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HETEROGENEOUS REACTOR CALCULATION METHODS

Quarterly Progress Report No. 2

Carl N. Klahr
Lawrence B. Mendelsohn

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ABSTRACT

New work directed towards practical use of heterogeneous reactor physics calculations is here reported. The most important result is given in Section 4 in which thermal utilization and resonance escape probability are calculated for infinite multi-component complex lattices. These calculations permit for the first time, we believe, straightforward and simple analysis of certain reactor cores with multi-component lattices.

A description of an IBM-704 code now being written, which will do realistic heterogeneous calculations is given in Section 1. Several methods for calculating the fuel element thermal absorption parameter are given in Section 2. The calculation of more precise rod-to-rod kernels, using transport theory, is developed in Section 3.

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Section 1. Heterogeneous Reactor Calculation Code

1.1 Code Input and Output

Analysis on the initial code for heterogeneous reactor calculations has been completed and flow charts have been written. This code is designated HET 1 and is being coded for the IBM-704. The code will have the following capabilities. It will handle up to 80 types of fuel elements and up to 2000 individual fuel elements. It will solve two types of problems: finite core configurations and infinite lattice properties. The inputs and outputs of the code will be as follows:

Inputs

(1) Infinite line kernels in an infinite moderator will be specified by giving the kernel values at the rod surface and at a series of mesh points to be specified. Four types of kernels will be given in this way -- F_{nm}, f_{nm}, $g_{nm}^{(r)}$, $F_{nm}^{(\eta)}$, corresponding respectively to slowing down from fission followed by thermal diffusion, thermal diffusion alone, slowing down to resonance, and slowing down from resonance followed by thermal diffusion.

(2) Fuel element (or absorbing element) parameters including * γ, η, and A for each individual element. HET 1 will treat only one equivalent resonance occurring at the same energy in each rod. It will not include fissions at resonance energies and all fissions are assumed to occur at thermal energies.

(3) Input information concerning the geometry of the reactor lattice.

* All notation in this report will be identical to that used in Quarterly Progress Report No. 1 NYO-2673 except for the kernel subscripts. The kernel subscripts have been reversed in significance to conform with conventional matrix notation. F_{nm} give the contributions from a fission neutron at the m-th rod to the thermal flux at the n-th rod.

Output

The outputs of HET 1 will be as follows if the problem configuration is that of a finite lattice:

(1) The reactivity of the configuration, obtained as the maximum eigenvalue of a certain matrix.

(2) The relative absorptions in the individual rod types, obtained as the eigenvector corresponding to the reactivity.

If the problem configuration is that of an infinite lattice the outputs will be the following:

(1) The reactivity of the configuration, k_∞

(2) The relative absorptions in the individual rod types for the complex (multi-component) lattice

(3) The lattice parameters η, p, and f for the complex lattices.

The basic assumptions implicit in the code are:

(a) The source rod can be represented by a line source, i.e., volume source effects and volume absorption effects within the rod are not explicitly considered.

(b) Displacement of moderator by fuel is not considered.

(c) Fission at non-thermal energies is ignored.

(d) Only one equivalent resonance is considered.

(e) The rod parameters are independent of the inter-rod separation distances.

(f) The fuel and absorbing rods are assumed infinitely long in the axial direction.

(g) The moderator is assumed infinite in extent.

The code will be written in separately contained sections to allow replacement of many of these assumptions one by one as the generality of the formulation is extended. Although initially the kernels to be used will be derived from age-diffusion theory, the code will be able to use kernels of arbitrary type, e.g. transport theory kernels, as long as they are displacement kernels, i.e., functions of only the source and receiver points.

1.2 Mathematical Treatment

In matrix notation the HET-1 code solves the following problem:

$$\underline{\underline{\gamma}}\ \underline{i} = \frac{1}{k}\ \underline{\underline{G}}\ \underline{i} - \underline{\underline{Z}}\ \underline{i} \qquad (1.1)$$

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 HET-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 (1.1). 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 $\underline{i}$ 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

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

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.

$$G_{nm} = \sum_{\beta} F^*_{na, m\beta} \, \eta_m$$

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 $S^r_{nm} = \sum_{\beta} g^r_{n\alpha, m\beta}$

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

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

$$\underline{\underline{G}} = (\underline{\underline{T}} - \underline{\underline{T}}^r \, \underline{\underline{A}} \, \underline{\underline{S}}^r) \, \underline{\underline{\eta}} \qquad (1.2)$$

Equation (1.1) can be written as

$$\underline{\underline{L}}\ \underline{i} = \frac{1}{k}\,\underline{\underline{G}}\ \underline{i} \tag{1.3}$$

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

$$\underline{\underline{L}}^{-1}\underline{\underline{G}}\ \underline{i} = k\ \underline{i} \tag{1.4}$$

The procedure in HET-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.[1] The first guess at the reciprocal matrix is formed by a Gaussian elimination procedure. Subsequent iterations use the following algorithm

$$\underline{\underline{R}}_{j+1} = \underline{\underline{R}}_j(2\underline{\underline{I}} - \underline{\underline{L}}\ \underline{\underline{R}}_j) \tag{1.5}$$

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. When this procedure has iterated to convergence (according to a criterion specified in the code), the code goes on to the next step.

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 (1.4). The power method iteration technique[2] 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. From the relative absorptions the code calculates the ratios of power generation in the various rod types. This concludes the calculation for a finite reactor.

When the problem is that of an infinite lattice an option is available in the code to calculate the lattice parameters f, p, and η. The code follows the calculation scheme presented in Section 4.

Section 2. Determination of the Rod Parameter γ

2.1 Discussion of γ

γ is a physical property of a given rod in a given moderator which is utilized in heterogeneous calculations. γ_n is defined as follows:

$$\gamma_n = \frac{\phi_{asy_n}}{i_n} \qquad (2.1)$$

where ϕ_{asy_n} = asymptotic thermal flux at the nth rod due to all the rods in the lattice. This asymptotic flux differs from the actual flux in that the source rods are considered to be line sources which only see moderator surrounding them.

$i_n = \frac{\text{thermal absorptions in } n^{th} \text{ rod}}{\text{cm sec}}$

In this section we will consider three different methods of obtaining γ for a particular rod-moderator combination. In a loosely packed lattice, γ is independent of the distance between rods (lattice spacing) and the number of rods present. Thus we can consider any lattice arrangement of the rod and calculate γ for the rod in this configuration. In this way we obtain the γ for the rod in the moderator. Since one of the simplest lattice configurations to study is an infinite square array, we have developed methods of calculating γ for this type of rod configuration. It should be noted that an infinite square lattice of one rod type has only one symmetry. Thus, as in

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Author's Note: The subscript u is used to indicate that the symbol refers to uranium.

heterogeneous diffusion theory, an effective cylindrical cell can be associated with any rod "n" in the lattice.

2.2 Method 1 - Evaluating $\frac{\phi_{asy}}{\bar{\phi}_{mod}}$

The first method we shall discuss utilizes the equation

$$\gamma = \frac{1}{\sigma_{au} A_u} \left(\frac{\phi_{asy_n}}{\bar{\phi}_{mod}} \right) D \tag{2.2}$$

where

A_u = cross section area of the n^{th} rod

σ_{au}= macroscopic absorption cross-section of the n^{th} rod

$\sigma_{a\ mod}$ = macroscopic absorption cross-section of the moderator

$\phi_{asy}(\vec{r}_m)$ = asymptotic thermal flux due to all rods at any point $\vec{r}_m$ of the moderator surrounding the n^{th} rod

$\phi(\vec{r}_m)$ = actual thermal flux due to all rods at any point $\vec{r}_m$ of the moderator surrounding the n^{th} rod

$\bar{\phi}_{mod}$ = average flux in the moderator included in the equivalent cylindrical cell surrounding the n^{th} fuel rod

$\bar{\phi}$ = average flux in the n^{th} fuel rod

D(disadvantage factor) = $\frac{\bar{\phi}_{mod}}{\bar{\phi}_u}$.

We can obtain equation 2.2 from 2.1 by substituting $i_n = \sigma_{au} A_u \bar{\Phi}$ into 2.1 and multiplying numerator and denominator by $\bar{\bar{\Phi}}_{mod}$.

