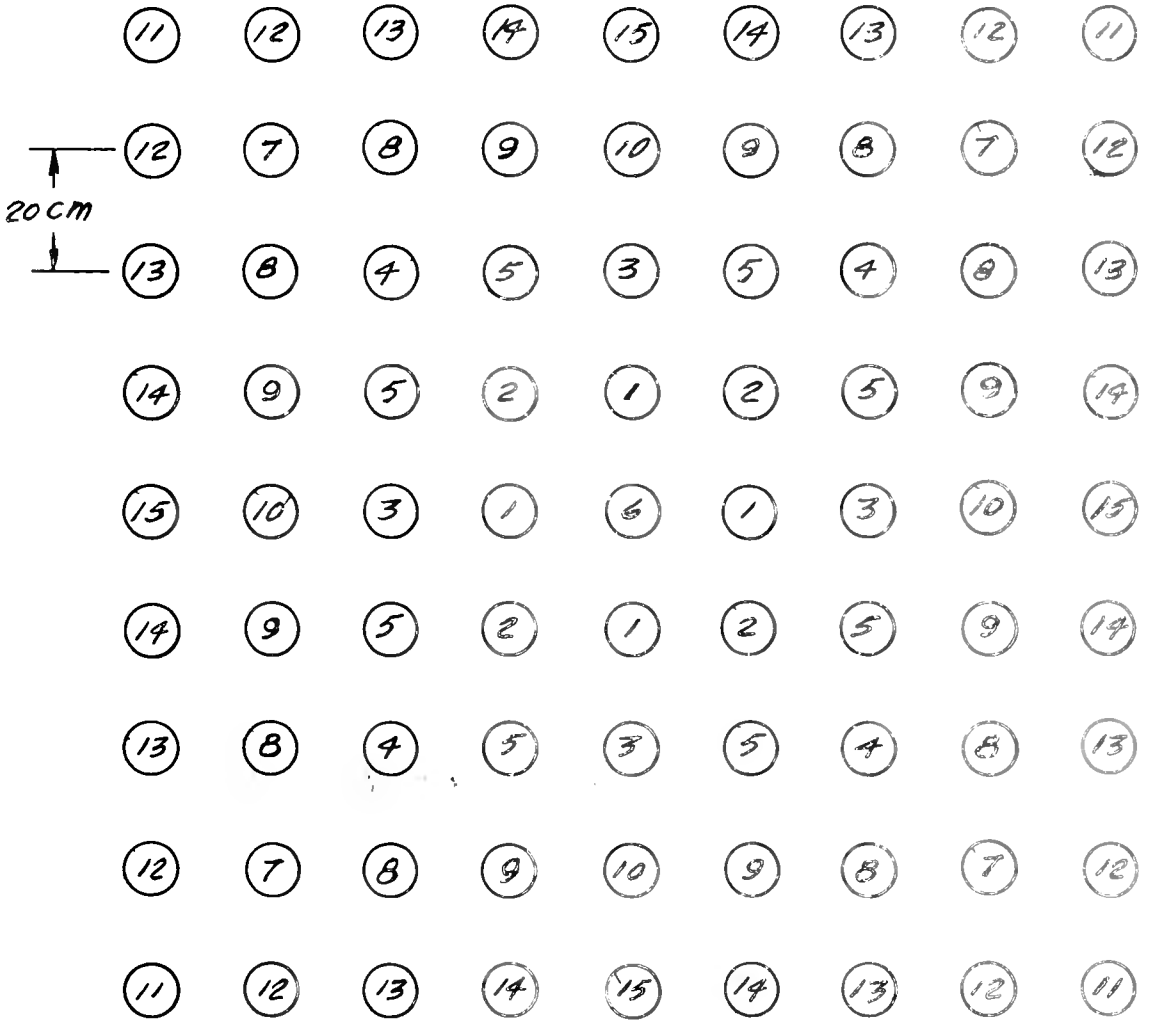


Fig. 4 Rod Symmetries in Configuration 5



Section 4. Study of Spiked Cores for Power Flattening

A study of spiked cores has been made by heterogeneous calculation methods using HERESY 1. The purpose of this study is to show how heterogeneous calculation methods can be used to investigate flux flattening and the variation of reactivity for a number of spiking patterns. In this study the numbers of enriched and unenriched rods are held constant while the pattern of placement of the enriched rods in the lattice is varied.

An array of 81 rods arranged in a square lattice in graphite is considered. This lattice with unenriched rods is shown in Figure 4 corresponding to configuration 5 of the last section. Two series of calculations have been made. In Series I 20 of the rods are enriched and the remaining 61 are unenriched. In Series II 24 of the rods are enriched and the remaining 57 are unenriched. By distributing the enriched rods in various ways within this array the reactivity and the average-to-maximum power ratio can be varied considerably. A number of spiked configurations of these types have been calculated. By studying the results of such computations the optimum spiking pattern can be chosen.

This optimum pattern will depend on the objective of the core designer. In general, in order to increase the average-to-maximum power ratio one will diminish the reactivity of the configuration. Putting the enriched rods near the boundary

increases average-to-maximum power but decreases reactivity, relative to placement of the enriched rods in the interior of the lattice.

