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CROSS SECTION SPACE SHIELDING IN DOUBLY HETEROGENEOUS HTGR SYSTEMS

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ABSTRACT

Collision probability methods using rational approximations for space shielding of cross sections in nuclear reactor codes allowing for one level of heterogeneity are first reviewed. A Dancoff factor for a cylindrical HTGR fuel pin with grain structure is then derived. A new simple method for cross section space shielding in a doubly heterogeneous HTGR system using collision probabilities and rational approximations is subsequently presented and calculations based on it are compared with calculations based on more elaborate methods.

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I. INTRODUCTION

Cross section space shielding using collision probability methods and rational approximations for heterogeneous nuclear reactor systems have been in use for some time. Their virtue has been simplicity of application due to equivalence relations with homogeneous systems as well as good accuracy for most reactor calculations.

Recently, High-Temperature Gas-Cooled Reactor (HTGR) systems, using a heterogeneous mixture of fuel grains and moderator in the fuel rods, have been designed in the United States and abroad and the neutronic calculations associated with such systems have required consideration of the "double-heterogeneity" problem created by the geometry of such systems. Various methods of varying degrees of difficulty in implementation have been proposed,¹⁻¹⁹ some of which have been incorporated in HTGR design calculations in the United States and abroad.

Presented here is a simple method which can be incorporated in most multigroup cross section generation codes and which produces double-heterogeneity space shielding corrections to homogeneous neutron cross sections that compare very well with results given by much more elaborate methods.

II. COLLISION PROBABILITY METHODS AND RATIONAL APPROXIMATIONS

A. General Relations

Consider an array of fuel lumps in a homogeneous infinite moderator region. In order to calculate the escape probability[†] from all lumps, let us define the following quantities:

P_{esc} - Escape probability from one fuel lump.

$P_{F,i}$ - Probability that a neutron incident on a fuel rod after i previous fuel traversals will collide in the fuel rod.

$P_{M,i}$ - Probability that a neutron incident on the moderator after i previous fuel traversals will collide in the moderator.

Then, the probability that a neutron will escape from all fuel lumps can be written as:

$$P_{esc}^* = P_{esc} [P_{M,1} + (1-P_{M,1})(1-P_{F,2}) P_{M,2} + (1-P_{M,1})(1-P_{F,2})(1-P_{M,2})(1-P_{F,3}) P_{M,3} + \dots] \quad (1)$$

[†]The derivation included here is similar to that given by Bell and Glasstone (Ref. 20).

The various values of $P_{F,i}$ and $P_{M,i}$ are not equal, but it is customary to approximate all $P_{F,i}$ by an average value P_F and all $P_{M,i}$ by an average value P_M . Consequently, we can approximate P_{esc}^* in Eq. (1) by

$$P_{esc}^* = P_{esc} [P_M + (1-P_M)(1-P_F)P_M + \dots] \\ = \frac{P_{esc} P_M}{1 - (1-P_M)(1-P_F)} \quad (2)$$

where

$$1 - P_M = C \quad (3)$$

C being the usual Dancoff correction. Then P_{esc}^* can be written as

$$P_{esc}^* = P_{esc} \frac{1 - C}{1 - C(1-P_F)} \quad (4)$$

This expression is based on "first collision" probabilities and is valid for an infinite array of lumps of any shape and composition. For a regular lattice of fuel rods, the relationship between P_{esc} and P_F , as well as the probabilities themselves, depends on lattice pitch, on the fuel rod shape and composition.

B. Regular Array of Homogeneous Convex Lumps

Case et al.²¹ have shown that, for a homogeneous convex gray lump, P_F and P_{esc} are related by the following expression

$$P_F = \Sigma_F \bar{\ell}_F P_{esc} \quad (5)$$

where Σ_F is the total macroscopic fuel lump cross section, and $\bar{\ell}_F$ is the mean fuel lump chordlength, i.e.,

$$\bar{\ell}_F = \frac{4V_F}{S_F} \quad (6)$$

V_F and S_F being the volume and the surface area of the lump, respectively.

