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On the Theory of Space Dependent Neutron Spectra in Heterogeneous Reactors

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An analytical method is developed for determining the energy dependent neutron flux in homogeneous and heterogeneous media. Using the heavy gas model scattering operator, neutron spectra in two-dimensional rod reactors of various types are calculated in the diffusion approximation. They show a strong spatial dependence even in the epithermal region, which fact is neglected in the numerical treatment of the problem by Honeck and Kaplan. It is just this epithermal part of the spectrum, which mainly influences the values of the thermal utilization and the η-factor. The value obtained for the latter quantity is too large if the correct neutron spectra in moderator and fuel are replaced by Maxwellian distributions at moderator-temperature or a suitably displaced temperature, for example.

INTRODUCTION

Many attempts have been made to obtain analytical solutions of the thermalization problem for various scattering models. Usually this is done for infinite, homogeneous media neglecting all effects of heterogeneity or finiteness of the system under consideration. A first step in the determination of stationary neutron spectra in heterogeneous assemblies has been made by Häfele (*1*), who has semi-analytically solved the problem for one-dimensional slab reactors with weak absorption in the heavy gas scattering model. The same geometry has been treated by an improved multigroup iteration procedure by Meetz, Ott, and Sanatani using the Wigner-Wilkins scattering operator (*2*). The completely numerical work of Honeck and Kaplan (*3*) will be discussed briefly at the end of this paper.

The aim of the present work was to find the analytical solution of the problem for heterogeneous reactors with infinitely long, cylindrical fuel elements arranged in a regular square lattice. Although the method derived below can be extended to a far more general character, we shall perform the calculation in the diffusion approximation, as far as the spatial dependence of the neutron flux is concerned, and use the heavy gas differential operator in order to describe the scattering of the neutrons by the molecules of the moderator. Furthermore all neutron absorptions shall follow a $1/v$-law.

The special difficulty one faces in a treatment of the energy dependence of the neutron flux is that in neutron thermalization a slowing down and an equilibration process are superposed, as has been stated by Häfele (*1*). At high energies the slowing down process is predominant; at low energies, however, the equilibration process prevails. The method described below treats these two phenomena separately by the appropriate mathematical methods and joins them continuously.

First we shall calculate the neutron spectrum in a homogeneous, infinite, absorbing medium in order to explain the idea of our method. Then we shall apply the method to heterogeneous reactor structures as considered by Meetz (*4*). The spatial dependence of the neutron flux is treated by means of Meetz's method. The neutron spectra thus obtained are used for calculating the thermal utilization and the η-factor.

In a two-dimensional problem the stationary neutron flux $\phi(x, y, E)$ obeys the following equation, if no sources are present:

$$D\Delta\phi(x, y, E) + \int \Sigma(x, y, E' \to E)\phi(x, y, E')\, dE' - \Sigma_{\text{tot}}(x, y, E)\phi(x, y, E) = 0. \quad (1)$$

x and y are space variables and E represents the neutron energy. If we introduce a dimensionless energy variable

$$\epsilon = \frac{E}{kT},$$

where T is the temperature of the moderator, and describe the scattering by the heavy gas model, we can write:

$$\begin{aligned}\int \Sigma(\epsilon' \to \epsilon)\phi(x, y, \epsilon')\, d\epsilon' - \Sigma_S(x, y, \epsilon)\phi \\ = 2\mu\Sigma_S^0 \left(\epsilon \frac{\partial^2}{\partial\epsilon^2} + \epsilon \frac{\partial}{\partial\epsilon} + 1\right)\phi(x, x, \epsilon) \\ = \mathfrak{L}\phi(x, y, \epsilon).\end{aligned} \tag{2}$$

μ is the ratio of the neutron mass to the mass of the molecule of the moderator. Σ_S^0 is the macroscopic low energy scattering cross section of the moderator. Thus we obtain the following equation determining the neutron flux:

$$\begin{aligned}D\Delta\phi(x, y, \epsilon) + \mathfrak{L}\phi(x, y, \epsilon) \\ - \Sigma_a(x, y, \epsilon)\phi(x, y, \epsilon) = 0.\end{aligned} \tag{3}$$

In the reactor model described below $\mathfrak{L}$ is spatially independent. The diffusion constant D is regarded as energy independent in this work. We shall use the eigenfunctions of the heavy gas operator $\mathfrak{L}$:

$$\mathfrak{L}\omega_p(\epsilon) = w_p \cdot \omega_p(\epsilon). \tag{4}$$

These are the Laguerre functions of the first kind:

$$\omega_p(\epsilon) = \epsilon \cdot e^{-\epsilon} L_p^{(1)}(\epsilon) \tag{5}$$

with (see (5), where they are defined with an additional factor $\sqrt{p+1}$; our normalization is more convenient for the purposes of this paper):

$$\begin{aligned}L_p^{(1)}(\epsilon) = \sqrt{p+1} \sum_{n=0}^{p} (-1)^n \\ \cdot \frac{p!}{n!(n+1)!(p-n)!} \cdot \epsilon^n.\end{aligned} \tag{6}$$

Furthermore,

$$w_p = -2\mu\Sigma_s^0 \cdot p. \tag{7}$$

THE INFINITE, HOMOGENEOUS MEDIUM

The neutron flux in a homogeneous, infinite, source-free medium is independent of the space variables. Thus, under the above mentioned assumption of a $1/v$-absorption law, we have to solve the following second order differential equation:

$$\left(\epsilon \frac{d^2}{d\epsilon^2} + \epsilon \frac{d}{d\epsilon} + 1\right)\phi(\epsilon) - p_t \cdot \epsilon^{-1/2}\phi(\epsilon) = 0 \tag{8}$$

with the abbreviation

$$p_t = \frac{\Sigma_a(\epsilon = 1)}{2\mu\Sigma_s^0}. \tag{9}$$

The conditions to be imposed on the solution of Eq. (8) are that the slowing-down density should vanish at $\epsilon = 0$ and the flux should be positive for positive energies. These conditions are satisfied if

$$\phi(\epsilon) \to 0 \quad \text{for} \quad \epsilon \to 0 \tag{10}$$

and

$$\phi(\epsilon) > 0 \quad \text{for} \quad \epsilon > 0 \tag{11}$$

The solution of Eq. (8) satisfying (10) and (11) is determined uniquely except for a positive factor.

Let us try now to find this solution. First we shall look for an asymptotic representation of the neutron flux at high energies:

$$\phi_{as}^{(1)}(\epsilon) = \sum_{\nu=0}^{N} \frac{g_\nu}{\epsilon^{1+\nu/2}}. \tag{12}$$

Equation (12) is the semiconvergent, asymptotic expansion of a particular solution $\phi^{(1)}(\epsilon)$ of Eq. (8). The coefficients g_ν are determined by the following recursion formula:

$$g_{\nu+2} = \frac{2}{\nu+2}\left[\left(1 + \frac{\nu}{2}\right)\left(2 + \frac{\nu}{2}\right)g_\nu - p_t \cdot g_{\nu+1}\right]. \tag{13}$$

$g_0 > 0$ is an arbitrary normalization constant. We obtain:

$$g_1 = -2p_t \cdot g_0, \qquad g_2 = 2(1 + p_t^2)g_0 \cdots.$$

A second linearly independent solution $\phi^{(2)}(\epsilon)$ of Eq. (8) may be written asymptotically in the form:

$$\phi_{as}^{(2)}(\epsilon) = \epsilon \cdot e^{-\epsilon} \sum_{\nu=0}^{N} \frac{g_\nu'}{\epsilon^{\nu/2}}. \tag{14}$$

The solution of Eq. (8) required here is a linear combination of the two particular solutions $\phi^{(1)}$ and $\phi^{(2)}$, both being singular at $\epsilon = 0$:

$$\phi(\epsilon) = \phi^{(1)}(\epsilon) + \lambda\phi^{(2)}(\epsilon). \tag{15}$$

$\phi(\epsilon)$ is regular at $\epsilon = 0$, but it does not belong to the space of the eigenfunctions of the heavy gas operator because of the contribution $\phi^{(1)}(\epsilon)$ in (15), as can be seen from (5) and (12).