Since $\Phi_{asy}(\vec{r}_m)$ will differ from $\Phi(\vec{r}_m)$ only very near the rod itself, it is valid to replace $\Phi(\vec{r}_m)$ by $\Phi_{asy}(\vec{r}_m)$ when averaging $\Phi(\vec{r}_m)$ over the entire cell. This is true because the volume of the moderator in an equivalent cell of a loosely packed lattice is large. Therefore the error incurred by using an incorrect representation for $\Phi(\vec{r}_m)$ over a small part of this volume is small. Since we are considering infinite rods, we need only average over the area. Thus,

$$\bar{\bar{\Phi}}_{mod} = \frac{1}{A_{mod}} \int_{A_{mod}} d\vec{r}_m \, \Phi_{asy}(\vec{r}_m) \tag{2.3}$$

where A_{mod} = cross section area of the moderator in the n^{th} cell. We obtain $\Phi_{asy}(\vec{r}_m)$ as a second order Taylor expansion about the rod n. To facilitate this calculation, the quantities $\Delta f_n(\vec{r}_m)$ and $\Delta F_n(\vec{r}_m)$ were introduced (defined below). The Taylor expansions of these quantities and the results for $\overline{\Delta f}_n$ and $\overline{\Delta F}_n$ for age diffusion kernels are cited in appendix 2.2. Below is the result for Φ_{mod}/Φ_{asy_n} in terms of $\overline{\Delta f}_n$, $\overline{\Delta F}_n$ and reactor constants.

$$\frac{\bar{\bar{\Phi}}_{mod}}{\Phi_{asy_n}} = 1 - \frac{\overline{\Delta f}_r - \eta p \overline{\Delta F}_n}{\eta p \sum_q F_{nq} - \sum_q f_{nq}} \tag{2.4}$$

where

$$\overline{\Delta f}_n = \frac{1}{A_{mod}} \int_{A_{mod}} \Delta f_n(\vec{r}_m) d\vec{r}_m = \frac{1}{A_{mod}} \int_{A_{mod}} d\vec{r}_m \left(\sum_q f(\vec{r}_m - \vec{r}_q) - f_{nq}\right)$$

$$\overline{\Delta F}_n = \frac{1}{A_{mod}} \int_{A_{mod}} \Delta F_n(\vec{r}_m) d\vec{r}_m = \frac{1}{A_{mod}} \int_{A_{mod}} d\vec{r}_m \left(\sum_q F(\vec{r}_m - \vec{r}_q) - F_{nq}\right)$$

$\vec{r}_m$ is a point in moderator surrounding the n^{th} rod

q is taken over all rods

$\eta = \frac{\text{fission neutrons emitted}}{\text{thermal neutron absorbed in the rod}}$

p = resonance escape probability

F_{nq} and f_{nq}, are the rod to rod kernels discussed in section I.

The disadvantage factor can be calculated directly from the thermal utilization which can be computed analytically or determined experimentally.

$$D = \frac{1-f}{Cf} \tag{2.5}$$

where f = thermal utilization

$$C = \frac{\sigma_{a\ mod} A_{mod}}{\sigma_{au} A_u}$$

From D and the ratio $\frac{\bar{\Phi}_{mod}}{\Phi_{asy_n}}$, we can readily calculate γ_n using equation 2.2.

2.3 Method 2 - Heterogeneous Technique

For the case of an infinite lattice, the criticality equations can be stated as:[3]

$$\gamma_m i_m = \frac{1}{k} \sum_{n=1}^{\infty} F^*_{mn} \eta_n i_n - \sum_{n=1}^{\infty} f_{mn} i_n \qquad \text{for } m, 1, 2 \to \infty \tag{2.6}$$

For an infinite square lattice where all the rods are physically identical, the constants η and γ do not differ from one rod to the next. Since there is only one symmetry, the absorptions in all the rods must be the same. Thus we can drop subscripts, cancel the i's and obtain for this case,

$$\gamma = \frac{\eta}{k} \sum_{n=1}^{\infty} F^*_{mn} - \sum_{n=1}^{\infty} f_{nm} \tag{2.7}$$

We have proved in appendix 2.1 that for an infinite square lattice,

$$\sum_{n=1}^{\infty} F^*_{nm} = p \sum_{n=1}^{\infty} F_{mn} \tag{2.8}$$

Substituting for $\sum_{n=1}^{\infty} F^*_{mn}$ from equation 2.8 and noting $k = \eta p f$, equation 2.7 becomes,

$$\gamma = \frac{1}{f} \sum_{n=1}^{\infty} F_{mn} - \sum_{n=1}^{\infty} f_{mn} \tag{2.9}$$

When the above equation is utilized to find γ, it is referred to as the heterogeneous technique since the heterogeneous kernels F_{mn} and f_{mn} are used. For an infinite square lattice where we consider only age and diffusion kernels, the sums in equation 2.9 are readily evaluated by the Poisson Summation

Formula.[4] For an infinite square lattice of lattice constant a and rod radius R_o, we obtain

$$\sum_n F_{mn} = \frac{1}{a^2 \sigma_{a\,mod}} \qquad (2.10a)$$

$$\sum_n f_{mn} = \frac{1}{a^2 \sigma_{a\,mod}} \left[1 + \frac{a^2}{4\pi L^2} \left\{ \ln\left(\frac{a^2}{\pi R_o^2}\right) + \frac{\pi R_o^2}{a^2} - 1.48 \right\} \right] \qquad (2.10b)$$

where L = diffusion length in the moderator.

Since the kernel sums are known, if the thermal utilization is calculated or experimentally determined, we can obtain γ directly from equation 2.9.

Note that no assumptions have gone into the derivation of 2.9. This method is also completely independent of resonance absorption effects. Furthermore an extremely important result concerning γ when it is obtained by equation 2.9 is shown in appendix 2.3. In this appendix we see that defining γ by equation 2.9 will give the correct k even if the kernels used are incorrect. Thus the γ, obtained from equation 2.9 when incorrect kernels are used, tends to balance out the effect of the incorrect kernels when both are used in the eigenvalue equation.

From the foregoing discussion, it may seem that this second method represents a panacea for obtaining γ for all rod-moderator combinations. However, we shall later show that γ as obtained from equation 2.9 has such a large dependence on the

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thermal utilization (the same is true for the first method) that it may be less useful for calculating γ's for rods in a D_2O moderator.

2.4 Method 3 - Diffusion Calculation of γ

Multiplying the numerator and denominator of the term on the right of equation 2.1 by $\Phi_{diff}(R_o)$ and $\bar{\Phi}_{u\ diff}$ where

$\Phi_{diff}(R_o)$ = flux on the periphery of the rod calculated by diffusion theory

$\bar{\Phi}_{u\ diff}$ = average flux in the rod calculated by diffusion theory

we obtain after rearranging:

$$\gamma = \frac{1}{\sigma_{au} A_u} \frac{\Phi_{diff}(R_o)}{\bar{\Phi}_{udiff}(R_o)} \cdot R \cdot S \qquad (2.11)$$

where $R = \dfrac{\Phi_{asyn}}{\Phi_{diff}(R_o)}$

$$S = \frac{\bar{\Phi}_{udiff}}{\bar{\Phi}_u}$$

$\bar{\Phi}_u$ = actual average flux in the rod.

The simplest type of γ calculation is to ignore R and S in equation 2.11. Doing this, calculating $\dfrac{\Phi_{diff}(R_o)}{\bar{\Phi}_{udiff}}$ for an infinite source rod of radius R_o, we obtain

$$\gamma = \frac{1}{2\pi R_o} \frac{L_u}{D_u} \frac{I_o(R_o/L_u)}{I_1(R_o/L_u)} \qquad (2.12)$$

This is the way γ is calculated by Galanin[5] and others. However, this is only an approximation and should be recognized as such. From physical reasoning we know that S will be slightly greater than one. We do not know, however, in which direction and by how much R differs from one.

2.5 Applying Methods 1, 2, 3 to a Uranium-Graphite Lattice

We have performed computations on a realistic lattice which was one of the configurations studied by Brookhaven National Laboratory.[6] We took a = 8-3/8 in. and R_o = 1 cm. We have considered our moderator to be AGOT graphite, whose properties have been determined experimentally. The experimental value of L^2 is 2800 cm^2; $\sigma_{a_{mod}} = 4 \times 10^{-4} cm^{-1}$ for this type of graphite. We used the values of the thermal cross-sections for natural uranium as quoted in Weinberg-Wigner.

Since f(r) is a more rapidly varying function of distance than F(r), we found that when we applied method 1 to this lattice that $\overline{\Delta f}_n >> \overline{\Delta F}_n$. Thus $\overline{\Delta F}_n$ can be ignored in the second term of equation 2.4. Utilizing the equations in appendix 2.2 we found $\overline{\Delta f}_n = .254\ cm^{-1}$. Then substituting our diffusion value of p = .94; $\sum_m F_{nm} = 5.49\ cm^{-1}$; $\sum_m f_{nm} = 5.74\ cm^{-1}$ into equation 2.4 we obtained $\frac{\phi_{asy}}{\bar{\phi}_{mod}} = .813$. Calculating D from our diffusion value of the thermal utilization (f = .826), we obtained $\gamma = .95\ cm^{-1}$ from equation 2.2 for a uranium rod of radius 1 cm in an AGOT graphite lattice. Utilizing the values of the thermal utilization, $\sum_m F_{nm}$ and $\sum_m f_{nm}$ referred to above, we obtained $\gamma = .91\ cm^{-1}$ from equation 2.9 of method 2. The diffusion theory result was $\gamma = .93\ cm^{-1}$. It should be noted that the diffusion theory result becomes more inaccurate as the rod becomes blacker - as the radius is increased.