Inserting Eq. (5) into (4) gives P_{esc}^* in terms of the unknown quantity P_{esc}

$$P_{esc}^* = \frac{P_{esc}}{1 + \frac{C}{1-C} \Sigma_F \bar{\ell}_F P_{esc}} \quad (7)$$

Expressions for P_{esc} for homogeneous fuel lumps of various geometries have been calculated by many investigators.²¹⁻²³ On the other hand, Wigner²⁴ has proposed a "rational" approximation for P_{esc} which is exact only in the two limits as $\bar{\ell}_F \rightarrow 0$ and $\bar{\ell}_F \rightarrow \infty$

$$P_{esc}^W = \frac{1}{1 + \Sigma_F \bar{\ell}_F} \quad (8)$$

Advantages of this form in calculating narrow resonance integrals will be seen later. Improved versions of rational approximations for P_{esc} were later proposed by Bell,^{25,26} Levine,²⁷ Otter,²⁸ Kelber,^{29,30} Leslie et al.,³¹ and others. The form given by Levine²⁷ is

$$P_{esc} = \frac{1}{1 + \frac{\Sigma_F \bar{\ell}_F}{A}} \quad (9)$$

where A , known as the Levine (or Bell) factor, is dependent on the shape of the lump. To show this, let us find a rational approximation for P_{esc} for a homogeneous spherical lump of radius R and macroscopic total cross section Σ_F . The exact equation given by Case et al.²¹ is

$$P_{esc}^{sphere} = \frac{3}{8(R\Sigma_F)^3} \\ \times [2(R\Sigma_F)^2 - 1 + (1+2R\Sigma_F)e^{-2R\Sigma_F}] \quad (10)$$

and can be rewritten as

$$P_{esc}^{sphere} = \frac{3}{X^3} \left[\frac{X^2}{2} - 1 + (1+X)e^{-X} \right] \quad (11)$$

where

$$X \equiv \frac{3}{2} \Sigma_F \bar{\ell}_F \quad (12)$$

and $\bar{\ell}_F$ for a sphere is

$$\bar{\ell}_F = \frac{4V_F}{S_F} = \frac{4R}{3} \quad (13)$$

For $X \ll 1$, a series expansion for $p_{\text{esc}}^{\text{sphere}}$ yields

$$p_{\text{esc}}^{\text{sphere}} \approx 1 - \frac{3}{8} X + \frac{1}{10} X^2 \dots, \quad (14)$$

for which a very good approximation is

$$p_{\text{esc}}^{\text{sphere}} \approx \frac{1}{1 + \frac{3}{8} X} = \frac{1}{1 + \frac{9}{16} \Sigma_F \bar{\ell}_F}. \quad (15)$$

Consequently, we find $16/9$ to be a good value of A to use in the rational form (9) for a spherical homogeneous fuel lump. Good approximations for all values of $\Sigma_F \bar{\ell}_F$ were given by Otter²⁸

$$A_{\text{sphere}} \approx \frac{16}{9} - 0.2625 \Sigma_F \bar{\ell}_F + 0.0258 (\Sigma_F \bar{\ell}_F)^3$$

$$(0 \leq \Sigma_F \bar{\ell}_F < 1.36), \quad (16)$$

$$A_{\text{sphere}} \approx 1 + 1.09 \frac{1}{\Sigma_F \bar{\ell}_F} - 0.591 \frac{1}{(\Sigma_F \bar{\ell}_F)^2}$$

$$(1.36 \leq \Sigma_F \bar{\ell}_F < \infty). \quad (17)$$

We observe that, in general, A depends not only on the fuel lump geometry, but also on energy. For small fuel grains, as used in an HTGR, however, it is easy to establish that Eq. (15) is an excellent approximation to Eq. (10).