The unenriched rods used in these calculations are identical with those considered in Section 3. The enriched rods correspond to 1.3% enrichment and are identical with the enriched rods considered in the previous report.[9] The enriched rod parameters are as follows:

$$\eta = 1.605$$
$$\gamma = 0.178 \text{ cm}^{-1}$$
$$A = 51 \text{ cm}^2$$
$$R_o = 2 \text{ cm}$$

The configurations studied in Series I are shown in Figures 5 to 11. These figures show one quadrant of the core, the lower right hand side. The configurations studied in Series II are shown in Figures 12 to 15. The calculation results for configurations 6 to 12 of Series I (20 enriched rods) are given in Table 2. The calculation results for configurations 13 to 16 of Series II are given in Table 3. Each of these tables gives the reactivity, lattice parameters and relative power in the various rod types of each configuration.

Figure 16 is a plot of the average-to-maximum power versus k-1 for the various configurations of Series I. This figure demonstrates the necessity of trading off reactivity and higher power density for each other in spiked cores for the types of configurations

considered.

It is important to note that a series of calculations such as are shown in Tables 2 and 3 can be used to develop successive spiking configurations with flatter power distributions. The following iterative procedure is suggested. One first surveys the possible spiking patterns to prepare a table like Table 2. For any configuration presented in this table one can hope to improve the average-to-maximum power by enriching those rods with the smallest power. Enriched rods in high power areas of the core can be replaced by unenriched rods. Thus one can make a series of calculations, starting from any configuration, that will reveal how to change the pattern of spiking to increase the average-to-maximum power.

For example, among the Series I configuration, configuration 11 has the largest average-to-maximum power, 0.861. To increase this ratio one notes that rod types 7 and 8 contribute the least to the power, with .7182 and .7932 respectively. This suggests that rod type 7 should be enriched. One should next calculate a configuration in which configuration 11 is changed by making rod type 7 enriched. If one wished to do this subject to the limitation that only 20 rods are to be enriched one could simultaneously change rod type 11 from enriched to unenriched.

This discrete iterative procedure can be expected to lead usually, though not always, to configurations with higher average

power. When a change decreases this ratio, one simply goes back to the initial configuration and makes another change. While this procedure has a certain element of trial-and-error in it, this can be reduced to a minimum by starting from a set of calculations representing a fairly comprehensive design survey, e.g., Table 2. The individual configuration calculations are quite cheap. The discrete iterative procedure has several advantages over methods previously proposed for power flattening based on homogeneous reactor physics calculations:

1. It calculates the power distribution among the individual rods directly, by obtaining the relative absorptions in the discrete rods.
2. A simple series of configuration calculations is carried out using HERESY 1. No complicated differential equations with spatially varying cross sections (to represent the variable fuel loading) need be solved. No variational calculations need be carried out. Table 2 represents less than 10 minutes running time on the IBM 704.

TABLE 2 - Series I Spiked Core Results

Enriched Rod Symmetries	3, 9, 13	8, 11, 12
Configuration No.	6	7
k	1.037	1.020
η	1.413	1.405
p	.8928	.8948
f	.8221	.8109
Average Power/Max. Power	.771	.856
i_1 (4 rods)	.9313	.9883
i_2 (4 rods)	.9217	.9767
i_3 (4 rods)	1.	.9312
i_4 (4 rods)	.7960	.8650
i_5 (8 rods)	.8524	.9252
i_6 (1 rod)	.9621	1.
i_7 (4 rods)	.6193	.7035
i_8 (8 rods)	.6957	.9201
i_9 (8 rods)	.8820	.8310
i_{10} (4 rods)	.7731	.8514
i_{11} (4 rods)	.5468	.7792
i_{12} (8 rods)	.5869	.8191
i_{13} (8 rods)	.7766	.7697
i_{14} (8 rods)	.7183	.8140
i_{15} (4 rods)	.7507	.8265

TABLE 2 - Series I Spiked Core Results (continued)

Enriched Rod Symmetries	11, 12, 13	2, 3, 4, 5
Configuration No.	11	12
k	1.018	1.059
η	1.405	1.427
p	.8959	.8901
f	.8091	.8332
Average Power/Max. Power	.861	.678
i_1	.9783	.8880
i_2	.9710	1.
i_3	.9171	.9277
i_4	.8733	.8134
i_5	.9246	.8968
i_6	1.	.9344
i_7	.7182	.5189
i_8	.7932	.6032
i_9	.8385	.6651
i_{10}	.8600	.6892
i_{11}	.7984	.4315
i_{12}	.8279	.4772
i_{13}	.9097	.5539
i_{14}	.8215	.6075
i_{15}	.8425	.6273

TABLE 2 - Series I Spiked Core Results (continued)