For a 1 cm Nat U rod in AGOT graphite	$\gamma_1(\frac{\Phi_{asy}}{\Phi_{mod}})$	γ_2(het)	γ_3(diff)
	.95	.91	.93

Let us evaluate the error in the γ computed by method 2, assuming that the thermal utilization calculated by diffusion theory is 1% too large. To do this we shall use equation 4 of appendix 2.4 Substituting the values quoted above for $\sum_m F_{nm}$, $\sum_m f_{nm}$ and f_D, we find a relative error in γ of about 7%. Thus a 1% error in f generates a 7% error in γ. This indicates the importance of starting out with a correct thermal utilization, measured experimentally if possible.

When methods 1 and 2 are applied to a D_2O moderator, the error introduced in γ by using an incorrect thermal utilization is larger than in the case of a graphite moderator. However, the thermal utilization is known more precisely for a D_2O moderator since for practical lattices its value lies between .95 and 1. Thus it is reasonable to assume these methods for determining γ will be valid when the moderator is D_2O.

Returning to our definition of γ,

$$i = \frac{1}{\gamma} \phi_{asy} \tag{2.13}$$

we can make some qualitative observations as to how γ varies when the radius and enrichment of a uranium rod are changed, assuming the properties of the moderator are fixed. As we increase the radius of the rod, for a given ϕ_{asy} we expect an increase in absorptions. Thus γ must decrease with increasing rod radius. For precisely the same reasons we expect γ to decrease with increasing enrichment.

2.6 Thermal Utilization for an infinite square lattice

If we set the two relations for γ (equations 2.2 and 2.9) equal to each other, we can solve for the thermal utilization, in this simple case, entirely in terms of the heterogeneous kernels. Doing this, we obtain

$$f = \frac{\sigma_{a_u} A_u C - \frac{G}{\Sigma F_{mn}}}{\sigma_{a_u} A_u CQ - \frac{G}{\Sigma F_{mn}}} \tag{2.14}$$

where

$$Q = \frac{\Sigma f_{mn}}{\Sigma F_{mn}} > 1$$

$$G = \frac{\Phi_{asy}}{\bar{\Phi}_{mod}} < 1$$

From 2.10, $\Sigma F_{mn} = \frac{1}{\sigma_{a_{mod}} a^2} = \frac{1}{\sigma_{a_{mod}} A_{mod}}$

for a heterogeneous system.

Also $C\sigma_{a_u} A_u = \sigma_{a_{mod}} A_{mod}$.

Substituting these into equation 2.14 we obtain the desired result

$$f = \frac{1-G}{Q-G} \tag{2.15}$$

For a given moderator-rod configuration where the properties of the moderator are fixed, the largest value of the thermal utilization occurs for $G \rightarrow 0$. This leads to

$$f_{max} = \frac{\sum_n F_{mn}}{\sum_n f_{mn}} \tag{2.16}$$

It should be noted that the same result can be obtained directly with equation 2.9 since $\gamma = 0$ is a lower bound on γ. Equation 2.16 indicates that no matter how much you increase the uranium enrichment, there is an upper bound to the thermal utilization which is determined by the properties of the moderator and the geometrical arrangement of the rods.

Section 3. Transport Kernels

3.1 Transport Point Kernels

A transport theory approximation to the flux from a unit point isotropic source in an infinite moderator is [8]:

$$\phi(r) = \frac{\beta e^{-\kappa r}}{4\pi Dr} + \frac{e^{-\sigma' r}}{4\pi r^2} \qquad (3.1)$$

where $\kappa = \sqrt{3\sigma\sigma_a(1-\bar{\mu})} \cdot (1-2\sigma_a/5\sigma)$

$$\sigma' = \frac{5}{4}\sigma; \qquad \beta = 1 - \frac{4\sigma_a}{5\sigma}$$

At large values of r, the first term predominates. This term is of the same form as the diffusion point kernel multiplied by a constant β. ($\beta < 1$). In the region near the source, however, diffusion theory is inapplicable and gives a smoothed out flux with 1/r dependence which is much too small. Thus the second term in the transport approximation gives a more realistic $\frac{1}{r^2}$ dependence for the flux close to the source. We can determine the transport kernel for a line source of thermal neutrons in an infinite moderator by integrating over point sources. We shall do this for infinite and finite line sources. These kernels can be substituted for the simple diffusion kernel in the heterogeneous equations.

3.2 Transport Kernels for Line Sources

Let us define the following integrals for the flux at the center of a rod of length $2\ell_0$ at a radial distance r_0 away.

Let z be the distance along the rod measured from its center. Let r be the distance between any point on the rod and the point r_o. Then for a rod of length $2\ell_o$ the transport kernel is of the form,

$$\phi_{line}(r_o) = \frac{\beta}{4\pi D} \int_{-\ell_o}^{\ell_o} \frac{e^{-\varkappa r}}{r} dz + \int_{-\ell_o}^{\ell_o} \frac{e^{-\sigma_a' r}}{4\pi r^2} dz \qquad (3.2)$$

define $$f_1(r_o) = \int_{-\ell_o}^{\ell_o} \frac{e^{-\varkappa r}}{r} dz \qquad (3.3a)$$

$$f_2(r_o) = \int_{-\ell_o}^{\ell_o} \frac{e^{-\sigma_a' r}}{4\pi r^2} dz \qquad (3.3b)$$

The second integral (3.3b) has been evaluated numerically in connection with gamma ray uncollided dose theory. We have,[9]

$$f_2(r_o) = \frac{1}{2\pi r_o} F(\tan^{-1} \frac{\ell_o}{r_o}, \sigma_a' r_o) \qquad (3.4)$$

where the F functions can be found in graphical form. The only difficulty with using these graphs is that the F is not plotted on a fine enough mesh over the range $0 < \sigma_a' r_o \leq 1$, which is the range of interest for graphite or D_2O moderators. For an infinite rod,

$$f_2(r_o) = \frac{1}{2\pi r_o} F(\pi/2, \sigma_a' r_o) \qquad (3.5)$$

It can be shown using the Feynman Technique (Appendix 3.1) that

$$F(\tfrac{\pi}{2}, \sigma_a' r_o) = \frac{\pi}{2} - K_{jo}(\sigma_a' r) \tag{3.6}$$

where $K_{jo}(\sigma_a' r)$ are integrals evaluated[10] for small values of the argument.. Thus for an infinite rod we have:

$$f_2(r_\theta) = \frac{1}{2\pi r_o}\left[\frac{\pi}{2} - K_{jo}(\sigma_a' r_o)\right] \tag{3.7}$$

Let us evaluate the integral (3.3a)

$$f_1(r_o) = \int_{-\ell_o}^{\ell_o} \frac{e^{-\mathcal{H}\sqrt{z^2 + r_0^2}}}{\sqrt{z^2 + r_0^2}}\,dz \qquad \text{since } r^2 = z^2 + r_0^2 \tag{3.8}$$

Now the integral is an even function of z,

$$f_1(r_o) = 2\int_0^{\ell_o} \frac{e^{-\mathcal{H}\sqrt{z^2 + r_o^2}}}{\sqrt{z^2 + r_o^2}}\,dz \tag{3.9}$$

separating $f_1(r_o)$ into 2 integrals,

$$f_1(r_o) = 2\left[\int_0^{\infty} \frac{e^{-\mathcal{H}\sqrt{z^2 + r_o^2}}}{\sqrt{z^2 + r_o^2}}\,dz - \int_{\ell_o}^{\infty} \frac{e^{-\mathcal{H}\sqrt{z^2 + r_o^2}}}{\sqrt{z^2 + r_o^2}}\,dz\right] \tag{3.10}$$

Let us look at the first integral. Pulling r_o out of the square root we have

$$\int_0^\infty \frac{e^{-\varkappa r_o \sqrt{1 + \frac{z^2}{r_o^2}}}}{r_o \sqrt{1 + z^2/r_o^2}} dz \qquad (3.11)$$

Now make the variable substitution $\mu^2 = 1 + z^2/r_o^2$;

Then we obtain

$$\int_1^\infty \frac{e^{-\varkappa r_o \mu}}{\sqrt{\mu^2 - 1}} d\mu = K_o(\varkappa r_o) \text{ (11)} \qquad (3.12)$$

For an infinite rod (3.10) would be the only term in $f_1(r_o)$.