If Eq. (9) is inserted into Eq. (7), it follows that

$$P_F = \frac{1}{1 + \frac{\Sigma_F}{\Sigma_e}}, \quad (18)$$

where Σ_e is an "effective" macroscopic cross section dependent only on geometric parameters

$$\Sigma_e = \frac{(1-C)A}{\bar{\ell}_F[1+C(A-1)]}. \quad (19)$$

It should be noted that if A is set equal to unity, one obtains the Wigner rational approximation for Σ_e as given by Bell²⁶

$$\Sigma_e^{\text{Bell}} = \frac{1-C}{\bar{\ell}_F}. \quad (20)$$

Equations (19) and (20) are used in a variety of computer codes (e.g., Refs. 32 and 33) for making heterogeneity corrections to homogeneous medium cross sections. This is possible because of a well-known "equivalence" theorem³⁴ derived here, for convenience, in the one-speed approximation.[†]

The collision rate in the fuel region of volume V_F for neutrons of energy E is $V_F \Sigma_F(E) \phi_F$. It is the result of contributions from the moderator

$$P_M(E) V_M \int_E^{E/\alpha_{mM}} \frac{\Sigma_{mM} \phi_M(E')}{(1-\alpha_{mM})E'} dE',$$

and from the fuel

$$[1-P_F(E)] V_F \int_E^{E/\alpha_{mF}} \frac{\Sigma_{mF} \phi_F(E')}{(1-\alpha_{mF})E'} dE' + \int_E^{E/\alpha_a} \frac{\Sigma_{SF} \phi_M(E')}{(1-\alpha_a)E'} dE',$$

or

$$V_F \Sigma_F(E) \phi_F = (1-P_F) V_F \times \left\{ \int_E^{E/\alpha_{mF}} \frac{\Sigma_{mF} \phi_F}{(1-\alpha_{mF})E'} dE' + \int_E^{E/\alpha_a} \frac{\Sigma_{SF} \phi_F}{(1-\alpha_a)E'} dE' \right\} + P_M V_F \int_E^{E/\alpha_{mM}} \frac{\Sigma_{mM} \phi_M}{(1-\alpha_{mM})E'} dE', \quad (21)$$

where V_M and V_F are the moderator and fuel volumes, respectively, and P_M and P_F are collision probabilities as defined above. The quantity α is given by

[†] This derivation is similar to one given in Ref. 20.

$$\alpha = \left(\frac{1-A}{1+A} \right)^2, \quad (22)$$

where A is the scatterer mass number and subscripts mF, mM, and a refer to moderator material in the fuel region, in the moderator region, and the absorber, respectively. Σ_{SF} is the scattering cross section in the fuel.

The general reciprocity theorem,

$$\Sigma_{mM}^V P_M^P = \Sigma_F^V P_F^P, \quad (23)$$

can be used to eliminate P_M in Eq. (21),

$$\begin{aligned} \Sigma_F \phi_F &= (1-P_F) \\ &\times \left[\int_E^{E/\alpha_a} \frac{\Sigma_{SF} \phi_F}{(1-\alpha_a)E'} dE' + \int_E^{E/\alpha_{mF}} \frac{\Sigma_{mF} \phi_F}{(1-\alpha_{mF})E'} dE' \right] \\ &+ P_F \Sigma_F \int_E^{E/\alpha_{mM}} \frac{\phi_M}{(1-\alpha_{mM})E'} dE'. \end{aligned} \quad (24)$$

Various approximations can be used for the fluxes in the moderator and in the fuel rod moderating material. According to the narrow resonance approximation (NR), these fluxes are replaced by the asymptotic value

$$\phi_{asy} = \frac{1}{E}, \quad (25)$$

which, when inserted into Eq. (24), yields

$$\begin{aligned} \Sigma_F \phi_F &= (1-P_F) \int_E^{E/\alpha_a} \frac{\Sigma_{SF} \phi_F}{(1-\alpha_a)E'} dE' \\ &+ [\Sigma_{mF} + P_F(\Sigma_{aF} + \Sigma_{SF})] \frac{1}{E}, \end{aligned} \quad (26)$$

where

$$\Sigma_F = \Sigma_{aF} + \Sigma_{SF} + \Sigma_{mF} \quad (27)$$

is the total fuel cross section.