It follows from Eq. (8) and the boundary condition (10) that the neutron flux $\phi(\epsilon)$ can be expanded in a power series in terms of $\epsilon^{1/2}$ beginning linearly in ϵ:

$$\phi = A\epsilon + B\epsilon^{3/2} + C\epsilon^2 + D\epsilon^{5/2} + \cdots. \tag{16}$$

Let us now determine a three-times differentiable function $\bar{\phi}^N(\epsilon)$ in such a way that

$$\bar{\phi}^N(\epsilon) = \phi_{as}^{(1)}(\epsilon) \qquad \text{for } \epsilon \geqq \epsilon_0 \tag{17}$$

and

$$\bar{\phi}^N(\epsilon) = a\epsilon + b\epsilon^{3/2} + c\epsilon^2 + d\epsilon^{5/2} \qquad \text{for } \epsilon \leqq \epsilon_0 . \tag{18}$$

The continuity condition for $\bar{\phi}^N(\epsilon)$ and its first three derivatives at $\epsilon = \epsilon_0$ determine the coefficients a, b, c, d. N is a finite, fixed upper limit of summation in (12).

The difference $\phi(\epsilon) - \bar{\phi}^N(\epsilon)$ can be determined from an inhomogeneous differential equation because $\bar{\phi}^N(\epsilon)$ does not satisfy Eq. (8) for $\epsilon < \epsilon_0$ and only approximately for $\epsilon \geqq \epsilon_0$:

$$\epsilon \frac{d^2}{d\epsilon^2}[\phi(\epsilon) - \bar{\phi}^N(\epsilon)] + \epsilon \frac{d}{d\epsilon}[\phi(\epsilon) - \bar{\phi}^N(\epsilon)] + [\phi(\epsilon) - \bar{\phi}^N(\epsilon)] - p_t \cdot \epsilon^{-1/2}[\phi(\epsilon) - \bar{\phi}^N(\epsilon)] = S^N(\epsilon). \tag{19}$$

$\phi(\epsilon) - \bar{\phi}^N(\epsilon)$ has to satisfy the boundary conditions

$$\phi - \bar{\phi}^N \to 0 \quad \text{for} \quad \epsilon \to 0 \tag{20}$$

and

$$\epsilon(\phi - \bar{\phi}^N) \to 0 \quad \text{for} \quad \epsilon \to \infty . \tag{21}$$

This can be seen from (12), (14), and (15). The "source function" $S^N(\epsilon)$ is found by inserting $-\bar{\phi}^N(\epsilon)$ into the left-hand side of Eq. (8).

For $\epsilon \geqq \epsilon_0$ one obtains from (12), (13), and (8):

$$S^N(\epsilon) = -\left\{ \frac{g_N(1 + \frac{1}{2}N)(2 + \frac{1}{2}N)}{\epsilon^{1+(N+2)/2}} + \frac{g_{N-1}[1 + \frac{1}{2}(N-1)][2 + \frac{1}{2}(N-1)]}{\epsilon^{1+(N+1)/2}} - p_t \cdot \frac{g_N}{\epsilon^{1+(N+1)/2}} \right\}. \tag{22}$$

One recognizes from Eq. (22) that $S^N(\epsilon)$ cannot be expanded in the eigenfunctions of the heavy gas operator.

As is shown in (7) the source function $S^N(\epsilon)$ can be made zero for $\epsilon \geqq \epsilon_0$, if instead of the $1/v$-absorption law assumed in Eq. (8) a slightly changed absorption cross section is used. N and ϵ_0 can be chosen in such a way that this deviation of the absorption cross section from the original $1/v$-law is negligibly small. Thus we may neglect $S^N(\epsilon)$ for $\epsilon \geqq \epsilon_0$ in Eq. (19). It is then possible to expand the source function $S^N(\epsilon)$ as well as the solution $\phi(\epsilon) - \bar{\phi}^N(\epsilon)$ of Eq. (19) in the Laguerre orthogonal functions. We write:

$$S^N(\epsilon) = \sum_{p=0}^{\infty} c_p \cdot \omega_p(\epsilon) \tag{23}$$

and make the ansatz

$$\phi(\epsilon) - \bar{\phi}^N(\epsilon) = \sum_{p=0}^{\infty} a_p \cdot \omega_p(\epsilon). \tag{24}$$

Equation (19) is transformed into the following infinite system of linear equations for the coefficients a_p :

$$-pa_p - p_t \sum_{q=0}^{\infty} V_{pq} a_q = c_p . \qquad (p = 0, 1, 2 \cdots) \tag{25}$$

Here we have introduced (8):

$$V_{pq} = (\omega_p , \epsilon^{-1/2}\omega_q) = \int_0^{\infty} L_p^{(1)}(\epsilon) \cdot \epsilon^{-1/2} \cdot \epsilon \cdot e^{-\epsilon} L_q^{(1)}(\epsilon)\, d\epsilon. \tag{26}$$

We shall take into consideration only $p_0 + 1$ modes in the expansions (23) and (24). Experience shows the result to be independent of p_0 for $p_0 \geqq 4$. The expansion coefficients a_p of the function $\phi(\epsilon) - \bar{\phi}^N(\epsilon)$ are then determined uniquely as the solution of the finite, inhomogeneous system of linear equations:

$$-pa_p - p_t \sum_{q=0}^{p_0} V_{pq} a_q = c_p . \qquad (p = 0, 1, 2, \cdots, p_0) \tag{27}$$

We have now obtained the solution of Eq. (8) satisfying the boundary conditions (10) and (11) with sufficient accuracy in the form:

$$\phi(\epsilon) = \bar{\phi}^N(\epsilon) + \sum_{p=0}^{p_0} a_p \cdot \omega_p(\epsilon). \tag{28}$$

$\bar{\phi}^N(\epsilon)$ is given by (12), (17) and (18); the coefficients a_p are determined from (27).