Now let us evaluate the second integral which is of importance for finite rods. Making a substitution of variable $t^2 = \varkappa^2(z^2 + r_o^2)$ we have,

$$\int_{\ell o}^\infty \frac{e^{-\varkappa\sqrt{z^2 + r_o^2}}}{\sqrt{z^2 + r_o^2}} dz = \frac{1}{\varkappa} \int_{\varkappa\sqrt{\ell_o^2 + r_o^2}}^\infty \frac{e^{-t} \, dt}{\sqrt{t^2 \varkappa^2 + r_o^2}} \qquad (3.13)$$

Taking $t/\varkappa$ out of the square root we obtain

$$\int_{\varkappa\sqrt{\ell_o^2 + r_o^2}}^\infty \frac{e^{-t} \, dt}{t\sqrt{1 - r_o^2 \varkappa^2/t^2}} \qquad (3.14)$$

We know $t^2/\varkappa^2 \geq \ell_o^2 + r_o^2$. Thus for $\ell_o >> r_o$, $\frac{r_o^2}{t^2/\varkappa^2} << 1$.

Expanding the square root in powers of $\left(\frac{r_o}{t/\mathcal{H}}\right)^2$ we have,

$$\int_{\mathcal{H}\sqrt{\ell_o^2 + r_o^2}}^{\infty} \frac{dt\, e^{-t}}{t} \left[1 + 1/2 \frac{r_o^2 \mathcal{H}^2}{t^2} + \frac{3}{8} \quad \frac{r_o^4 \mathcal{H}^4}{t^4} + \cdots + \right] \tag{3.15}$$

Keeping terms of first order in $\frac{r_o^2 \mathcal{H}^2}{t^2}$, the integral 3.15 becomes

$$E_1 \left(\mathcal{H}\sqrt{\ell_o^2 + r_o^2}\right) + 1/2 \left(\frac{r_o^2}{r_o^2 + \ell_o^2}\right) E_3 \left(\mathcal{H}\sqrt{\ell_o^2 + r_o^2}\right) + \cdots + \tag{3.16}$$

where $E_n(b) = b^{n-1} \int_b^{\infty} \frac{e^{-t}}{t^n}\, dt$ and has been evaluated numerically. Now,

$$E_n(b) = \frac{1}{n-1} \left[e^{-b} - bE_{n-1}\right] \tag{3.17}$$

is a recursion relation which enables us to obtain E_3 in terms of E_1 and exponentials. Thus we obtain for the second integral in equation 3.10,

$$\int_{\ell_o}^{\infty} \frac{e^{-\mathcal{H}\sqrt{z^2 + r_o^2}}}{\sqrt{z^2 + r_o^2}}\, dz = \left(1 + \frac{\mathcal{H}^2 r_o^2}{4}\right) E_1(t') + 1/4\left(\frac{\mathcal{H}^2 r_o^2}{t'^2}\right) (1-t')\ e^{-t'} + \cdots + \tag{3.18}$$

where $t' = \mathcal{H}\sqrt{\ell_o^2 + r_o^2}$

Substituting 3.12 and 3.18 into 3.10,

$$f_2(r_o) = 2\left[K_o(\varkappa r_o) - \left(1 + \frac{\varkappa^2 r_o^2}{4}\right)E_1(t') - 1/4\,\frac{\varkappa^2 r_o^2}{t'^2}\,(1-t')e^{-t'}\right] \quad (3.19)$$

Substituting 3.19 and 3.4 into 3.2

$$\Phi_{line}(r_o) = \frac{1}{2\pi r_o}\,F\left(\tan^{-1}\frac{\ell_o}{r_o},\ \sigma'_a R_o\right) \quad (3.20)$$

$$+ \frac{\beta}{2\pi D}\left[K_o(\varkappa r_o) - \left(1+\frac{\varkappa^2 r_o^2}{4}\right)E_1(t') - 1/4\left(\frac{\varkappa^2 r_o^2}{t'^2}\right)(1-t')e^{-t'}\right]$$

For an infinite rod, we obtain the simpler expression

$$\Phi_{line}(r_o) = \frac{\beta}{2\pi D}\,K_o(\varkappa r_o) + \frac{1}{2\pi r_o}\,F(\pi/2, \sigma'_a r_o) \quad (3.21)$$

Equations 3.20 and 3.21 express more accurate approximations for the f_{nm} moderator kernels for both finite and infinite rods. These kernels will be incorporated in some future problems handled by the heterogeneous code. In this way, we will determine how sensitive the eigenvalue results are to a kernel modification.

Section 4. Calculations for Complex Lattices

The heterogeneous method of reactor physics analysis can be used to calculate thermal utilization and resonance escape probability for complex lattices, i.e., those with several different kinds of lattice rods. These parameters can then be used in homogeneous calculations. The procedure would be as follows: First one calculates η, f, and p for an infinite complex lattice by the methods to be described. Then one calculates the effects of the finite size of the reactor by homogeneous methods.

No systematic exploration of the properties of complex lattices seems to have been carried out. Yet, complex lattices with rods of high and low enrichment are of interest for a number of potential applications, e.g., extending core lifetime, power flattening, increasing the conversion ratio, and taking the effects of burnup into account. Complex lattices with fuel and poison rods are of interest for control applications.

The heterogeneous method provides a direct means of calculating the properties of complex lattices with many types of rods. Formulas were obtained in our previous Quarterly Progress Report No. 1 for p and f in an infinite lattice. These parameters can be used in the following way to carry out homogeneous calculations consistently for complex lattices.

We assume an unreflected (bare) core infinite in longitudinal extent, for simplicity. Then by the conventional two group homogeneous methods one obtains

$$k = \frac{k_{\infty} e^{-B^2 \tau_{hom}}}{1 + L_{hom}^2 B^2} \tag{4.1}$$

where

B^2 = geometrical buckling

L_{hom} = thermal diffusion length for the homogenized system

τ_{hom} = age to thermal in the homogenized system

k_{∞} = infinite lattice multiplication constant

we shall use

$$k_{\infty} = \eta p f \tag{4.2}$$

where the fast fission factor has been absorbed into η. This expression for k_{∞} assumes that resonance fission is negligible.

The relations between L_{hom}^2 and τ_{hom} for the homogenized calculation and L^2 and τ for an infinite moderator (which are used in heterogeneous calculations) are

$$L_{hom}^2 = L^2(1-f) \tag{4.3}$$

τ_{hom} = τ(mixture), i.e. one calculates τ for the homogeneous mixture actually present.

Thus if η, f, and p have been obtained for a complex lattice one can calculate k and L^2_{hom} for a homogeneous calculation. A homogeneous calculation of the geometrical buckling, B^2, is then necessary to apply homogeneous reactor calculation methods to a finite reactor core with a complex lattice.

The formulas for f and p obtained in Reference 3 are as follows for an infinite lattice

$$f = \frac{\sum_{m=1}^{\infty} i_m}{\sum_{m=1}^{\infty} i_m \left[1 + \sum_{n=1}^{\infty} \frac{1}{\gamma_n} f_{nm}\right]} Q \qquad (4.4)$$

where

$$Q = \frac{\sum_{m=1}^{\infty}\left[i_m \eta_m + \sum_{r=1}^{R} i_{mr}\eta_{mr}\right]\left[\sum_{n=1}^{\infty} \frac{1}{\gamma_n} F^*_{nm}\right]}{\sum_{m=1}^{\infty}\left[i_m\eta_m + \sum_{r=1}^{R} i_{mr}\eta_{mr}\right]\left[1 - \sum_{r}\sum_{t=1}^{\infty} A_{tr} g_{tm}^{(r-1)}\right]} \qquad (4.5)$$

$$\frac{1}{p} - 1 = \frac{\sum_{m=1}^{\infty}\sum_{r=1}^{R} i_{mr}}{\sum_{m=1}^{\infty} i_m\left[1 + \sum_{n=1}^{\infty}\frac{1}{\gamma_n} f_{nm}\right]} Q \qquad (4.6)$$

η is the average number of fission neutrons per absorption. Thus

$$\eta = \frac{\sum_{m=1}^{\infty} i_m \eta_m}{\sum_{m=1}^{\infty} i_m}$$

We shall apply these formulas to cylindrical fuel elements of infinite axial length in an infinite two dimentional lattice. One equivalent lumped resonance is assumed and fission at resonance energies will be neglected, since only low enrichment fuels will be considered. We define the following matrices:

$\underline{\underline{Z}}$, whose elements Z_{ij} give the contribution of all thermal sink kernels f_{nm} of type j to a rod of type i.

That is, $Z_{ij} = \sum_m f_{in, jm}$, from all rods m of the j-th type to any rod n of the i-th type. Z_{ij} is independent of n by definition of a rod type.

$\underline{\underline{T}}$, whose elements T_{ij} give the contribution of the slowing down-thermal diffusion kernels F_{nm} of type j to a rod of type i. That is,

$$T_{ij} = \sum_m F_{in,jm} ,$$

from all rods m of the j-th type to any rod n of the i-th type.