Enriched Rod Symmetries	5, 10, 13	4, 9, 12	3, 9, 12
Configuration No.	8	9	10
k	1.041	1.030	1.032
η	1.416	1.410	1.411
p	.8924	.8933	.8930
f	.8240	.8177	.8192
Average Power/Max. Power	.767	.826	.768
i_1	.9463	.9874	.9282
i_2	.9195	.9708	.9147
i_3	.8530	.9220	1.000
i_4	.7835	.9861	.7940
i_5	1.000	.9017	.8441
i_6	.9765	1.000	.9519
i_7	.6115	.6718	.6160
i_8	.6952	.7512	.6992
i_9	.7483	.9428	.8752
i_{10}	.9098	.8231	.7587
i_{11}	.5355	.6038	.5496
i_{12}	.5760	.7583	.6912
i_{13}	.7669	.7283	.6676
i_{14}	.7134	.7768	.7167
i_{15}	.7375	.7969	.7374

TABLE 3 - Series II Spiked Core Results (continued)

Enriched Rod Symmetries	4, 8, 11, 12	5, 7, 11, 13
Configuration No.	15	16
k	1.032	1.042
η	1.420	1.424
p	.8944	.8937
f	.8132	.8191
Average Power/Max. Power	.859	.784
i_1	.9895	.9356
i_2	.9758	.9112
i_3	.9327	.8536
i_4	.9993	.7894
i_5	.9184	1.
i_6	1.	.9644
i_7	.6985	.7386
i_8	.9094	.7070
i_9	.8277	.7607
i_{10}	.8499	.7884
i_{11}	.7690	.6740
i_{12}	.8115	.6055
i_{13}	.7641	.7971
i_{14}	.8083	.7288
i_{15}	.8204	.7523

TABLE 3 - Series II Spiked Core Results

Enriched Rod Symmetries	8, 12, 14	4, 9, 11, 12
Configuration No.	13	14
k	1.034	1.034
η	1.422	1.414
p	.8948	.8936
f	.8128	.8186
Average Power/Maximum Power	.874	.841
i_1	.9921	.9812
i_2	.9824	.9699
i_3	.9440	.9144
i_4	.8764	.9992
i_5	.9369	.9065
i_6	1.	1.
i_7	.7092	.6905
i_8	.9313	.7693
i_9	.8428	.9533
i_{10}	.8697	.8299
i_{11}	.6648	.7084
i_{12}	.8262	.7719
i_{13}	.7767	.7482
i_{14}	.9725	.7909
i_{15}	.8456	.8083

The next 11 figures represent the lower right hand quadrant of configuration 5 where certain natural uranium rods have been replaced by rods of enriched uranium. The enriched uranium rods are explicitly designated by a ○ . Configurations 6-12 refer to Series I where there are 20 enriched rods in the entire lattice. Configurations 13-16 refer to Series II where 24 rods are enriched.