The method of the determination of the neutron spectrum in an infinite, homogeneous medium as described in this section has been applied to the example $p_t = 0.25$. We have chosen $\epsilon_0 = 16$, $N = 10$, and $p_0 = 5$. Figure 1 shows the result of the calculation completely agreeing with the solution obtained numerically by Hurwitz, Nelkin, and Habetler (6). The figure shows $\epsilon\phi(\epsilon)$ in its dependence on $\sqrt{\epsilon}$. Furthermore, $\epsilon\bar{\phi}^{10}(\epsilon)$ has also been drawn. One recognizes that this function, representing the main part of the solution at high energies, essentially

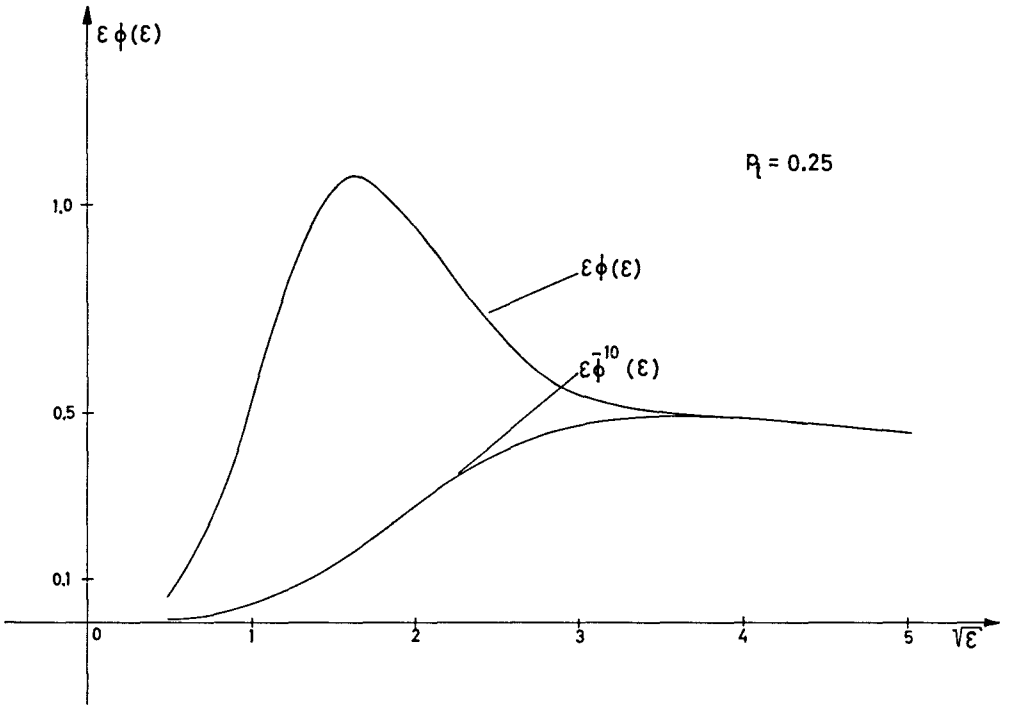

FIG. 1. Neutron spectrum in an infinite, homogeneous, source-free medium. The lower curve represents $\epsilon\bar{\phi}^{10}(\epsilon)$, giving essentially the contribution of the neutrons slowed down from higher energies. The difference $\epsilon\phi(\epsilon) - \epsilon\bar{\phi}^{10}(\epsilon)$ describes the contribution of the neutrons nearly in thermal equilibrium with the moderator.

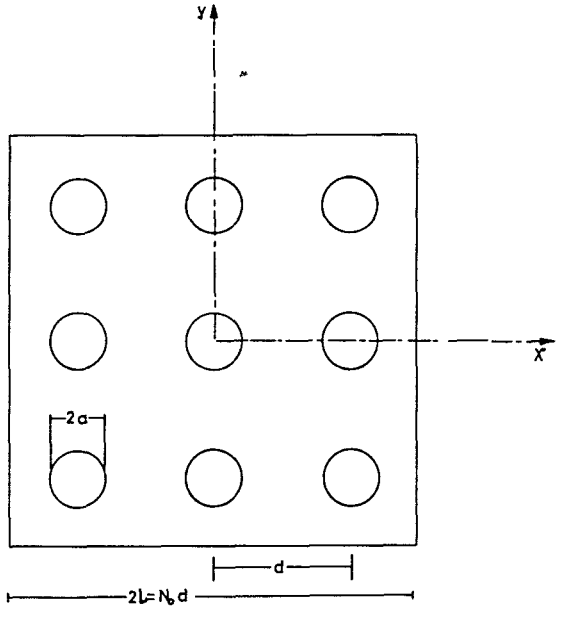

FIG. 2. Arrangement of the fuel elements in the two-dimensional rod reactor.

gives the contribution to the total flux of those neutrons which are slowed down from higher energies by collisions with the molecules of the moderator. On the other hand, the function $\sum_{p=0}^{p_0} a_p\omega_p(\epsilon)$ describes the contribution of those neutrons which are nearly in thermal equilibrium with the moderator. By continuing the function $\bar{\phi}^N(\epsilon)$ steadily to the origin of the energy scale according to Eq. (18), we were able to compose these two functions, representing physically completely different contributions to the neutron flux, continuously to the entire solution of Eq. (8).

THE TWO-DIMENSIONAL ROD REACTOR

It is now our task to combine the method of treating the energy dependence of the neutron flux, as developed in the last section, with Meetz's theory describing the spatial behavior of the neutron flux. We shall use here the notation of Häfele (*1*).

Meetz considers a reactor of the following type: the reactor is infinitely long in the z-direction and has a square cross section. There are $N_0^2 = (2n+1)^2$ cylindrical fuel elements of radius a, likewise infinitely long in the direction of the reactor axis which form a regular square lattice with the lattice parameter d. The side length of the reactor cross section is $2L = N_0 d$. Figure 2 shows the arrangement of the fuel elements in the reactor.

The space between the fuel slugs is filled with non-absorbing moderator. The absorption effect of the fuel elements is described in its spatial dependence by Dirac δ-functions, i.e., the fuel rods are considered

as linear sinks for the neutrons. This has as a consequence that the neutron flux has logarithmic singularities at the lattice points of the reactor thus idealized. Therefore it may not be identified with the real physical flux inside the fuel elements but only in the moderator and at the boundary of the fuel slugs. The neutron absorption rate in a fuel element has to be determined from the mean value $\phi^R(\epsilon)$ of our solution over the boundary of the rod and an appropriately chosen effective absorption cross section Σ_a^{eff}. It has to be determined in such a way that the absorption rate calculated from it agrees with that obtained using the real neutron flux ϕ_U in the fuel and the real absorption cross section $\Sigma_a{}^U$. Thus the equation determining Σ_a^{eff} is:

$$\pi a^2 \iint\limits_{\substack{\text{fuel}\\ \text{element}\\ (kd,ld)}} \Sigma_a^{\text{eff}}(\epsilon)\phi^R(kd, ld; \epsilon)\delta(x - kd)\delta(y - ld)\, dx\, dy = \iint\limits_{\substack{\text{fuel}\\ \text{element}\\ (kd,ld)}} \Sigma_a^U(\epsilon)\phi_U(x, y, \epsilon)\, dx\, dy. \tag{29}$$

The effort to be applied in the determination of ϕ_U depends on the accuracy required in the calculation. For a first estimate we may use an energy independent diffusion approximation inside the fuel elements. The determination of the effective cross section is a point to be improved later on.

The energy of the fission neutrons is assumed as infinite. Thus the reactor is source-free. As we shall see below this assumption, together with the postulate of positivity of the neutron flux, has as a consequence a simple $\cos(\alpha_0 x)\cos(\alpha_0 y)$-behavior of the flux in the limit of an infinite neutron energy. This does not describe the real physical situation in a reactor. Häfele (*1*) has treated the heterogeneous slowing down problem assuming the energy of the fission neutrons as finite at $\epsilon_F \approx 10^8$. At an intermediate energy $\epsilon \approx 10^6$ the neutrons then show the above mentioned simple spatial distribution. This energy being extremely high in comparison with the thermal energies $\epsilon \approx 1$ of interest here, we may assume it to be infinite, thus justifying our assumption of infinite fission energy coincidentally.