$\underline{\underline{S}}^r$, whose elements S^r_{ij} give the contribution of the slowing down kernels to resonance energy at r^{th} resonance from all rods of type j to type i.

$\underline{\underline{T}}^r$, whose elements T^r_{ij} give the contribution of the r^{th} resonance-to-thermal kernels from all rods of type j to type i.

$\underline{\underline{\eta}}$, a diagonal matrix whose elements are the η's for the individual types

$\underline{\underline{\gamma}}$, a diagonal matrix whose elements are the γ's for the individual types

$\underline{\underline{A}}$, a diagonal matrix whose elements are the A's for the individual types

$\underline{\underline{G}}$, which is defined as

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

$\underline{H}$, will denote a row vector whose elements are the relative number of rods of each type in the lattice

$\underline{i}$, will denote a column vector whose components are the relative absorptions in each type of rod.

In this matrix notation expressions (4.4), (4.5), (4.6) become the following:

$$f = \frac{\underline{H} \cdot \underline{i}}{\underline{H} \cdot \underline{i} + \underline{H} \cdot \underline{\underline{\gamma}}^{-1} \cdot \underline{\underline{Z}} \cdot \underline{i}} \, Q \tag{4.7}$$

$$Q = \frac{\underline{H} \cdot \underline{\underline{\gamma}}^{-1} \cdot \underline{\underline{G}} \cdot \underline{i}}{\underline{H} \cdot \underline{\underline{\eta}} \cdot \underline{i} - \underline{H} \cdot \underline{\underline{A}} \cdot \underline{\underline{S}}^{r} \cdot \underline{\underline{\eta}} \cdot \underline{i}} \tag{4.8}$$

$$P = \frac{\underline{H} \cdot \underline{\underline{A}} \cdot \underline{\underline{S}}^{r} \cdot \underline{\underline{\eta}} \cdot \underline{i}}{\underline{H} \cdot \underline{\underline{\eta}} \cdot \underline{i}} \tag{4.9}^{*}$$

* (4.9) is obtained as follows. (4.6) becomes

$$\frac{1}{p} - 1 = \frac{\underline{H} \cdot \underline{\underline{A}} \cdot \underline{\underline{S}}^{r} \cdot \underline{\underline{\eta}} \cdot \underline{i}}{\underline{H} \cdot \underline{i} + \underline{H} \cdot \underline{\underline{\gamma}}^{-1} \cdot \underline{\underline{Z}} \cdot \underline{i}} \, \frac{Q}{k}$$

If one takes $k = \eta p f$ and uses the expressions above for Q, F and η, one obtains (4.9) after some manipulation.

$$\eta = \frac{\underline{H} \cdot \underline{\underline{\eta}} \cdot \underline{i}}{\underline{H} \cdot \underline{i}} \tag{4.10}$$

We have applied these expressions to the two lattices shown in Figure 1. A square lattice (20 cm on a side) of natural uranium rods (2 cm in radius) in a graphite moderator, with 1.3% enriched rods in interstitial positions has been considered. The inter-rod spacing for the enriched rods is (Case I) equal to, or (Case II) double that of the square lattice.

For the special case of infinite, square, interstitial lattices, the elements of the Z, S^r, T and T^r matrices have been calculated using the Poisson Summation Formula[(4)] for diffusion age kernels. This technique greatly facilitates a hand calculation since it converts the unwieldy sums usually encountered in computing these matrix elements to sums which converge much more rapidly. Noting that the subscript 1 denotes the rod type with the smaller inter-rod spacing, Poisson Formula Results are cited below for the matrix elements Q_{11}, Q_{22}, Q_{21} where Q represents Z, S^r, T or T^r. For a two component lattice we obtain Q_{12} from Q_{21} utilizing the relation

$$H_1 Q_{12} = H_2 Q_{21}$$

which holds for any displacement kernel. H_1 and H_2 are the relative numbers of rods of types 1 and 2.

<u>S^r Matrix</u>

$$S^r_{ii} = \frac{1}{a_i^2}\left[1 + 2e^{-4\pi^2 \tau_r / a_i^2}\right] \qquad i = 1,2 \tag{4.11}$$

$$S^r_{21} = \frac{1}{a_1^2}\left[1 - 2e^{-4\pi^2 \tau_r / a_1^2}\right]$$

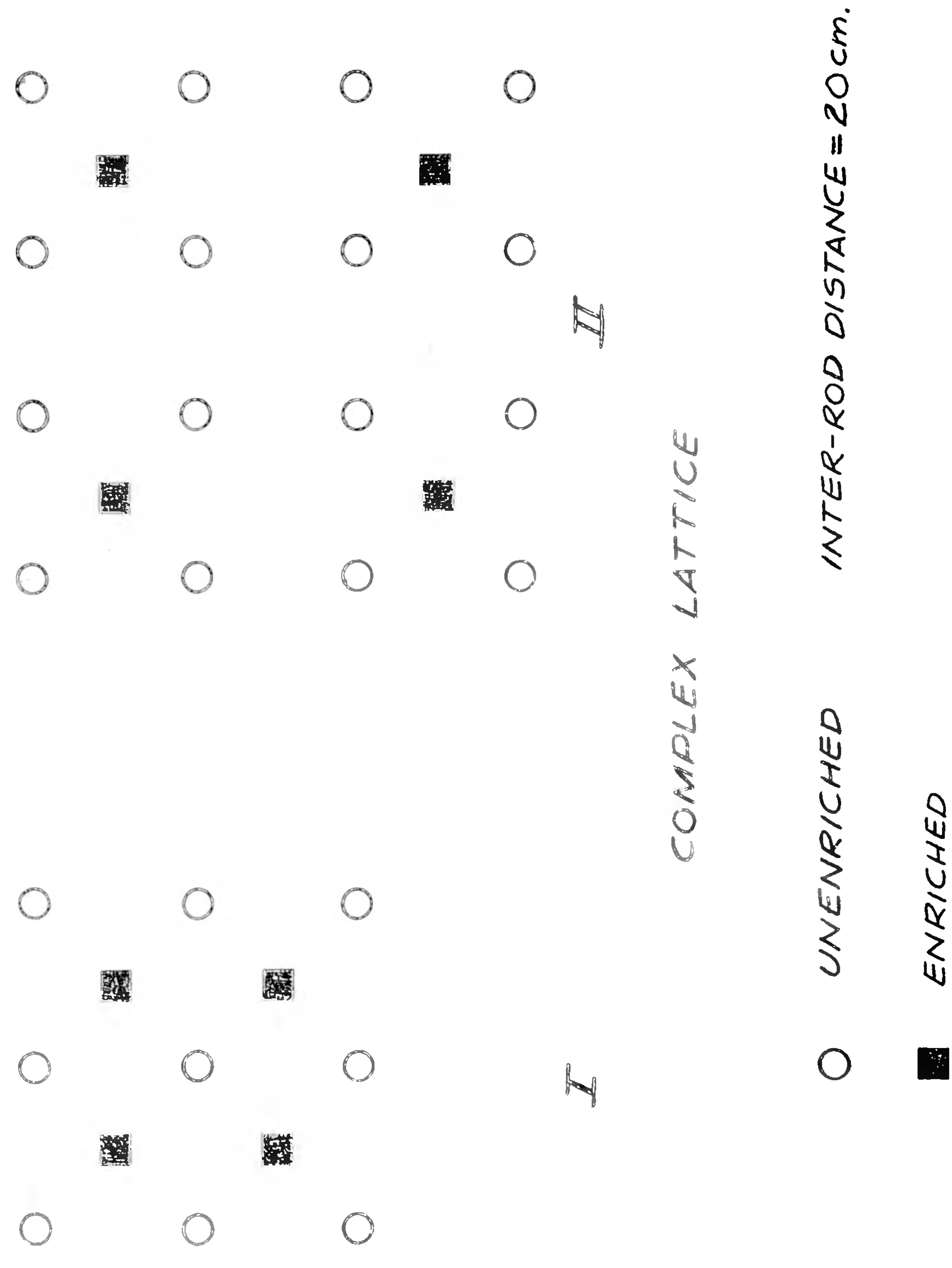

FIG. 1

COMPLEX LATTICE

These expressions assume that $\frac{4\pi^2\tau_r}{a_i^2} >> 1$. a_i^2 is the lattice area per unit rod for the i^{th} rod type.

Z Matrix

$$Z_{ii} = \frac{1}{a_i^2\sigma_a}\left[\frac{a_i^2}{4\pi L^2}\left(\ln\left(\frac{a_i^2}{\pi R_{oi}^2}\right) + \frac{\pi R_{oi}^2}{a_i^2} - 1.48\right) + 1\right] \quad i = 1,2$$

$$Z_{21} = \frac{1}{a_1^2\sigma_a}\left[1 + \frac{a_1^2}{4\pi L^2}\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}{}' (-1)^{m+n}\frac{1}{m^2+n^2}\right] \tag{4.12}$$

where the prime indicates m = n = o not allowed.