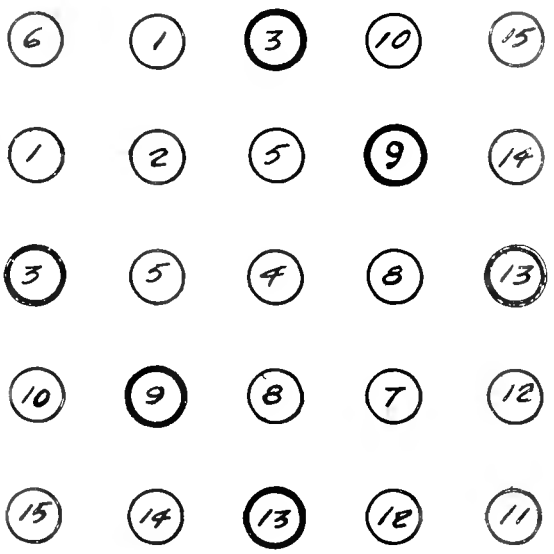


Fig. 5 Configuration 6

Fig. 6 Configuration 7

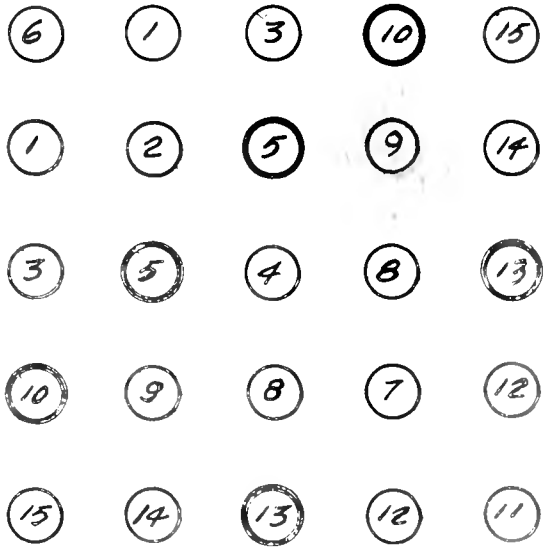


Fig. 7 Configuration 8

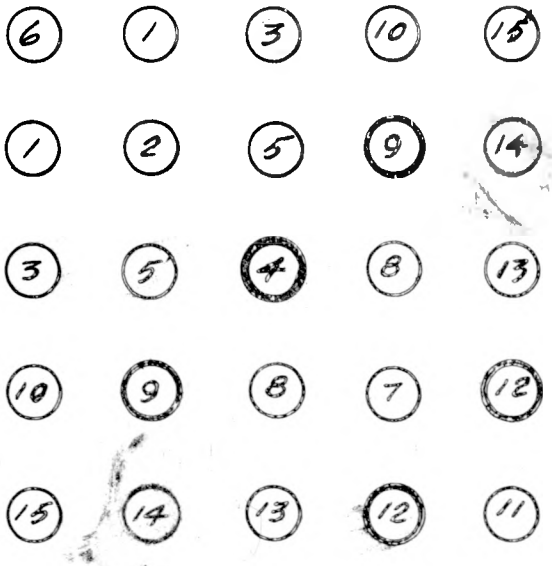


Fig. 8 Configuration 9

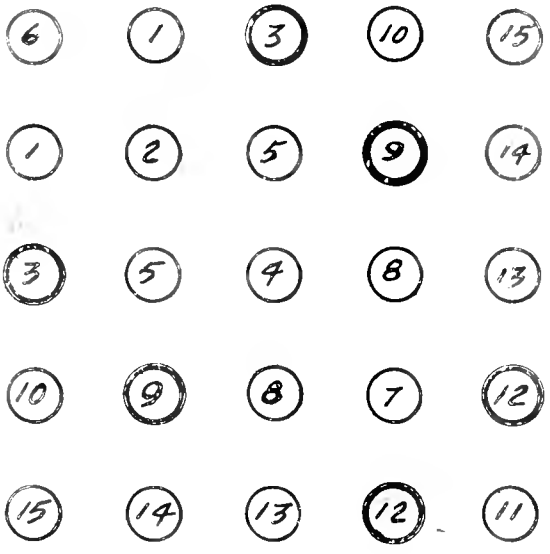


Fig.9 Configuration 10

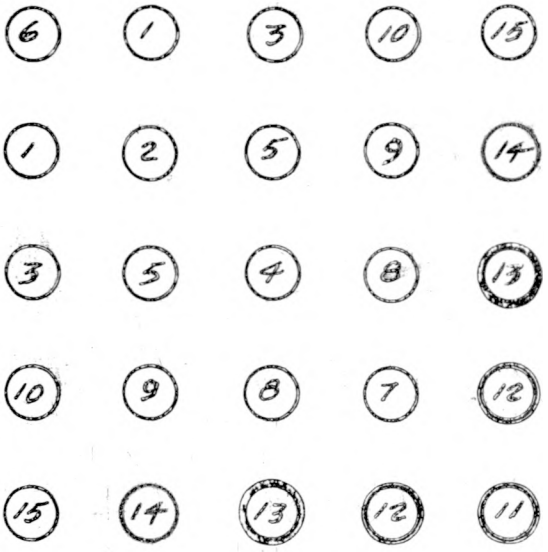