With the abbreviations

$$p_t = \frac{\Sigma_a^{\text{eff}}(\epsilon = 1) \cdot \pi a^2}{d^2 2\mu\Sigma_s{}^0} \tag{30}$$

and

$$x_0{}^2 = \frac{D}{2\mu\Sigma_s{}^0} \tag{31}$$

we obtain from (3) the equation determining the neutron flux in our reactor model:

$$x_0{}^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\phi(x, y, \epsilon) + \frac{1}{2\mu\Sigma_s{}^0}\mathfrak{L}\phi(x, y, \epsilon) - p_t \cdot \epsilon^{-1/2}\sum_{k=-n}^{+n}\sum_{l=-n}^{+n} d^2\delta(x - kd)\delta(y - ld) \cdot \phi^R(kd, ld, \epsilon) = 0. \tag{32}$$

The boundary conditions to be imposed on the solution of Eq. (32) are (1) energetically: regularity of the flux at $\epsilon = 0$, i.e.,

$$\phi(x, y, \epsilon) \to 0 \quad \text{for} \quad \epsilon \to 0, \tag{33}$$

and (2) spatially: vanishing of the flux at the reactor boundaries, i.e.,

$$\begin{aligned}\phi(x, \pm L, \epsilon) &= 0\\ \phi(\pm L, y, \epsilon) &= 0.\end{aligned} \tag{34}$$

Equation (34) means that the reactor has no reflector. Furthermore the neutron flux has to be positive all over the reactor. From the symmetry of the problem it follows that the flux is an even function of x and y. A main result of Meetz's work is a representation of the neutron flux by a double Fourier series, which in our energy dependent case takes the form (cf. (*4*)):

$$\phi(x, y, \epsilon) = \sum_{r,s=-\infty}^{+\infty}\varphi_{N_0 r,\, N_0 s}(\epsilon)\ \cos(\alpha_{N_0 r}x)\cos(\alpha_{N_0 s}y) \tag{35}$$

with

$$\alpha_{N_0 r} = \frac{2N_0\, r + 1}{2L}\,\pi \tag{36}$$

We obtain from (32) the following system of second order differential equations for the Fourier coefficients $\varphi_{N_0 r, N_0 s}(\epsilon)$:

$$\frac{1}{2\mu\Sigma_s{}^0}\mathfrak{L}\varphi_{N_0 r, N_0 s}(\epsilon) - (\alpha_{N_0 r}^2 + \alpha_{N_0 s}^2)x_0{}^2\varphi_{N_0 r, N_0 s}(\epsilon) - p_t\,\epsilon^{-1/2}\sum_{m,t=-\infty}^{+\infty}\varphi_{N_0 m, N_0 t}(\epsilon)[\cos(\alpha_{N_0 m}x)\cos(\alpha_{N_0 t}y)]^{R_0} = 0,\ (r, s = -\infty, \cdots, -1, 0, +1, \cdots, +\infty). \tag{37}$$

The superscript R_0 means that the mean value over the boundary of the central rod is to be taken.

The boundary conditions for the solution of Eqs.

(37) are:

$$\varphi_{N_0 r,N_0 s}(\epsilon) \to 0 \quad \text{for} \quad \epsilon \to 0 \qquad (r, s = -\infty, \cdots, -1, 0, 1, \cdots, +\infty) \tag{38}$$

$$\epsilon^{1-2\alpha_0{}^2 x_0{}^2}\varphi_{00}(\epsilon) \to \text{const.} > 0 \text{ for } \epsilon \to \infty \tag{39}$$

$$\epsilon^{1-2\alpha_0{}^2 x_0{}^2}\varphi_{N_0 r,N_0 s}(\epsilon) \to 0 \quad \text{for} \quad \epsilon \to \infty. \qquad ((r, s) \neq (0, 0)) \tag{40}$$

The connection between the postulate that the flux should be positive all over the reactor and the boundary conditions (39)–(40) becomes obvious later on.

In order to obtain the asymptotic solution of the system (37), we make the ansatz (cf. (1)):

$$\underset{\text{as}}{\varphi^{(1)}_{N_0 r,N_0 s}} = \sum_{\nu=0}^{N} \frac{g^{\nu}_{N_0 r,N_0 s}}{\epsilon^{1+\beta+(\nu/2)}} \tag{41}$$

and get a recursion formula for the coefficients $g^{\nu}_{N_0 r,N_0 s}$:

$$g^{\nu}_{N_0 r,N_0 s} = -p_t \frac{G^{\nu-1}}{(\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2 + \beta + \frac{1}{2}\nu} + \frac{(\frac{1}{2}\nu + \beta)(\frac{1}{2}\nu + \beta + 1)g^{\nu-2}_{N_0 r,N_0 s}}{(\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2 + \beta + \frac{1}{2}\nu}. \tag{42}$$

$G^0 > 0$ is an arbitrary constant. We have furthermore introduced in (42):

$$G^{\nu} = \sum_{r,s=-\infty}^{+\infty} g^{\nu}_{N_0 r,N_0 s}[\cos(\alpha_{N_0 r}x)\cos(\alpha_{N_0 s}y)]^{R_0}. \tag{43}$$

For $\nu = 0$, Eq. (42) must be replaced by:

$$g^{0}_{N_0 r,N_0 s}(\beta + (\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2) = 0. \tag{44}$$

Equation (44) determines the indices of the nonvanishing coefficients $g^0_{N_0 r,N_0 s}$. In order that the flux be positive in the high energy range the indices of the sole nonvanishing coefficient $g^0_{N_0 r,N_0 s}$ have to be zero. This means that the spatial behavior of the neutron flux in our geometry is given by a simple $\cos(\alpha_0 r)\cos(\alpha_0 y)$-distribution at high energies. We see that the asymptotic solution (41) satisfies the boundary conditions (39), (40). Thus we obtain:

$$\beta = -2\alpha_0{}^2 x_0{}^2. \tag{45}$$

From (42), together with (45), the $g^{\nu}_{N_0 r,N_0 s}$'s can be easily determined.