Inserting the rational approximation form of Eq. (18) for P_F in Eq. (26) yields, after some algebra,

$$\begin{aligned} (\Sigma_F + \Sigma_e) \phi_F(F) &= \int_E^{E/\alpha_a} \frac{\Sigma_{SF} \phi_F}{(1-\alpha_a)E'} dE' \\ &+ (\Sigma_{mF} + \Sigma_e) \frac{1}{E}. \end{aligned} \quad (28)$$

If the sum $\Sigma_{mF} + \Sigma_e$ in Eq. (28) is replaced by Σ_m , Eq. (28) becomes identical to the collision rate in a homogeneous medium with moderator cross section Σ_m . This established the equivalence between a homogenized system and a heterogeneous system in the NR approximation.

This equivalence theorem has been used in a number of codes correcting homogenized cross sections for space shielding due to one level of heterogeneity.

In the Bondarenko formalism³⁵ of multigrouping cross sections in the narrow resonance approximation, the epithermal weighting flux is given by

$$\phi(E) = \frac{1}{\sigma_t(E) + \sigma_0}, \quad (29)$$

where $\sigma_t(E)$ is the total microscopic cross section and σ_0 is an effective cross section accounting for the energy shielding due to large absorber concentrations in a homogeneous medium. In this formalism, it is particularly easy to further correct for cross section space shielding when the fuel resonance escape probability can be written in the rational form of Eq. (18). Then, the weighting flux simply becomes

$$\phi(E) = \frac{1}{\sigma_t(E) + \sigma_0 + \sigma_e}, \quad (30)$$

where

$$\sigma_e = \frac{\Sigma_e}{N_F}, \quad (31)$$

and N_F is the absorber concentration in the fuel rod.

A better approximation for the weighting flux in a homogenized region is provided by the intermediate resonance approximation according to which, in a composition independent approach,

$$\phi(E) = \frac{1}{\sigma_a(E) + \lambda \sigma_s(E) + \tau_0}, \quad (32)$$

where all microscopic cross sections are given per absorber atom.

For heterogeneous configurations and for heavy moderators (like carbon), Seghal and Goldstein³⁶ have proposed a weighting flux

$$\psi(E) = \frac{1}{\sigma_a(E) + \lambda \sigma_s(E) + k \sigma_{m,a} + \tau_0}, \quad (33)$$

where subscript m,a refers to moderator admixed in fuel.

Parameters λ , k , and τ_0 are related by transcendental equations which, in the unbroadened Breit-Wigner approximation without interference,³⁶ are

$$k = 1 - X_{k\lambda u}^{(am)},$$

$$\lambda = 1 - X_{k\lambda u}^{(f)},$$

and

$$\tau_0 = 1 - [1 - \tau_0 + (\tau_0 / \sigma_m)] X_{k\lambda u}^{(m)}, \quad (34)$$

where

$$X_k^{(i)} = \frac{\arctan x_{k\lambda u}^{(i)}}{x_{k\lambda u}^{(i)}}, \quad (35)$$

and

$$x_{k\lambda u}^{(i)} = 2 E_r (1 - \alpha_i) / [\Gamma (\Gamma_{111} + \beta_{k\lambda u})], \quad (36)$$

$$\beta_{k\lambda u}^2 = 1 + \frac{\sigma_0}{k \sigma_{am} + \lambda \sigma_p + \tau_0 \sigma_e} \left(\frac{\Gamma_Y + \lambda \Gamma_n}{\Gamma - \tau_0} \right). \quad (37)$$

Quantities Γ_Y , Γ_n , and Γ are the gamma width, neutron width, and total width of the resonance, respectively. Superscripts am, f, and m correspond to admixed moderator, resonance absorber, and outside moderator, respectively.