Fig.10 Configuration 11

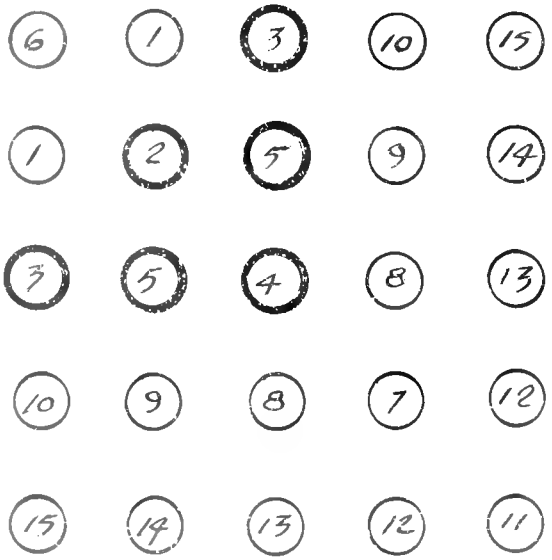


Fig. 11 Configuration 12

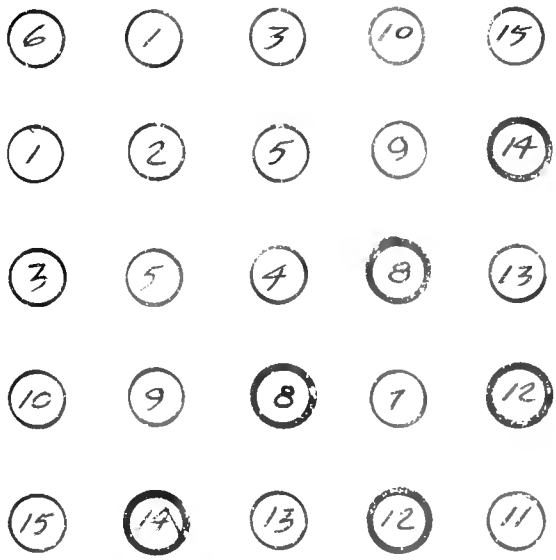


Fig. 12 Configuration 13

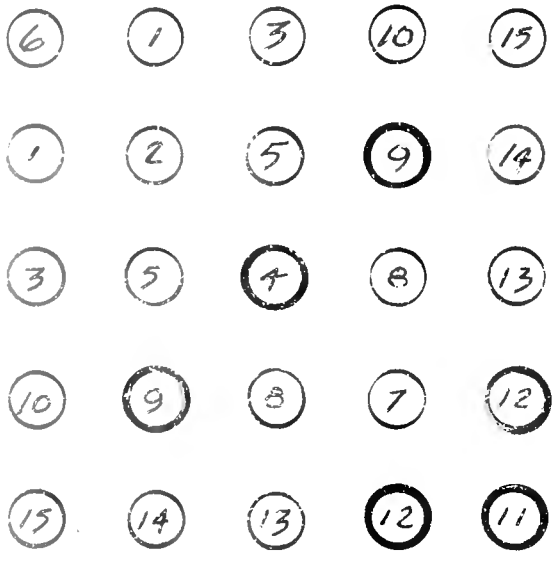


Fig. 13 Configuration 14

Fig. 14 Configuration 15

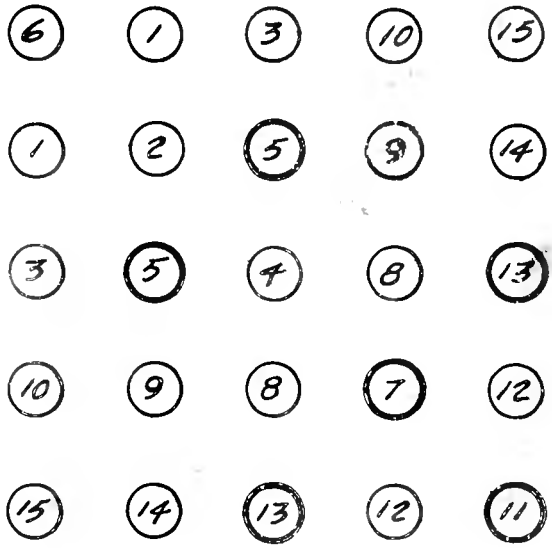
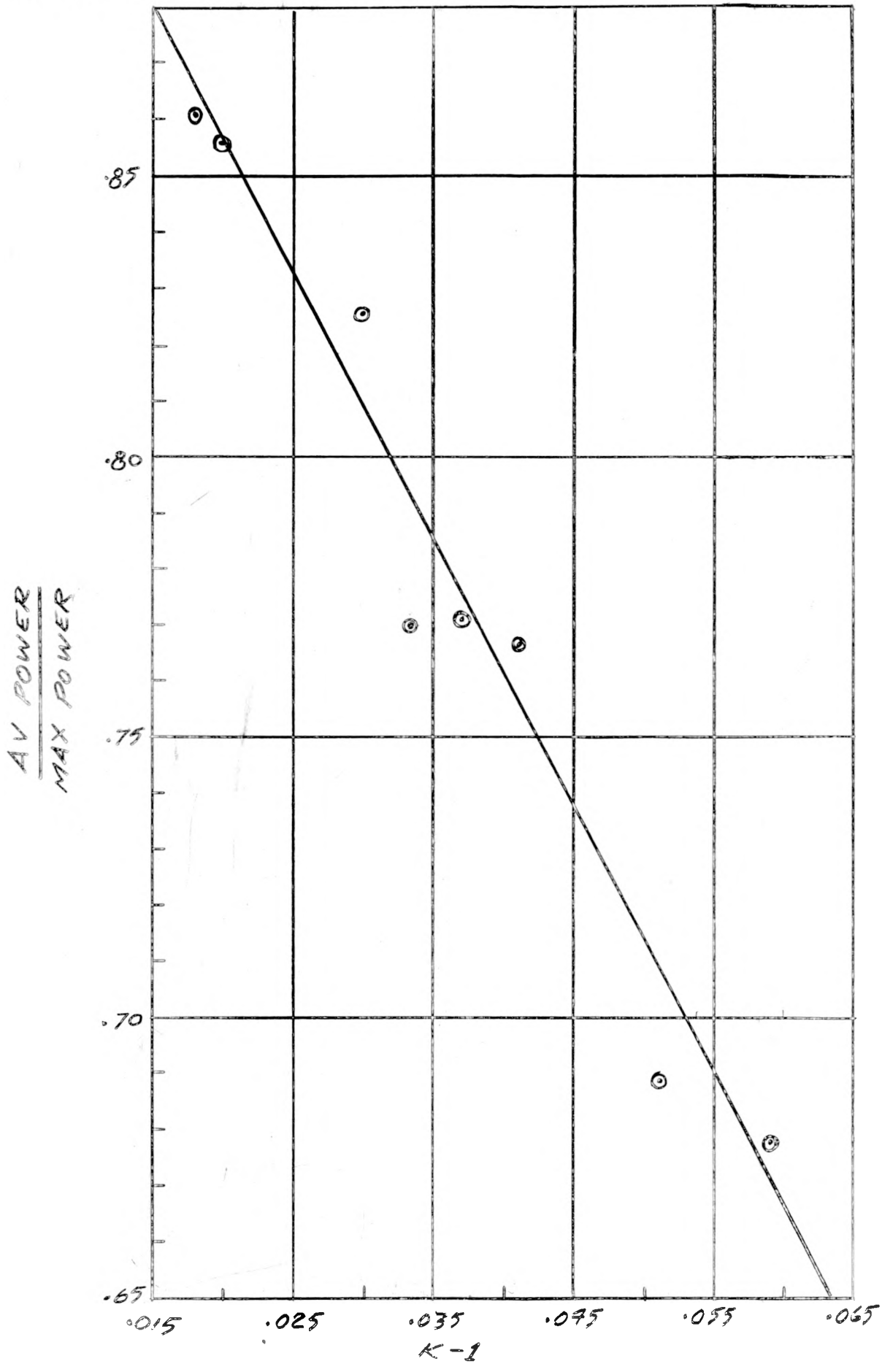