R_{oi} is the radius of the i^{th} rod type.

T Matrix

$$T_{ii} = \frac{1}{a_i^2\sigma_a} \quad i = 1,2$$

$$T_{21} = e^{\tau/L^2} Z_{21} + \frac{e^{\tau/L^2}}{2\pi L^2\sigma_a}\sum_{n_1=-\infty}^{\infty}\sum_{n_2=-\infty}^{\infty} S(n_1, n_2) \tag{4.13}$$

$$S(n_1, n_2) = \frac{\tau}{2L^2} \exp - \frac{a_1^2}{4\tau}\left[(1/2-n_1)^2 + (1/2-n_2)^2\right]$$

$$- 1/2\left\{ 1 + \frac{a_1^2}{4L^2}\left[(1/2-n_1)^2 + (1/2-n_2)^2\right]\right\} E_1\left[\frac{a_1^2}{4\tau}\left[(1/2-n_1)^2\right.\right.$$

$$\left.\left. +(1/2 - n_2)^2\right]\right]$$

We can obtain T^r by replacing τ by $\tau - \tau_r$.

The rod parameters used in these calculations are as follows:

<u>Enriched rod</u> (numbered 2)

radius = 2 cm

$\gamma = 0.178\ cm^{-1}$

$A = 51.0\ cm^2$

$\tau_r = 262.5\ cm^2$ in graphite

$\eta = 1.605$, including fast fission factor

Enrichment = 1.30%

Unenriched rod (numbered 1)

radius = 2 cm

$\gamma = 0.255\ cm^{-1}$

$A = 51.0\ cm^2$

$\tau_r = 262.5\ cm^2$ in graphite

$\eta = 1.340$, including fast fission factor

Natural uranium enrichment

These rod parameters were calculated as follows:

Calculation of γ

To calculate γ for rod 1, for example, we assume an infinite lattice composed of such rods, i.e., a one component infinite lattice. The heterogeneous equation becomes

$$\gamma = \frac{1}{f} T_{ii} - Z_{ii}$$

f is assumed known for the rod. In this schematic calculation f was obtained from diffusion theory.

Calculation of A

To calculate A it was assumed that the resonance escape probability p was available. A was calculated from

$$p = 1 - \frac{A}{\sigma}$$

where σ is the lattice area per unit rod in the one component infinite lattice for which p was calculated. p was calculated by standard techniques using the values of the U^{238} resonance integral given by Macklin and Pomerance.[12]

Calculation of η

η was calculated as the product of ϵ, the fast fission factor, and the conventional η, obtained from measurements by Kouts.[(13)]

Figure 1 shows configurations I and II.

The H vector is the following:

Configuration I

$$H = \begin{bmatrix} 1 & 1 \end{bmatrix}$$

Configuration II

$$H = \begin{bmatrix} 4 & 1 \end{bmatrix}$$

Other matrices are:

$$A = \begin{bmatrix} 51 & 0 \\ 0 & 51 \end{bmatrix} \qquad \eta = \begin{bmatrix} 1.34 & 0 \\ 0 & 1.605 \end{bmatrix}$$

The results of the calculation are given in Table I

TABLE I CALCULATION RESULTS FOR COMPLEX LATTICE

	Unenriched Lattice		Enriched Lattice		Complex Lattice	
	I	II	I	II	I	II
f	.940	.940	.953	.794	.978	.957
p	.872	.872	.872	.968	.745	.841
η	1.34	1.34	1.605	1.605	1.489	1.400
$\frac{i_2}{i_1}$					1.214	1.127
k	1.095	-	1.330	1.235	1.084	1.122

The columns of Table I labelled "unenriched lattice" give the properties of the one-component unenriched lattice for the two configurations. Since the unenriched lattice is the same for both configurations these two columns are identical. The ratio of absorptions i_2/i_1 is not applicable to the single component lattices. k is the infinite lattice static multiplication factor.

The columns of Table I labelled "enriched lattice" give the properties of the one component enriched lattice in the two configurations. Since the configurations are different columns I and II are not identical. Configuration I is more tightly packed than Configuration II, hence f is larger for I and p is larger for II.

The columns of Table I labelled "Complex lattice" are of primary interest. This gives the properties of the two component lattices made up of enriched and unenriched rods. Since Configuration I is more tightly packed than II, f is larger in I and p is larger in II. η is larger in I where the ratio of absorptions in the enriched to unenriched rods is 1.214 to 1, as compared to 1.122 to 1 in the less tightly packed Configuration II. The ratios i_2/i_1 for these two configurations could not have been predicted by homogeneous calculations.

The interesting and surprising conclusion demonstrated for the complex lattice in Table I is that k_∞ is actually smaller for the more tightly packed lattice Configuration I, than for the loose packed Configuration II. This is due to the lower p in I, which is not sufficiently compensated by a higher η.

Appendix 2.1

"To Show $\sum_{q=1}^{\infty} F_{mq}^{*} = p\sum_{q=1}^{\infty} F_{mq}$ for an infinite square lattice".

Let us look at the heterogeneous equations for an infinite square lattice with only one rod type when resonance absorption is present (subscript 1) and when it is not (subscript 2). We assume that γ and η of the rods are known. Cancelling the i's, we have

$$\gamma = \frac{\eta}{k_1} \sum_{q=1}^{\infty} F_{mq}^{*} - \sum_{q=1}^{\infty} f_{mq} \qquad (1)$$

$$\gamma = \frac{\eta}{k_2} \sum_{q=1}^{\infty} F_{mq} - \sum_{q=1}^{\infty} f_{mq} \qquad (2)$$

Setting the two expressions for γ equal to one another, we obtain

$$\frac{k_1}{k_2} = \frac{\sum_{q=1}^{\infty} F_{mq}^{*}}{\sum_{q=1}^{\infty} F_{mq}} \qquad (3)$$

For an infinite square lattice with no resonance absorption present, utilization of the Poisson Summation Formula yields the result that the asymptotic slowing down density at thermal energies is a constant throughout the moderator. For resonance absorption present, we find that the asymptotic thermal showing down density is again a constant (with smaller magnitude) throughout the moderator if the condition

$$\frac{4\pi^2 \tau_r}{a^2} >> 1 \tag{4}$$

where τ_r is the age from the resonance energy to thermal

a is the lattice constant

is satisfied. This condition is fulfilled unless the lattice constant a is unreasonably large. Thus we see for the case of the infinite square lattice that the spacial distribution of the thermal slowing down density is not affected by the presence of resonances. It then follows for this case that the thermal utilization, calculated by the heterogeneous method, is invariant to the presence of resonances. Therefore, reactivities in the two cases, with and without resonance absorption present, reduce to

$$k_1 = \eta f p \tag{5a}$$

$$k_2 = \eta f \tag{5b}$$

Returning to equation 3, we obtain the immediate result

$$\sum_{q=1}^{\infty} F^{*}_{mq} = p \sum_{q=1}^{\infty} F_{mq} \tag{6}$$

Appendix 2.2

"Calculation of $\frac{\bar{\Phi}_{mod}}{\Phi_{asy_n}}$."

A. Derivation of equation 2.4

We represent $\Phi(\vec{r}_m)$ by $\Phi_{asy}(\vec{r}_m)$ throughout the moderator when averaging Φ. Thus,

$$\bar{\Phi}_{mod} = \frac{1}{A_{mod}} \int_{\text{Area of moderator}} \Phi_{asy}(\vec{r}_m)\, d\vec{r}_m \qquad (1) \qquad dA$$

We define a quantity $\Delta\Phi_{asy}(\vec{r}_m)$ from the following equation.

$$\Delta\Phi_{asy}(\vec{r}_m) = \Phi_{asy}(\vec{r}_m) - \Phi_{asy_n} \qquad (2)$$

For an infinite square lattice, where each rod has 1 thermal absorption/cm sec,

$$\Phi_{asy}(\vec{r}_m) = \eta \sum_q F^*(|\vec{r}_m - \vec{r}_q|) - \sum_q f(|\vec{r}_m - \vec{r}_q|) \qquad (3a)$$

$$\Phi_{asy_n} = \eta \sum_q F^*_{nq} - \sum_q f_{nq} \qquad (3b)$$

where q is over all rods.