Using the empirical correlations of Seghal³⁷

$$\frac{1}{\lambda} = \left[1 + \frac{2.2195}{R_a (\sigma_0)^{0.449}} \right]^2, \quad (38)$$

where

$$R_a = \frac{E_r (1 - \alpha_a)}{\Gamma_p}, \quad (39)$$

$$\Gamma_p = \Gamma \left[\frac{\sigma_1}{\sigma_{pth} + 2 \sigma_{poxy} + \frac{Nc}{N_{th}} \sigma_c + \frac{\tau_0 \sigma_e}{N_{th}}} \right]^{\frac{1}{2}}, \quad (40)$$

and

$$\frac{1}{k} = \left[1 + \frac{2.2195}{R_{\tau_0} (\sigma_0)^{0.449}} \right]^2, \quad (41)$$

where

$$R_{\tau_0} = \frac{E_r (1 - \alpha_m)}{\Gamma_p}, \quad (42)$$

M. Becker of Rensselaer Polytechnic Institute (RPI) has estimated parameters λ and k for the important low-lying ^{232}Th resonance (at 23.4 eV) in a graphite moderated system to be 0.92 and 0.996, respectively. These results warrant the use of the NR approximation for the ^{232}Th resonances in an HTGR system, i.e., assuming λ and k to both be equal to unity.

C. Uniform Spherical-Grain Distribution in a Moderator Matrix

Let us consider a uniform distribution of equal size spherical fuel grains in an infinite moderator medium. Equation (7) can then be written as

$$P_g = P_e \frac{1 - C_0}{1 - C_0 (1 - \Sigma_0 \bar{V}_0 P_e)}, \quad (43)$$

where

P = escape probability from all grains;

P_e = escape probability from one grain;

C_0 = grain-structure Dancoff factor;

Σ_0 = grain total macroscopic cross section;

$\bar{V}_0$ = mean grain chordlength, i.e., $\frac{4V_0}{S_0}$;

V_0 = grain volume;

S_0 = grain surface area.

Using the rational approximation form of Eq. (9) for P_e

$$P_e = \frac{1}{1 + \frac{\Sigma_0^0}{a}} \quad (44)$$

where a good energy-independent approximation of a for small grains is 16/9 as discussed in Sec. II-B, we obtain for P_g

$$P_g = \frac{1}{1 + \frac{\Sigma_0^0}{C_0}} \quad (45)$$

where

$$\Sigma_0^0 = \frac{(1 - C_0)a}{V_0[1 + (a - 1)C_0]} \quad (46)$$

The Dancoff factor C_0 for such an infinite medium was calculated by Lane et al.⁶ to be

$$C_0 = \frac{1}{1 + \frac{N_0 \sigma_m}{1 - f_0}} \quad (47)$$

where N_0 , σ_m , and f_0 are the absorber density in the grains, moderator cross section per absorber atom, and grain volume fraction, respectively.

III. DOUBLE HETEROGENEITY CORRECTIONS TO HOMOGENEOUS CROSS SECTIONS THROUGH EQUIVALENCE RELATIONS

A. General Expressions

We now wish to simultaneously consider the two levels of heterogeneity, the grain heterogeneity in the fuel rod, and the fuel pin heterogeneity in the reactor core, and to derive an overall absorber escape probability in terms of rational approximations. For this purpose, we will define the following average quantities:

- P_e - escape probability from one grain;
- P_{ng} - probability that a neutron leaving a grain will not collide again with a grain in the same fuel pin;
- $P_{f,0}$ - probability that a neutron incident on a fuel rod will re-emerge outside the rod either uncollided or after any number of collisions in the fuel-rod moderator;
- P_M - probability that a neutron incident on the moderator outside a fuel pin will collide with it;

- P_e^* - escape probability from all grains in all rods (i.e., overall fuel absorber escape probability) for a neutron born in any grain;
- P_0 - probability that a neutron incident on a grain will collide in the grain;
- $P_{g,0}$ - probability that a neutron produced in a grain will escape from that grain and will not collide again in any grain of the same fuel pin;
- P_1 - probability that a neutron incident on the fuel pin moderator outside a grain will collide in it;
- C_0 - Dancoff factor of grain structure in a rod;
- C - Dancoff factor of the array of cylindrical rods in the reactor core;
- P_g - probability that a neutron incident on a fuel rod will also be incident on any grain in that rod;
- $P_{0,g}$ - probability that a neutron incident on a fuel rod will collide in at least one grain of that rod.