Fig.15 Configuration 16

Fig. 16 Average-to-Maximum Power vs K-1 for Series 1 Configurations



Section 5. The Self-Consistent Procedure: Sensitivity to Kernel Errors

An important consideration in the use of heterogeneous reactor physics calculations (as exemplified in HERESY 1) is the sensitivity of the calculation results to errors in the input quantities. If the reactivity and power distribution among rods turn out to be relatively insensitive to errors in the kernels and the rod parameters this would provide an important additional incentive to use the method.

The previous quarterly reports[1] describe a method for calculating rod parameters that we have dubbed the "Self-Consistent Heterogeneous Procedure". This method, it is hoped, will give results that are relatively insensitive to certain input errors. In this section we report some preliminary calculations to test the sensitivity of the self-consistent method to certain input errors. It is important to emphasize, however, that one cannot yet draw general conclusions about the accuracy of the self-consistent method.

The principle of the self-consistent method is the following: We consider errors in the rod-to-rod kernels. The rod parameter γ will be evaluated by measuring f, the thermal utilization in an infinite one-component lattice of the given rod type. In terms of the kernels F_{nm} and f_{nm} (which may be in error) one has

$$\gamma = \frac{1}{f} \Sigma F_{nm} - \Sigma f_{nm} \qquad (5.1)$$

where

f = thermal utilization in one-component infinite lattice of rod type n

F_{nm} = slowing down-diffusion kernel between rods m and n

f_{nm} = thermal diffusion kernel between rods m and n

Now if the kernels F_{nm} and f_{nm} are in error γ will be in error. But if this erroneous γ calculated from (5.1) is used in the heterogeneous equations for some other configuration, in which the erroneous kernel values F_{nm} and f_{nm} are also used, the errors introduced by the kernels may cancel the error in γ. This use of γ as calculated from a set of kernels (5.1) in the heterogeneous equations using the same kernels, we shall call the self-consistent method of calculating the rod parameter γ.

It was shown in the appendix to the last quarterly that for an infinite one-component lattice the reactivity is independent of the form of the thermal diffusion kernel when γ is evaluated by the self-consistent method. We have extended this investigation to finite lattices using HERESY 1. The following calculations have been carried out: Square lattices with 3, 5, 7, and 9 rods per side, respectively, corresponding to configurations 1, 2, 4, and 5 of Section 3 have been considered. These square lattices consist of the unenriched rods previously described in an infinite graphite moderator with a lattice pitch of 20 cm. The calculation results for these configurations are given in Section 3 corresponding to a thermal diffusion length of $L^2 = 2800\ cm^2$.

These calculations have been repeated with $L^2 = 5600\ cm^2$. Changing the thermal diffusion length in this way greatly alters the kernels. We call the altered kernel set "b" while the original set we call "a". γ is calculated from the new kernel set by the self-consistent method. Actually a third kernel set "c" was also considered with $L^2 = 1400\ cm^2$. The forms of the kernel function f(r) for these three cases is shown in Fig. 17. The values of γ for the unenriched and the enriched rods previously considered, as obtained by the self-consistent method, are shown in Table 4. We may consider kernel set "a" to be the correct set while kernel set "b" and "c" are erroneous.

The effect of the self-consistent procedure in cancelling the errors inherent in kernel set "b" is shown in Table 5. This table compares the results for configurations 1, 2, 4, and 5 when kernel set "a" (results of Section 3) and kernel set "b" are used with the self-consistent procedure. It is clear that a 100% error in L^2 and a large change in the kernels leads to small changes in k and changes in the power distribution not exceeding 15%. Thus the self-consistent procedures seem to minimize the effects of errors in the kernels.

Similar calculations have been carried out for the two complex lattices consisting of two superimposed infinite square lattices which were analyzed in the last Quarterly Report No. 2. Two cases are considered:

Case I: $\frac{\text{Pitch of enriched rods}}{\text{Pitch of unenriched rod}} = 1$

Case II: $\frac{\text{Pitch of enriched rods}}{\text{Pitch of unenriched rods}} = 2$

The results are given in Table 6 for the three kernel sets. The self-consistent procedure is followed in each case.