The first coefficients are (cf. (1)):

$$g^0_{N_0 r,N_0 s} = \frac{G^0}{\mathfrak{F}_0(\sqrt{2}\alpha_0 a)}\,\delta_{r0}\,\delta_{s0}$$

$$g^1_{N_0 r,N_0 s} = -p_t \frac{G^0}{(\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2 - 2\alpha_0{}^2 x_0{}^2 + \frac{1}{2}}$$

$$G^1 = -p_t H(-2\alpha_0{}^2 x_0{}^2 + \tfrac{1}{2}),$$

$$g^2_{N_0 r,N_0 s} = -p_t \cdot \frac{G^1}{(\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2 - 2\alpha_0{}^2 x_0{}^2 + 1} + \frac{(1 - 2\alpha_0{}^2 x_0{}^2)(2 - 2\alpha_0{}^2 x_0{}^2)}{(\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2 - 2\alpha_0{}^2 x_0{}^2 + 1}\,\delta_{r0} \cdot \delta_{s0} \cdot \frac{G^0}{\mathfrak{F}_0(\sqrt{2}\alpha_0 a)} \tag{46}$$

$$G^2 = -p_t \cdot G^1 \cdot H(-2\alpha_0{}^2 x_0{}^2 + 1) + (1 - 2\alpha_0{}^2 x_0{}^2)(2 - 2\alpha_0{}^2 x_0{}^2)G^0$$

Here we have introduced

$$H(\gamma) = \sum_{r,s=-\infty}^{+\infty} \frac{[\cos(\alpha_{N_0 r}x)\cos(\alpha_{N_0 s}y)]^{R_0}}{\gamma + (\alpha^2_{N_0 r} + \alpha^2_{N_0 s})x_0{}^2}. \tag{47}$$

The evaluation of this double series as well as that of all following Fourier series is discussed briefly at the end of this section. Furthermore the mean value $[\cos(\alpha_0 x)\cos(\alpha_0 y)]^{R_0}$ was replaced by a Bessel function of the first kind and zero order

$$\mathfrak{F}_0(\sqrt{2}\alpha_0 a) = \frac{1}{2\pi}\int_0^{2\pi} \cos(\alpha_0 a \cos\theta)\cos(\alpha_0 a \sin\theta)\, d\theta.$$

We now define a set of functions which have three continuous derivatives at $\epsilon = \epsilon_0$ by:

$$\bar{\varphi}^N_{N_0 r,N_0 s}(\epsilon) = \underset{\text{as}}{\varphi^{(1)}_{N_0 r,N_0 s}}(\epsilon) \quad \text{for } \epsilon \geqq \epsilon_0 \tag{48}$$

and

$$\bar{\varphi}^N_{N_0 r,N_0 s}(\epsilon) = a_{N_0 r,N_0 s}\cdot\epsilon + b_{N_0 r,N_0 s}\cdot\epsilon^{3/2} + c_{N_0 r,N_0 s}\cdot\epsilon^2 + d_{N_0 r,N_0 s}\cdot\epsilon^{5/2} \quad \text{for } \epsilon \leqq \epsilon_0. \tag{49}$$

The set of difference functions

$$\varphi_{N_0 r,N_0 s}(\epsilon) - \bar{\varphi}^N_{N_0 r,N_0 s}(\epsilon)$$

is then determined as the solution of an inhomogeneous system of differential equations obeying appropriate boundary conditions. As in the homogeneous medium the source functions $S_{N_0 r,N_0 s}(\epsilon)$ of these equations may be neglected for $\epsilon \geqq \epsilon_0$. $S_{N_0 r,N_0 s}(\epsilon)$, as well as the set of functions $\varphi_{N_0 r,N_0 s} - \bar{\varphi}^N_{N_0 r,N_0 s}$, can then be expanded in the eigenfunctions of the heavy gas operator $\mathfrak{L}$.

We write:

$$S_{N_0 r,N_0 s}(\epsilon) = \sum_{p=0}^{p_0} c_{N_0 r,N_0 s,p}\cdot\omega_p(\epsilon) \tag{50}$$

and

$$\varphi_{N_0 r,N_0 s}(\epsilon) - \bar{\varphi}^N_{N_0 r,N_0 s}(\epsilon) = \sum_{p=0}^{p_0} a_{N_0 r,N_0 s,p}\cdot\omega_p(\epsilon). \tag{51}$$

TABLE I

PARAMETERS OF THE TWELVE REACTORS

Reactor	Moderator	d (cm)	a (cm)	p (%)	gm/cm³	p_t	x_0/d	p_t^M
I	D_2O (40°C)	10	1.6	0.7115	18.4	0.1046	0.186	3.33×10^{-4}
II	D_2O (40°C)	16.8	1.6	0.7115	18.4	0.03705	0.1108	3.33×10^{-4}
III	D_2O (40°C)	20	1.6	0.7115	18.4	0.02614	0.093	3.33×10^{-4}
IV	D_2O (40°C)	10	1.6	2	18.4	0.2274	0.186	3.33×10^{-4}
V	D_2O (40°C)	16.8	1.6	2	18.4	0.08058	0.1108	3.33×10^{-4}
VI	D_2O (40°C)	20	1.6	2	18.4	0.05686	0.093	3.33×10^{-4}
VII	Graphite (300°C)	10	1.2	0.7115	18.4	0.1791	0.3925	4.34×10^{-4}
VIII	Graphite (300°C)	20	1.2	0.7115	18.4	0.04479	0.1962	4.34×10^{-4}
IX	Graphite (300°C)	30	1.2	0.7115	18.4	0.01991	0.1309	4.34×10^{-4}
X	Graphite (300°C)	10	1.2	2	10	0.212	0.3925	4.34×10^{-4}
XI	Graphite (300°C)	20	1.2	2	10	0.05299	0.1962	4.34×10^{-4}
XII	Graphite (300°C)	30	1.2	2	10	0.02356	0.1309	4.34×10^{-4}

This manipulation leads to an infinite system of linear equations for the unknown coefficients $a_{N_0r,N_0s,p}$:

$$a_{N_0r,N_0s,p} = -\frac{c_{N_0r,N_0s,p} + p_t \cdot \sum_{q=0}^{p_0} V_{pq} A_q}{p + (\alpha_{N_0r}^2 + \alpha_{N_0s}^2)x_0^2} \quad (52)$$

$$(r, s = -\infty, \cdots, -1, 0, +1, \cdots, +\infty)$$

$$(p = 0, 1, 2, \cdots, p_0)$$

with the abbreviation:

$$A_p = \sum_{r,s=-\infty}^{+\infty} a_{N_0r,N_0s,p}[\cos(\alpha_{N_0r}x)\cos(\alpha_{N_0s}y)]^{R_0} \quad (53)$$

Equation (52) is multiplied by

$$[\cos(\alpha_{N_0r}x)\cos(\alpha_{N_0s}y)]^{R_0}$$

and summed over r and s. This procedure results in a finite system of linear, inhomogeneous equations with the unknowns A_p :

$$A_p + p_t H(p) \cdot \sum_{q=0}^{p_0} V_{pq} A_q = -\sum_{r,s=-\infty}^{+\infty} \frac{c_{N_0r,N_0s,p}}{p + (\alpha_{N_0r}^2 + \alpha_{N_0s}^2)x_0^2} \cdot [\cos(\alpha_{N_0r}x) \cdot \cos(\alpha_{N_0s}y)]^{R_0}. \quad (54)$$

$$(p = 0, 1, 2, \cdots, p_0)$$

The coefficients $a_{N_0r,N_0s,p}$ are then obtained from (52). Thus the solution of (32) is found in the form:

$$\phi(x, y, \epsilon) = \sum_{r,s=-\infty}^{+\infty} \left[\bar{\varphi}_{N_0r,N_0s}^{N}(\epsilon) + \sum_{p=0}^{p_0} a_{N_0r,N_0s,p}\omega_p(\epsilon)\right] \cdot \cos(\alpha_{N_0r}x)\cos(\alpha_{N_0s}y). \quad (55)$$

All the coefficients of the above Fourier series can be written as linear combinations of terms of the form $\delta_{r0} \cdot \delta_{s0}$ and

$$\frac{1}{\gamma + (\alpha_{N_0r}^2 + \alpha_{N_0s}^2)x_0^2}.$$

In order to obtain $\phi^{R_0}(\epsilon)$ the mean value of the flux over the boundary of the fuel element is replaced by the mean value of the flux at the four intersections of the axes with the boundary of the slug (cf. (4)), which is a good approximation for small a/L.