All grains of the same type are assumed to be of equal size. From these definitions, the following relations are obvious

$$C_0 = 1 - P_1 \quad (48)$$

$$C = 1 - P_M \quad (49)$$

$$P_{g,0} = P_e P_{ng} \quad (50)$$

$$P_{0,g} = P_0 P_g \quad (51)$$

$$P_{f,0} = 1 - P_{0,g} \quad (52)$$

Since grains are assumed to have no structure, i.e., are homogeneous, we also can write

$$P_0 = \Sigma_0^0 \bar{\ell}_0 P_e \quad (53)$$

where Σ_0^0 is the total macroscopic grain cross section and $\bar{\ell}_0$ is the grain mean chordlength.

For a spherical grain of radius R , $\bar{\ell}_0$ is

$$\bar{\ell}_0 = \frac{4V}{S_0} = \frac{4}{3}R \quad (54)$$

The overall grain escape probability P_e^* is given by the series

$$P_e^* = P_{g,0} [P_M + (1 - P_M)P_{f,0}P_M + (1 - P_M)^2 P_{f,0}^2 P_M + \dots]$$

$$= P_{g,0} \frac{P_M}{1 - (1 - P_M)P_{f,0}} \quad (55)$$

Substituting Eqs. (49) and (52) into Eq. (55), we obtain

$$P_e^* = P_{g,0} \frac{1 - C}{1 - C(1 - P_{0,g})} \quad (56)$$

We can now relate P_g and P_{ng} through the reciprocity relation

$$P_g = \frac{\bar{\ell}_F}{\bar{\ell}_g} P_{ng} \quad (57)$$

where $\bar{\ell}_F$ is the mean fuel rod chordlength and λ_g is the geometric mean free path of the grains⁶

$$\lambda_g = \frac{1}{n\sigma_0} \quad (58)$$

where n is the number of grains per unit volume and σ_0 is the mean geometric cross section of one grain⁶

$$\sigma_0 = \frac{S_0}{4} \quad (59)$$

S_0 is the grain surface area and n is given by

$$n = \frac{f_0}{V_0} \quad (60)$$

where f_0 is the grains volume fraction in a fuel pin and V_0 the volume of one grain.

Then λ_g becomes

$$\lambda_g = \frac{V_0}{f_0} \frac{4}{S_0} = \frac{\bar{\ell}_0}{f_0} \quad (61)$$

and P_g of Eq. (57) becomes

$$P_g = f_0 \frac{\bar{\ell}_F}{\bar{\ell}_0} P_{ng} \quad (62)$$

If Eqs. (50), (51), (53), and (62) are substituted into Eq. (56), one obtains

$$P_e^* = \frac{P_{ng}}{1 + \frac{C}{1 - C} \Sigma_0 f_0 \bar{\ell}_F P_{ng}}$$

$$= \frac{1}{\frac{1}{P_{ng}} + \frac{C}{1 - C} \Sigma_0 f_0 \bar{\ell}_F} \quad (63)$$

Let us define P_{Cl} as the first collision probability anywhere in the fuel pin moderator outside the grains for neutrons escaping from a grain. The multiple collision probability P_{ng} then becomes

$$P_{ng} = P_{nC} + (1 - P_{nC})P_{Cl}(1 - P_0)P_{nC}$$

$$+ (1 - P_{nC})^2 P_{Cl}^2 (1 - P_0)^2 P_{nC} + \dots$$

$$= \frac{P_{nC}}{1 - (1 - P_{nC})P_{Cl}(1 - P_0)} \quad (64)$$

where

$$P_{Cl} = P_1 + (1 - P_1)(1 - P_0)P_1$$

$$+ (1 - P_1)^2 (1 - P_0)^2 P_1 + \dots$$

$$= \frac{P_1}{1 - (1 - P_1)(1 - P_0)} = \frac{1 - C_0}{1 - C_0(1 - P_0)} \quad (65)$$

and P_{nC} is the no-collision probability for a neutron escaping from a grain.