This entire set of computations indicates that knowing the correct thermal utilization for a one-component infinite lattice allows us to assign a γ to the rod by the self-consistent procedure for any assumed realistic kernel approximation f_{nm}, and that when this rod is a constituent of a complex lattice configuration of physical interest the resultant eigenvalue k is almost entirely independent of the kernel approximation used. It is also seen that even for extreme variations in the kernel functions, the difference in the relative absorptions between calculations "a", "b", and "c" was only of the order of 5%, to 10%.

TABLE 4

γ for Several Kernel Sets as Obtained by the Self-Consistent Method

L^2	Kernel Set Designation	γ Unenriched	γ Enriched
2800	a	.255	.178
5600	b	.328	.237
1400	c	.113	.0224

TABLE 5

Self-Consistent Procedure Comparisons
for Finite Square Lattices

Configuration 1 - 9 rods

	Kernel Set "a"	Kernel Set "b"
k	.649	.6735
f	.512	.5377
i_1	.977	.9833
i_2	1.0	1.0
i_3	.9315	.9489

TABLE 5 (Continued)

Self-Consistent Procedure Comparisons
for Finite Square Lattices

Configuration 2 - 25 rods

	Kernel Set "a"	Kernel Set "b"
k	.8428	.8576
f	.6899	.7018
i_1	.954	.965
i_2	.910	.932
i_3	.934	.95[illegible]
i_4	.856	.891
i_5	.893	.920
i_6	1.0	1.0

TABLE 5 (Continued)

Self-Consistent Procedure Comparisons
for Finite Square Lattices

Configuration 4 - 49 rods

	Kernel Set "a"	Kernel Set "b"
k	.9279	.9435
f	.7696	.7821
i_1	.965	.971
i_2	.931	.943
i_3	.871	.896
i_4	.760	.804
i_5	.841	.870
i_6	1.	1.
i_7	.683	.744
i_8	.729	.781
i_9	.805	.844
i_{10}	.8325	.868

TABLE 5 (Continued)

Self-Consistent Procedure Comparisons
for Finite Square Lattices

Configuration 5 - 81 rods

	Kernel Set "a"	Kernel Set "b"
k	.9772	.9923
f	.8169	.8289
i_1	.9781	.983
i_2	.9584	.966
i_3	.9023	.920
i_4	.8209	.850
i_5	.8900	.909
i_6	1.0	1.0
i_7	.6367	.697
i_8	.7236	.770
i_9	.7824	.823
i_{10}	.8058	.841
i_{11}	.5598	.636
i_{12}	.6052	.674
i_{13}	.6858	.774
i_{14}	.7394	.791
i_{15}	.7596	.809

TABLE 6

Self-Consistent Procedure - Infinite Complex Lattices

Results for Geom. I:	"a"	"b"	"c"
k	1.074	1.071	1.077
η	1.485	1.490	1.483
p	.745	.745	.745
f	.9705	.9629	.9750
i_1	.8248	.7673	.8485
i_2	1.0	1.0	1.0

Results for Geom. II:	"a"	"b"	"c"
k	1.111	1.111	1.104
η	1.395	1.400	1.391
p	.8406	.8406	.8406
f	.948	.9437	.944
i_1	.9644	.8542	1.0
i_2	1.	1.	.9526