Subtracting 3b from 3a

$$\Delta\Phi_{asy}(\vec{r}_m) = \eta \Delta F_n^*(\vec{r}_m) - \Delta f_n(\vec{r}_m) \qquad (4)$$

where we define

$$\Delta F_n^*(\vec{r}_m) = \sum_q \left[F^*(|\vec{r}_m - \vec{r}_q|) - F^*_{nq}\right] \qquad (5a)$$

$$\Delta f_n(\vec{r}_m) = \sum_q \left[f(|\vec{r}_m - \vec{r}_q|) - f_{nq}\right] \qquad (5b)$$

$$\Delta F_n(\vec{r}_m) = \sum_q \left[F(|\vec{r}_m - \vec{r}_q|) - F_{nq}\right] \qquad (5c)$$

It is the difference quantities (5) that we shall later expand in a Taylor Series. We want to obtain $\bar{\Phi}_{mod}$ in terms of these quantities. To do this let us return to equation 2 and integrate over $d\vec{r}_m$. When we do this substituting equation 4 for $\Delta\Phi_{asy}(\vec{r}_m)$,

$$\bar{\Phi}_{mod} = \Phi_{asy_n} + \eta \frac{1}{A_{mod}} \int_{A_{mod}} \Delta F_n^*(\vec{r}_m)\, d\vec{r}_m - \frac{1}{A_{mod}} \int_{A_{mod}} \Delta f_n(\vec{r}_m)\, d\vec{r}_m \qquad (6)$$

If we consider the integrals divided by the area as averages $\overline{\Delta F}_n^*$ and $\overline{\Delta f}_n$ respectively, then equation 6 becomes

$$\bar{\Phi}_{mod} = \Phi_{asy_n} + \eta \overline{\Delta F}_n^* - \overline{\Delta f}_n \qquad (6^1)$$

If we divide by Φ_{asy_n},

$$\frac{\bar{\Phi}_{mod}}{\Phi_{asy_n}} = 1 - \frac{\overline{\Delta f}_n - \eta \overline{\Delta F}_n^*}{\eta \sum_q F_{nq}^* - \sum_q f_{nq}} \qquad (7)$$

We show in appendix 2.1 that for the case of an infinite square lattice with one rod type,

$$\Sigma F_{nq}^* = p \Sigma F_{nq}$$

It follows that the same relations hold for $\overline{\Delta F}$. Making these substitutions we obtain

$$\frac{\bar{\Phi}_{mod}}{\Phi_{asy_n}} = 1 - \frac{\overline{\Delta f}_n - \eta p \overline{\Delta F}_n}{\eta p \Sigma F_{nq} - \Sigma f_{nq}} \qquad (8)$$

B. Evaluating $\overline{\Delta f}_n$ and $\overline{\Delta F}_n$ by a Taylor Expansion

Since the principal contributions to the kernel sums $\Delta f_n(\vec{r}_m)$ and $\Delta F_n(\vec{r}_m)$ (5) comes from the n^{th} rod itself, this contribution was evaluated exactly. For all other rods ($q \neq n$), the contributions to $\Delta f_n(\vec{r}_m)$ and $\Delta F_n(\vec{r}_m)$ were taken into account by a second order Taylor Expansion about the n^{th} rod. Defining ρ_m as the radial distance from the rod n to the point $\vec{r}_m$ in the moderator and summing over all rods in the infinite square lattice of pitch a, we obtain

$$\Delta f_n(\vec{r}_m) = f(\rho_m) + \rho_m^2 \Bigg[\sum_{q=1}^{\infty} \left(\frac{d^2 f(r)}{dr^2}\bigg|_{qa} + \frac{1}{qa} \frac{df(r)}{dr}\bigg|_{qa} \right)$$

$$+ \sum_{q=1}^{\infty} \left(\frac{d^2 f(r)}{dr^2}\bigg|_{qa\sqrt{2}} + \frac{1}{qa\sqrt{2}} \frac{df(r)}{dr}\bigg|_{qa\sqrt{2}} \right)$$

$$+ 2\sum_{q=2}^{\infty} \sum_{s=1}^{q-1} \left(\frac{d^2 f(r)}{dr^2}\bigg|_{a\sqrt{q^2+s^2}} + \frac{1}{a\sqrt{q^2+s^2}} \frac{df(r)}{dr}\bigg|_{a\sqrt{q^2+s^2}} \right) \Bigg]$$

$$-f(R_o) \qquad (9)$$

In equation 9, the first term on the right represents the contribution from the rod n itself. We can also see that the second order expansion depends on ρ_m^2, thus it's radially symmetric. We would obtain an exactly similar expression for $\Delta F_n(\vec{r}_m)$.

For any set of displacement kernels $\Delta f_n(\vec{r}_m)$ is of the form $f(\rho_m) + C_1\rho_m^2 + C_2$, where C_1 and C_2 are constants. This can be readily averaged over the equivalent circular cell if $f(\rho_m)$ is integrable. We cite the results for the case of diffusion and age theory kernels where $\varkappa$ is the reciprocal diffusion length in the moderator and R_o is the radius of the rods.

$$\overline{\Delta f}_n = \frac{1}{2\pi L^2 \sigma_{a_{mod}}} \left[- K_o(\varkappa R_o) + \frac{2}{(\frac{a^2}{\pi} - R_o^2)} \left[\frac{R_o}{\varkappa} K_1(\varkappa R_o) - \frac{a}{\pi} K_1\left(\frac{\varkappa a}{\sqrt{\pi}}\right)\right] + \frac{a^2}{2\pi} B \right] \tag{10}$$

$$\text{where } B = \varkappa^2 \left[\sum_{n=1}^{\infty} K_o(\varkappa na) + K_o(\varkappa na\sqrt{2}) + 2 \sum_{n=2}^{\infty} \sum_{j=1}^{n-1} K_o(\varkappa a\sqrt{n^2 + j^2}) \right]$$

$$\overline{\Delta F}_n = \frac{a^2}{2\pi} \frac{e^{\varkappa^2 \tau}}{4\pi L^2 \sigma_{a_{mod}}} \left[A - \frac{1}{4\tau} E_2(\varkappa^2 \tau) \right]$$

$$\text{where } A = \varkappa^2 \sum_{n=1}^{\infty} 2 \left[K_o(\varkappa na) + K_o(\varkappa na\sqrt{2}) \right]$$

$$- \frac{1}{\tau} (1-\varkappa^2\tau) \left[\exp - \frac{(na)^2}{4\tau} + \exp - \frac{(na\sqrt{2})^2}{4\tau} \right]$$

$$- \left[E_1\left(\frac{(na)^2}{4\tau}\right) + E_1\left(\frac{(na\sqrt{2})^2}{4\tau}\right) \right]$$

$$+ \varkappa^2 \sum_{n=2}^{\infty} \sum_{j=1}^{n-1} 2K_o(\varkappa a\sqrt{n^2 + j^2}) - \frac{1}{\tau}(1-\varkappa^2\tau) \exp - \frac{(n^2 + j^2)a^2}{4\tau} - E_1\left(\frac{\sqrt{(n^2+j^2)a^2}}{4\tau}\right)$$

Appendix 2.3

"To show k is independent of the diffusion kernel used when γ is obtained by Method 2"

Suppose we have 2 sets of kernels, the primed and the unprimed. For an infinite square lattice where the thermal utilization is known, we can obtain γ and γ' from equation 2.9 for each set of kernels.

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

$$\gamma' = \frac{1}{f}\Sigma F'_{mn} - \Sigma f'_{mn} \qquad (1b)$$

Substituting each of these γ's into the eigenvalue equation for the infinite square lattice with the appropriate kernels used in each case, we obtain

$$\frac{1}{f}\Sigma F_{mn} - \Sigma f_{mn} = \frac{\eta}{k}\Sigma F^{*}_{mn} - \Sigma f_{mn} \qquad (2a)$$

$$\frac{1}{f}\Sigma F'_{mn} - \Sigma f'_{mn} = \frac{\eta}{k'}\Sigma F^{*\prime}_{mn} - \Sigma f'_{mn} \qquad (2b)$$

Solving for k and k' from equations 2 and taking the ratio,

$$\frac{k'}{k} = \frac{\Sigma F^{*\prime}_{mn}/\Sigma F'_{mn}}{\Sigma F^{*}_{mn}/\Sigma F_{mn}} \qquad (3)$$

For the case of an infinite square lattice, with only one rod type and one effective resonance absorption, we can obtain the above summations in terms of the matrix elements discussed in section 1. If we did this, we would find that k is independent of the thermal diffusion kernel approximation used. However, this conclusion follows more readily from the result in appendix 2.1. That is,

$$p = \frac{\sum_n F^*_{nm}}{\sum_n F_{nm}},$$

Substituting this relation into equation 3, we have

$$\frac{k'}{k} = \frac{p'}{p} \qquad (4)$$

Since the p's only depend on the slowing down density distribution at resonance energies, they are independent of the thermal diffusion kernel approximation utilized. Thus the k's are also independent of the diffusion kernel approximation when γ is obtained from equation 2.9.