Substituting Eq. (65) into Eq. (64) gives

$$P_{ng} = \frac{P_{nC}[1 - C_0(1 - P_0)]}{P_0 + P_{nC}(1 - P_0 - C_0 + P_0 C_0)} \quad (66)$$

If Eqs. (66), (44), (53), and (63) are further combined, one obtains

$$P_e^* = \frac{1}{1 + \Sigma_0 \bar{\ell}_0 \left[\frac{C}{1 - C} f_0 \frac{\bar{\ell}_F}{\bar{\ell}_0} + \frac{1}{a} + \frac{\left(\frac{1}{P_{nC}} - 1 \right) \left(1 + \frac{\Sigma_0 \bar{\ell}_0}{a} \right)}{1 + \Sigma_0 \bar{\ell}_0 \frac{(1 - C_0)}{a}} \right]} \quad (67)$$

or alternately

$$P_e^* = \frac{1}{1 + \frac{\sigma_F}{\sigma_{eff}}} \quad (68)$$

where

$$\sigma_{eff} = \frac{1}{N_F \bar{\ell}_F \left[\frac{C}{1 - C} + \frac{1}{A^*} \right]} \quad (69)$$

and

$$\frac{1}{A^*} = \frac{\bar{\ell}_0}{\bar{\ell}_F f_0} \left[\frac{1}{a} + \frac{\left(\frac{1}{P_{nC}} - 1 \right) \left(1 + \frac{\Sigma_0 \bar{\ell}_0}{a} \right)}{1 + \frac{\Sigma_0 \bar{\ell}_0}{a} (1 - C_0)} \right] \quad (70)$$

and σ_F is the fuel pin total microscopic cross section per absorber atom. It will be shown later that P_{nc} and C_0 are related through the following equation

$$P_{nc} = \frac{\bar{\ell}_0}{\bar{\ell}_F \bar{\ell}_0} C_0 \quad (71)$$

We now make a final approximation in the equation for A^*

$$\Sigma_0 \approx \frac{1}{\lambda_g} \quad (72)$$

Then, we can write A^* as an approximately energy-independent quantity given by

$$\frac{1}{A^*} = \frac{\bar{\ell}_0}{\bar{\ell}_F \bar{\ell}_0} \left[\frac{1}{a} + \frac{\left(\frac{f_0 \bar{\ell}_F}{\bar{\ell}_0 C_0} - 1 \right) \left(1 + \frac{f_0}{a} \right)}{1 + \frac{f_0}{a} (1 - C_0)} \right] \quad (73)$$

This implies that double heterogeneity can be accounted for by simply replacing the Levine factor A by the new factor A^* in the single-heterogeneity space shielding correction. It should be noted that Eq. (69) is identical with Eqs. (19) and (31) if A^* replaces A .

Two problems yet unsolved are the calculation of C_0 and the accounting for scattering effects in the grains which usually contain absorber compounds with light elements, rather than pure fuel absorbers. These problems will be addressed next.

B. Dancoff Factor for Grain Structure in Infinite Cylindrical Rods

The Dancoff factor given by Eq. (47) was derived by Lane et al.⁶ on the basis of a uniform chordlength distribution in an infinite medium. We will now remove this restriction and derive a Dancoff factor averaged over the chordlength distribution in an infinite cylinder.

The Dancoff factor is defined as the probability that a neutron leaving an absorber lump will next collide in another absorber lump. In an infinite cylinder with grain structure, the Dancoff factor C_0 can be written as

$$C_0 = \int_0^\infty C_0(\ell) P(\ell) d\ell \quad (74)$$

where $P(\ell)$ is the chordlength distribution in the fuel rod, and $C_0(\ell)$ is the Dancoff factor along a specific chordlength ℓ in the cylinder. The actual chordlength distribution in an infinite cylinder as used by Case et al.²¹ is rather complicated, but Sauer³⁸ has found that the following simplified distribution works quite well