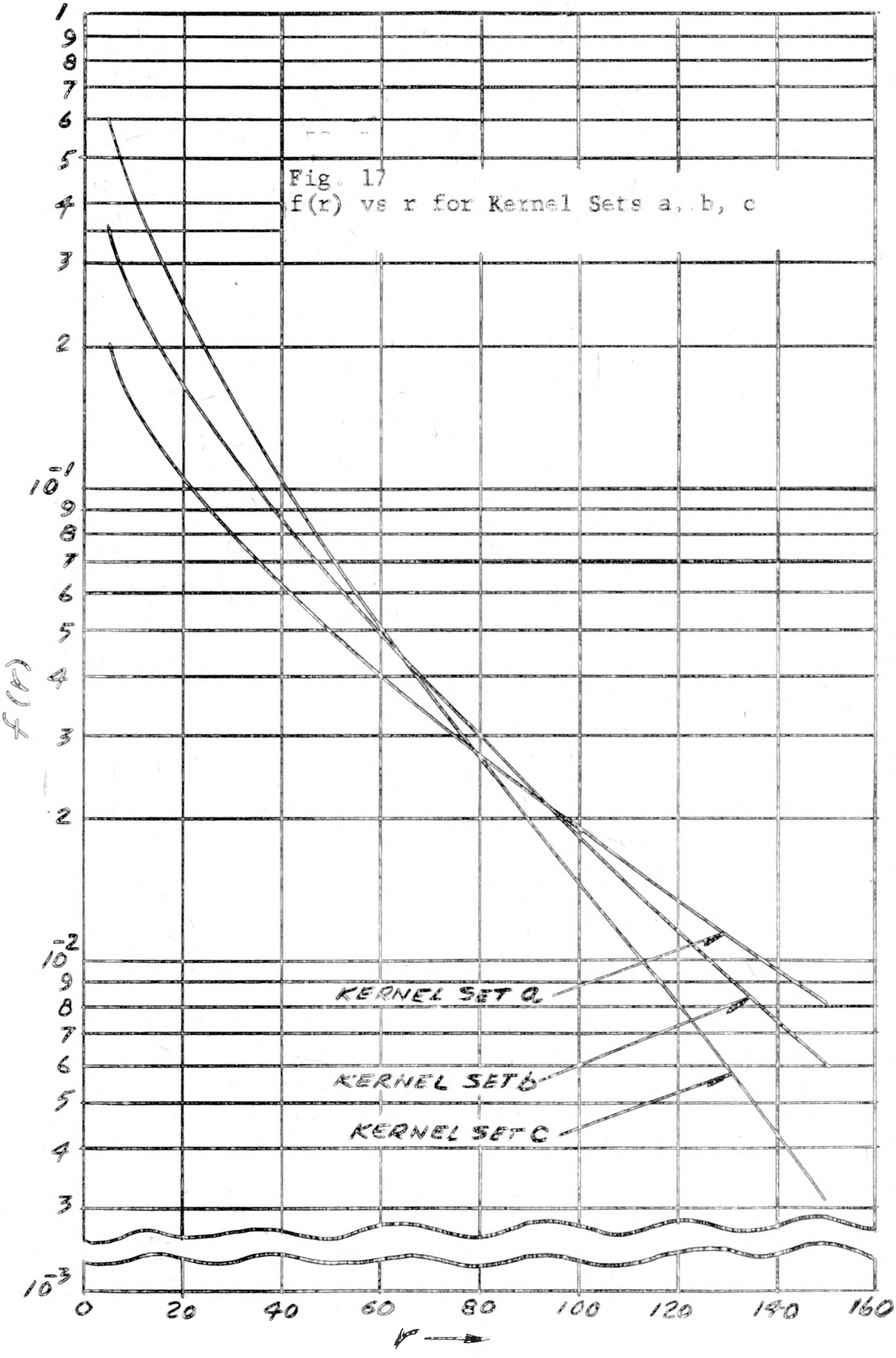


Fig. 17
f(r) vs r for Kernel Sets a, b, c

Appendix I. Third (Axial) Dimension in HERESY 1

For fuel elements of finite axial length the same set of equations may be used in HERESY 1 if several assumptions are made. Let (r, θ) be two dimensional polar coordinate in the central plane. Then the asymptotic flux becomes $\phi_{asy}(r,\theta,z)$ in place of $\phi_{asy}(r,\theta)$ for infinitely long fuel elements. The absorptions in the m-th rod centered at (r,θ) become $i_m(r,\theta,z) = \frac{1}{\gamma_m}\phi_{asy}(r,\theta,z)$. γ_m is assumed independent of z. The asymptotic flux is assumed to have a cosine-like variation in the z direction

$$\phi_{asy}(r,\theta,z) = \phi_{asy}(r,\theta)\cos(kz)$$

where

$$k = \frac{\pi}{H+2\Delta}$$

H = fuel element active length

Δ = reflector savings

$$i_m(r,\theta,z) = i_m(r,\theta)\cos(kz)$$

The code will obtain the reactivity and the relative absorptions $i_m(r,\theta)$ for the finite sized core if the following parameter substitutions are made.[10]

Replace $\frac{1}{L^2}$, the inverse squared thermal diffusion length for the infinite problem by

$$\frac{1}{L^2} + k^2$$

Replace η, the fast neutrons produced per absorption in the infinite problem by

$$\eta e^{-k^2\tau}$$

where τ is the age to the energy considered.

REFERENCES

1. The self-consistent procedure is discussed in Section 2.3 and Appendix 2.3 of the following reference: Klahr, C. N., and Mendelsohn, L. B., "Heterogeneous Reactor Calculation Methods" Quarterly Progress Report No. 2, NYO-2674, September 30, 1959.

2. The heterogeneous equations, kernel definitions, and rod parameter definitions are given in Reference 1 and in the following reference: Klahr, Carl N. "Heterogeneous Reactor Calculation Methods" Quarterly Progress Report No. 1, NYO-2673, June 30, 1959.

3. Bodewig, E. "Matrix Calculus" Interscience Publisher, Inc. New York (1956) Page 231.

4. Buckingham, R. A., "Numerical Methods" Sir Isaac Pitman and Sons Ltd., publishers, London (1957) Page 111.

5. Scarborough, J. B., "Numerical Mathematical Analysis" third edition, Oxford University Press (1955) Page 507. The iteration formula (2.7) for matrix inversion is given in Reference 3 Page 199.

6. Fortran Linear Equation Solution Subroutine LEQ-O-581009, AEC Computing Center, 4 Washington Place, New York City.

7. Reference 1, Section 4

8. Galinin, A. D., "Critical Size of Heterogeneous Reactor with Small Number of Rods", 1955 Geneva Conference Proceedings, Vol. 5, Page 461 United Nations, New York.

9. Reference 1, Pages 33-35

10. Feinberg, S. M., "Heterogeneous Methods for Calculating Reactors" 1955 Geneva Conference Proceedings, Vol. 5, Page 486.