Appendix 2.4

"Error in γ due to a Diffusion Theory Thermal Utilization"

Since the f calculated by diffusion theory is too large, the values γ_D of γ obtained using a diffusion theory thermal utilization must be too small. In the following discussion f = true thermal utilization; f_D = diffusion theory thermal utilization;

$$\Delta f = f_D - f;$$

A) Error in Method 2

$$\gamma_D = \frac{1}{f_D} \sum_n F_{mn} - \sum_n f_{mn} \tag{1a}$$

$$\gamma = \frac{1}{f} \sum_n F_{mn} - \sum_n f_{mn} \tag{1b}$$

Substituting for f_D in a and subtracting b-a,

$$\gamma - \gamma_D = \left[\frac{1}{f} \sum_n F_{mn} - \sum_n f_{mn}\right] - \left[\frac{1}{f+\Delta f} \sum_n F_{mn} - \sum_n f_{mn}\right] \tag{2}$$

Now $\Delta f \ll f$

$$\gamma - \gamma_D = \left[\frac{1}{f} \sum_n F_{mn} - \sum_n f_{mn}\right] - \frac{1}{f}\left[1 - \frac{\Delta f}{f}\right] \sum_n F_{mn} + \sum_n f_{mn} \tag{3}$$

$$\gamma - \gamma_D = \frac{\Delta f}{f^2} \sum_n F_{mn}$$ where the term on the right represents the error in using f_D. (4)

B) Error in Method 1

Following the same routine as before we obtain after a few steps:

$$\gamma - \gamma_D = \left(\frac{\Phi_{asy}}{\bar{\Phi}_{mod}}\right)\left(\frac{1}{\Sigma_{au} A_u C}\right)\left\{\frac{\Delta f}{f}\left[\frac{1}{f} - 1\right] + \frac{\Delta f}{f}\left[1 - \frac{\Delta f}{f}\right]\right\} \qquad (5)$$

Neglecting terms in $(\Delta f)^2$

$$\gamma - \gamma_D = \frac{\Phi_{asy}}{\bar{\Phi}_{mod}} \quad \frac{1}{\sigma_{a_u} A_u C} \quad \frac{\Delta f}{f^2} \qquad (6)$$

Now by definition $\sigma_{a_u} A_u C = \sigma_{a_{mod}} A_{mod}$. Since the area of the cell $a^2 \approx A_{mod}$ for most heterogeneous systems,

$$\sigma_{au} A_u C \approx \sigma_{a_{mod}} A^2 = \frac{1}{\sum_n F_{mn}} \text{ from equation 12 of Section 2.} \qquad (7)$$

Substituting (7) into (6)

$$\gamma - \gamma_D = \frac{\Delta f}{f^2} \left(\sum_n F_{mn} \right) \left(\frac{\Phi_{asy}}{\bar{\Phi}_{mod}} \right) \qquad (8)$$

Since $\frac{\Phi_{asy}}{\bar{\Phi}_{mod}} \lesssim 1$, the error in method 1 introduced by a diffusion theory f is slightly less than in method 2.

Appendix 3.1

Evaluating $f_2(r_o) = \frac{1}{4\pi} \int_{\text{inf. line}} \frac{e^{-\sigma' |\vec{r}-\vec{\ell}|} d\vec{\ell}}{|\vec{r}-\vec{\ell}|^2}$ by the Feynman Technique.

The solution to the helmholtz equation

$$\nabla^2 \phi_H(\vec{\rho}) - \sigma'^2 \phi_H(\vec{\rho}) = S(\vec{\rho}) \tag{1}$$

with an infinite line source of unit strength

$$\phi_H(r_o) = \int_{\text{inf. line}} \frac{e^{-\sigma' |\vec{r}-\vec{\ell}|} d\vec{\ell}}{4\pi |\vec{r}-\vec{\ell}|} \tag{2}$$

In the above equation $\vec{\ell}$ is the vector to any point of the line source; $\vec{r}$ is the vector to the point in the moderator at which we want to evaluate the kernel. r_o is the radial distance from the rod to the point $\vec{r}$. Since the line source is infinite we expect $\phi_H = \phi_H(r_o)$.

Suppose we consider $\phi_H(r_o)$ to be $\phi_H(\sigma', r_o)$ and integrate with respect to σ'.

$$\int_{\sigma}^{\infty} \phi_H(\sigma', r_o)\, d\sigma' = \int_{\text{line}} \frac{e^{-\sigma' |\vec{r}-\vec{\ell}|}}{4\pi |\vec{r}-\vec{\ell}|^2} d\vec{\ell} = f_2(r_o) \tag{3}$$

Thus if we can find ϕ_H by solving the helmholtz differential equation using the boundary conditions for an infinite rod, we can integrate ϕ_H with respect to σ' and obtain $f_2(r_o)$ as shown in equation 3.

Therefore, we look at the inhomogeneous helmholtz equation with only one independent variable - the radial distance r_o from the rod.

$$\frac{\partial^2 \phi_H}{\partial r_o^2} + \frac{1}{r_o}\frac{\partial \phi_H}{\partial r_o} - \sigma_a'^2 \phi(r_o) = -\delta(r_o)/2\pi r_o \qquad (4)$$

The homogeneous solution is:

$$\phi_H(r_o) = A\, K_o(\sigma_a' r_o) \qquad (5)$$

We apply the source boundary condition to evaluate A,

$$\lim_{r_o \to o} \vec{\nabla}\phi \cdot \vec{dS} = \lim_{r_o \to o} A\, \sigma_a' K_1(\sigma_a' r_o)\, 2\pi r_o = 1 \qquad (6)$$

We know $\lim_{r_o \to o} K_1(\sigma_a' r) = \frac{1}{\sigma_a' r_o}$. Thus

$$A = \frac{1}{2\pi} \qquad (7)$$

Substituting (7) into (5)

$$\phi_H(r_o) = \frac{K_o(\sigma_a' r_o)}{2\pi} \qquad (8)$$

Substituting $\phi_H(r_o) = \frac{K_o(\sigma_a' r_o)}{2\pi}$ into equation 3, we obtain

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$$f_2(r_o) = \int_{\sigma_a'}^{\infty} \frac{K_o(\sigma_a' \; r_o)}{2\pi} \, d\sigma_a' \tag{9}$$

Making a change of variable $z = \sigma_a' r_o$, we obtain

$$f_2(r_o) = \frac{1}{2\pi r_o} \int_{\sigma_a' r_o}^{\infty} K_o(z) \, dz \tag{10}$$

Restating equation 10,

$$f_2(r_o) = \frac{1}{2\pi r_o} \left[\int_0^{\infty} K_o(z) dz - \int_0^{\sigma_a' r_o} K_o(z) dz \right] \tag{10'}$$

In HW-30323 we find the integrals γ_o and K_{jo}

where

$$\gamma_o = \int_0^{\infty} K_o(z) dz$$

$$K_{jo}(x) = \int_0^{x} K_o(z) dz$$

evaluated numerically. Thus we can express $f_2(r_o)$ in terms of these quantities. That is,

$$f_2(r_o) = \frac{1}{2\pi r_o} \left[\gamma_o - K_{jo} \; (\sigma_a' \; r_o) \right] \tag{11}$$

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BIBLIOGRAPHY

1. E. Bodewig, "Matrix Calculus" (Interscience, 1959), p. 227

2. Ibid. p. 269

3. Carl Klahr, "Heterogeneous Reactor Calculation Methods, Quarterly Progress Report No. 1" (June 30, 1959), p. 12

4. Morse and Feshback, "Methods of Theoretical Physics", (McGraw-Hill, 1953), p. 466

5. Galanin, "Critical Size of Heterogeneous Reactor with Small Number of Rods", Paper No. 663, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy (New York: United Nations, 1956), Vol. 5, p. 462

6. Kaplan and Chernick, "Brookhaven Reactor", Paper No. 606, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy (New York: United Nations, 1956), Vol. 5, p. 295

7. P. Gast, "Uranium-Graphite Lattices", Paper No. 607, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy (New York: United Nations, 1956), Vol. 5, p. 288

8. Weinberg and Wigner, "The Physical Theory of Neutron Chain Reactions" (University of Chicago Press, 1958), p. 200

9. T. Rockwell, Reactor Shielding Design Manual (TID-7004, 1956), p. 348

10. G. Muller, "Table of the Function $K_{jn}(x)$", HW30323, Jan. 54

11. Morse and Feshback, "Methods of Theoretical Physics", (McGraw-Hill, 1953) p. 1323

12. Macklin and Pomerance, "Resonance Capture Integrals", Paper No. 833, Proceedings of the International Conference on the Peaceful Uses of Atomic Energy (United Nations, 1956), Vol. 5, p. 96

13. Kouts and Sher, "Experimental Studies of Slightly Enriched Uranium, Water Moderated Lattices", BNL 486, (to be published).