Thus series of the type

$$\sum_{r,s=-\infty}^{+\infty} \frac{\cos(\alpha_{N_0r}x)\cos(\alpha_{N_0s}y)}{\gamma + (\alpha_{N_0r}^2 + \alpha_{N_0s}^2)x_0^2}$$

have to be summed. As has been shown by Meetz one summation can be carried out exactly by means of the calculus of residues. The remaining single series converges rather rapidly inside the moderator, but its convergence is very poor at the boundary of the fuel rods because of the logarithmic singularities of the flux at the lattice points of the reactor. But the convergence of these Fourier series can be improved by usual methods such that all double series occurring in our theory can be determined with high accuracy.[1]

EXAMPLES

The theory derived in the last section has been applied to twelve types of reactors in the limit $N_0 = \infty$ (7). Besides the neutron spectra themselves, the values of the η-factor and the thermal utilization have been calculated. In determining the latter quantity a $1/v$-absorption law in the moderator has been assumed. The mean values of the absorption and fission cross sections of the fuel elements were

[1] For a detailed description of the numerical work involved in the method see (7).

taken in the energy interval $0 \leqq \epsilon \leqq 16$; in the moderator the spatial average of the absorption cross section has been calculated, too, by means of the spectrum determined neglecting the neutron absorption in the moderator.

The parameters of the twelve reactors considered here are given in Table I. a, d, p_t, x_0/d have the meaning defined in the text above; $p_t^M = \Sigma_a^M(\epsilon = 1)/2\mu\Sigma_s^0$ is the absorption parameter of the moderator; and ρ is the density of the fuel. In the calculation of the η-factor the fuel was assumed to consist of p% U^{235} and $(100 - p)$% U^{238}.

The values $p = 0.7115$, $\rho = 18.4$ gm/cm^3 correspond to those of natural uranium; $p = 2$ and $\rho = 10$ gm/cm^3 are the data of uranium oxide enriched up to 2% U^{235}. The macroscopic absorption cross section of natural uranium at the moderator temperature of 40°C was assumed to be $\Sigma_a^U(\epsilon = 1) = 0.3467$ cm^{-1}. At a fuel enrichment of 2 % we have $\Sigma_a^U(\epsilon = 1) = 0.7541$ cm^{-1} for metallic uranium at 40°C and $\Sigma_a^U(\epsilon = 1) = 0.3034$ cm^{-1} for enriched uranium oxide at 300°C. As the absorption cross section in heavy water has been used $\Sigma_a^M(\epsilon = 1) = 7.736 \times 10^{-5}$cm^{-1} at 40°C and in graphite at 300°C $\Sigma_a^M(\epsilon = 1) = 2.58 \times 10^{-4}$ cm^{-1}. Finally the Sachs-Teller mass has been used for heavy water.

Figures 3–10 show the neutron spectra in some of the reactors I–XII. The neutron flux ϕ is plotted versus the energy in double logarithmic scale. There is drawn the flux $\phi^{R_0}(\epsilon)$ at the boundary of the fuel rods and the spectrum $\phi(d/2, d/2, \epsilon)$ in the middle of the moderator, respectively.

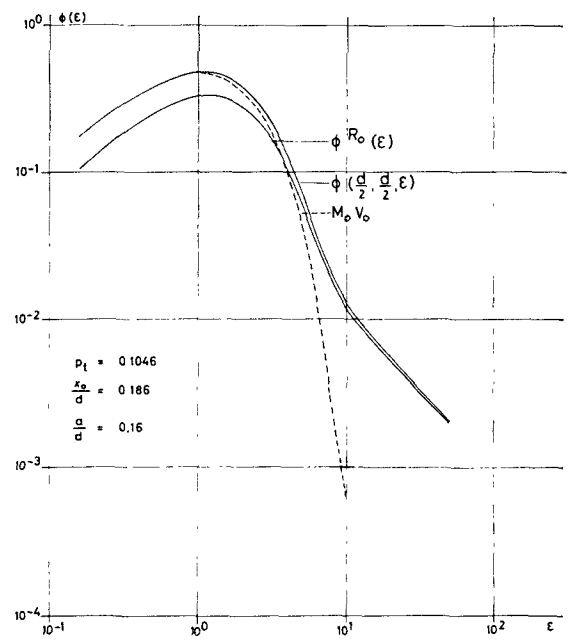

FIG. 3. Neutron spectrum in reactor I. The upper curve represents the spectrum in the middle of the moderator. M_0V_0 is a Maxwellian distribution fitted to the moderator spectrum at low energies. $\phi^{R_0}(\epsilon)$ gives the spectrum at the boundary of the fuel slugs.

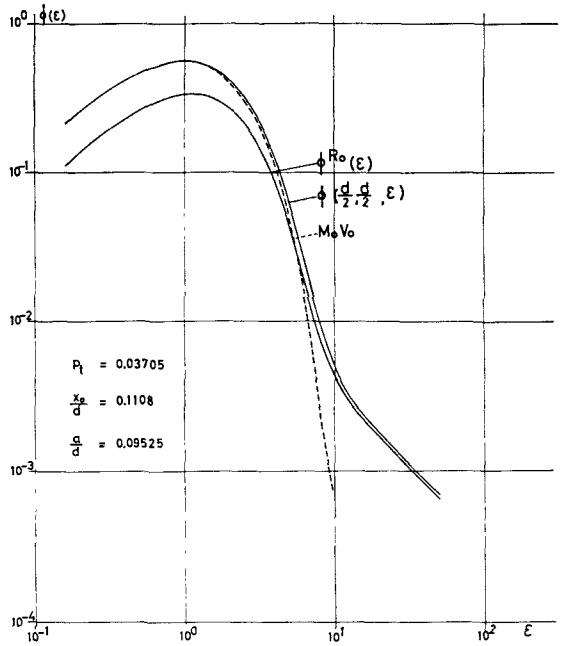

FIG. 4. Neutron spectrum in reactor II. According to the larger lattice parameter the spectrum is approximated by a Maxwellian distribution much better than in reactor I.

For comparison a Maxwellian distribution M_0V_0 has been fitted to the spectrum in the moderator at low energies. In the low energy range all the spectra have Maxwellian character, the maximum being usually displaced from $\epsilon = 1$. One recognizes clearly the change from the Maxwellian part of the spectrum to the characteristic $1/\epsilon$ slowing-down spectrum. Diminution of the lattice parameter d results in a simultaneous, almost equal, increase of the neutron temperature in fuel and moderator. The neutron temperature is here defined as the temperature of a Maxwellian distribution fitted to the given spectrum in its maximum. An increase in the absorption cross section of the fuel with unchanged geometry, on the contrary, has as a consequence a displacement of the maximum of the spectrum in the fuel but almost none in the moderator.

Figures 3–10 show that the spectra in fuel and moderator are far from being identical in the epithermal region. In an infinite reactor ($N_0 = \infty$) they tend to meet asymptotically, of course. But this becomes true only at very high energies. Honeck and Kaplan (*3*) made the assumption that the spectra in moderator and fuel are identical above

$\epsilon = 9$ in the numerical treatment of the problem in the Wigner-Seitz cell. This assumption was necessary because of the limited machine capacity. It seems to us to become dubious at least for strong absorption.

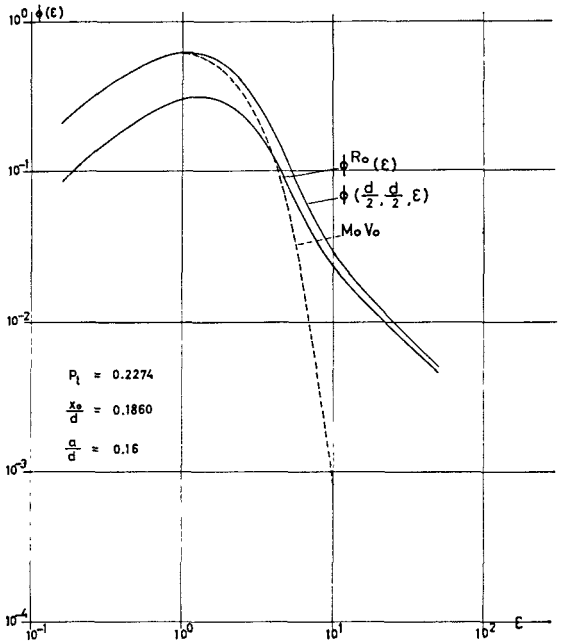

FIG. 5. Neutron spectrum in reactor IV, i.e., in an enriched, D_2O-moderated, heterogeneous reactor. The displacement of the maximum of the spectrum against $\epsilon = 1$ is obvious.

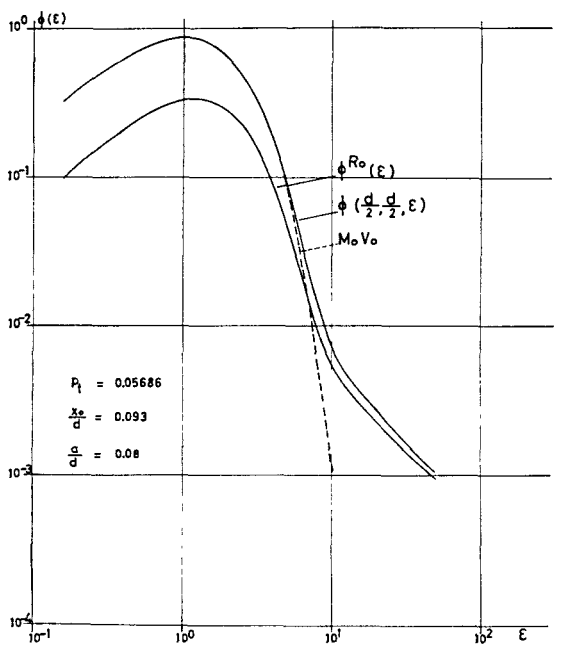

FIG. 6. Neutron spectrum in reactor VI. The neutron temperature nearly coincides with the moderator temperature.

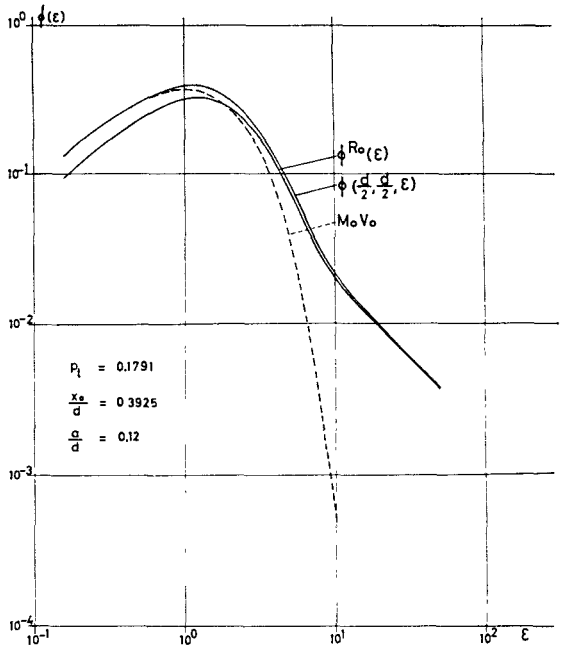

FIG. 7. Neutron spectrum in reactor VII, i.e., a graphite-moderated, natural uranium reactor. The neutron temperature differs much from the temperature of the moderator.

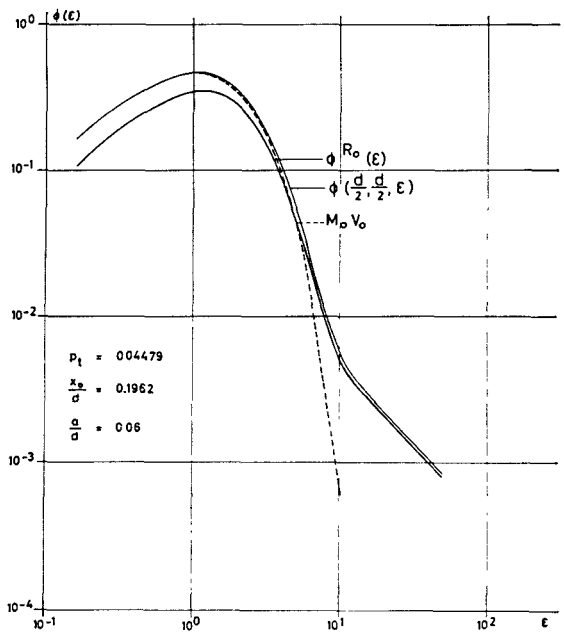

FIG. 8. Neutron spectrum in reactor VIII. Due to the diminution of the lattice parameter the neutron temperature approaches the moderator temperature.

According to the experience of the author a small inaccuracy in the calculation of the high energy part of the spectrum results in serious deviations from the rigorous solution in the thermal energy range.

This difficulty and a possible way of overcoming it has been discussed in the second and third sections of this paper for the homogeneous and heterogeneous case.

Table II gives the values of the thermal utilization f calculated for our twelve reactors I–XII. For comparison these quantities have been determined in a one-group diffusion calculation for the corresponding Wigner-Seitz cell. There can be no pretension of great accuracy in these values, of course. But at present the main aim of f-factor calculations tends to a refinement of transport-theoretical corrections, i.e., to an improvement of the treatment of the spatial dependence of the neutron density, whilst its energetic behavior is neglected. At most the absorption cross sections are averaged over a Maxwellian distribution the temperature of which, however, is dubious. Naturally, this procedure loses its meaning as soon as the error caused by neglecting the correct, space-dependent behavior of the neutron spectrum is larger than that of the monoenergetic transport-theoretical determination of the f-factor. An estimate of the improvement in accuracy to be expected from a rigorous consideration of the energy dependence of the neutron density can be obtained from a comparison of the f-factor values in Table II. The difference between these quantities determined by our method and the one group approximation, respectively, is negligibly small for D_2O-moderated reactors with natural uranium fuel elements (this is true only for a $1/v$-absorption law). But this is not the case in reactors with enriched fuel elements, especially in graphite-moderated reactors. In any case the accuracy of the monoenergetic, transport-theoretical calculation can be improved essentially if the absorption cross sections used are averaged over the neutron spectra determined in the diffusion approximation.

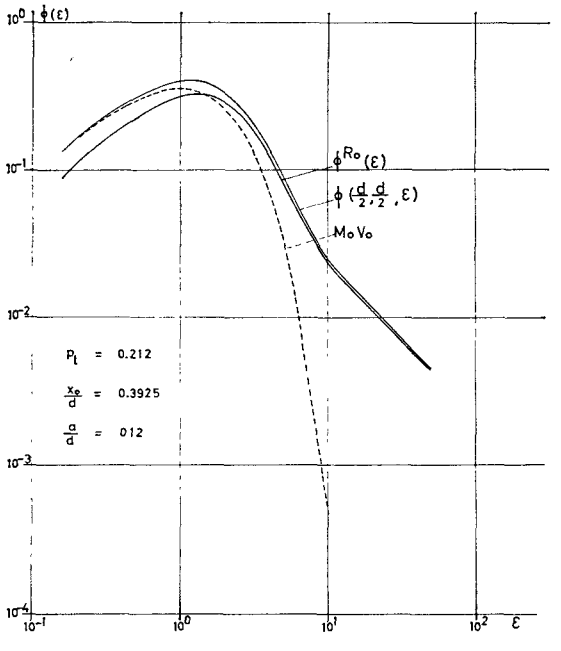

FIG. 9. Neutron spectrum in reactor X, i.e., an enriched, graphite-moderated, uranium oxide reactor. The difference between the spectra in moderator and fuel is large in the epithermal region.

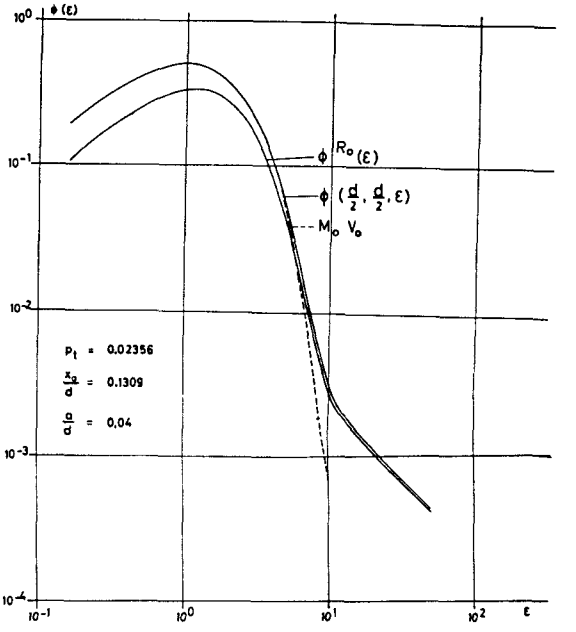

FIG. 10. Neutron spectrum in reactor XII. The neutrons are in good equilibrium with the moderator. The spectrum can be well approximated by a Maxwellian distribution.

In Table II the values of the η-factor determined by means of the neutron spectra shown in Figs. 3–10 and those calculated from Maxwellian distributions at moderator temperature and the temperature T_n^U of the neutrons at the boundary of the fuel rods are also given for comparison. Finally; the mean values of the fission and absorption cross section of U^{235} and of the absorption cross section of U^{238} are given as obtained from the three types of spectra just specified. As expected the mean values of these cross sections obtained from Maxwellian distributions are too large because these functions decrease so rapidly that the epithermal cross section values have no influence on the mean value. Consequently, the η-factors determined with Maxwellian distributions are too large.

CONCLUSION

An analytical method has been derived by which the energy dependent neutron flux in heterogeneous

TABLE II

VALUES OF f- AND η-FACTOR AND OF MEAN ABSORPTION AND FISSION CROSS SECTIONS

Reactor		f_{ws}^{igr}	$\bar{\sigma}_f^5$ (barns)	$\bar{\sigma}_a^5$ (barns)	$\bar{\sigma}_a^8$ (barns)	η
I	0.99648	0.99606	415.96	491.09	2.037	1.30965
II	0.98750	0.98655	446.82	526.56	2.171	1.31500
III	0.98125	0.97996	452.11	532.65	2.194	1.31585
IV	0.99807	0.99764	373.24	441.79	1.853	1.70659
V	0.99217	0.99117	422.12	497.82	2.067	1.71586
VI	0.98786	0.98649	430.90	507.89	2.105	1.71731
VII	0.97453	0.97215	271.48	322.74	1.427	1.27012
VIII	0.89185	0.88192	311.89	370.06	1.606	1.28157
IX	0.77493	0.75494	320.73	380.41	1.645	1.28373
X	0.97801	0.97554	263.40	313.27	1.392	1.68171
XI	0.90395	0.89361	307.96	365.49	1.589	1.69160
XII	0.79586	0.77458	317.96	377.20	1.634	1.69351
I	Maxwellian distribution at mod-		481.44	566.94	2.316	1.32037
II	erator-temperature		481.44	566.94	2.316	1.32037
III			481.44	566.94	2.316	1.32037
IV			481.44	566.94	2 316	1.72304
V			481.44	566.94	2.316	1.72304
VI			481.44	566.94	2.316	1.72304
VII			341.01	403.86	1.730	1 29026
VIII			341.01	403.86	1.730	1.29026
IX			341.01	403.86	1.730	1.29026
X			341.01	403.86	1.730	1.69962
XI			341.01	403.86	1.730	1.69962
XII			341.01	403.86	1.730	1.69962

Maxwellian distribution with displaced temperature

Reactor	T_n^U (°C)	$\bar{\sigma}_f^5$ (barns)	$\bar{\sigma}_a^5$ (barns)	$\bar{\sigma}_a^8$ (barns)	η
I	74	453.78	534.45	2.203	1.31578
II	65	460.74	542.62	2.231	1.31700
III	56	468.11	551.26	2.261	1.31823
IV	134	414.12	488.16	2.040	1.71469
V	109	429.69	506.29	2.104	1.71703
VI	105	433.59	510.85	2.120	1.71757
VII	443	301.10	358.68	1.556	1.27680
VIII	372	319.22	379.16	1.636	1.28306
IX	357	323.21	383.67	1.653	1.28440
X	472	294.68	351.42	1.527	1.68371
XI	386	315.32	374.74	1.619	1.69121
XII	346	326.56	387.47	1.668	1.69502

reactors of regular geometry can be determined. Of course, the theory can be applied to Wigner-Seitz cells, too. The calculation has been carried out in the diffusion approximation; nevertheless it can be extended to a P_L-approximation of arbitrarily high order, as has been shown in the one-dimensional case in the example of the P_1-approximation (7). As a first improvement of the diffusion calculation the diffusion constant D will be taken to be energy dependent. The heavy gas model has been used to describe the scattering law, but integral operators can be treated principally in the same way. Furthermore, a $1/v$-absorption law has been assumed. This, too, is not a necessary condition to the applicability of the theory. The author is working on an extension of the method in this direction at the moment. The inclusion of resonances like the Pu^{239} resonance at 0.3 eV will be described in a later paper.

Another important step improving the calculation described above should tend to a more accurate de-

termination of the effective absorption cross section from the real cross section values, as long as the model of linear fuel sinks is used. This coincides with a better calculation of the neutron flux inside the fuel from the spectrum at the boundary of the rods. Naturally the dependence of the neutron flux on a third space variable z can be taken into consideration. Thus it seems to us that many problems connected with neutron thermalization can now be solved by generalizations of the theory described in this paper.

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