$$P(\ell) d\ell = \frac{1}{n!} u^n e^{-u} du \quad (75)$$

where

$$u = \frac{(n+1)\ell}{\bar{\ell}_F} \quad (76)$$

Sauer has also found that a good value of n for an infinite cylinder is 3.58. In view of the fact that n is not an integer for the infinite cylinder, the normalized distribution [Eq. (75)] must be replaced by the following one

$$P(\ell) d\ell = \frac{1}{\Gamma(n+1)} u^n e^{-u} du \quad (77)$$

because

$$\int_0^\infty x^m e^{-ax} dx = \frac{\Gamma(m+1)}{a^{m+1}} \quad (78)$$

where $\Gamma(m+1)$ is the gamma function.

Using the same train of thought as Lane et al.,⁶ we can now derive an expression for $C_0(\ell)$. Let us first define λ_m as the mean free path for the fuel rod moderator outside the grains and λ_g as the geometric mean free path for the grains

$$\lambda_m = \frac{1}{N_1 \sigma_1} \quad (79)$$

and

$$\lambda_g = \frac{1}{n C_0} \quad (58)$$

where $N_1 \sigma_1 = \Sigma_1$ is the macroscopic cross section of the fuel rod moderator outside the grains. Then $C_0(\ell)$ can be written as

$$C_0(\ell) = \int_0^\ell e^{-\Sigma r} \frac{dr}{\lambda_g} \quad (80)$$

where

$$\bar{c} = \frac{1}{\lambda_m} + \frac{1}{\lambda_g} \quad (81)$$

Integration of Eq. (30) yields

$$C_0(\lambda) = \frac{1}{\lambda \bar{c}} [1 - e^{-\lambda \bar{c}}] \quad (82)$$

or

$$C_0(\lambda) = \frac{1}{1 + \frac{\Sigma_1 \bar{c}}{f_0}} \left[1 - \exp \left[-\frac{\lambda f_0}{\Sigma_1 \bar{c}} \left(1 + \frac{\Sigma_1 \bar{c}_0}{f_0} \right) \right] \right] \quad (83)$$

Substituting Eqs. (83) and (77) into Eq. (74) gives, after some algebra

$$C_0 = \frac{1}{1 + \frac{\Sigma_1 \bar{c}_0}{f_0}} \left\{ 1 - \left[1 + \frac{f_0 \bar{c}_F}{4.58 \bar{c}_0} \left(1 + \frac{\Sigma_1 \bar{c}_0}{f_0} \right) \right]^{-4.58} \right\} \quad (84)$$

This is the Dancoff factor to be used in Eq. (73).

The non-collision probability P_{nc} of Eq. (70) can now be related to C_0 because

$$P_{nc} = \frac{1}{\Sigma_1 \bar{c}_F} \int_0^\infty d\lambda P(\lambda) [1 - \exp(-\lambda \bar{c}_r)] \quad (85)$$

where Σ_1 is given by Eq. (81).

Upon examination of Eqs. (81), (80), and (74), we can immediately conclude that

$$P_{nc} = \frac{\bar{c}_0}{f_0 \bar{c}_F} C_0 \quad (71)$$

C. Scattering Effects in the Grains

So far, any collision in the grain was tacitly assumed to result in absorption. However, the grains used in HTGR's are chemical compounds with light elements and contain one or several light scattering atoms per absorber atom. It is, therefore, proper to replace P_e in Eq. (63) by a multiple collision quantity $P_{e,s}$ which accounts for multiple scatterings in the grains. The overall effect of this substitution on the corresponding absorber multigroup cross sections was seen to be significant although not very large, probably due to the relatively small size of the grains.

Let us first assume, for simplicity, that the ratio of the scattering to total cross section in the grain is energy independent. This restriction will be removed later. Then we can define an energy-independent scattering probability per collision in the grain as

$$q = \frac{\Sigma_{s,0}}{\Sigma_0} \quad (86)$$

In view of this, we can further write the multiple-collision escape probability from one grain as

$$P_{e,s} = P_e [1 + (1 - P_e)q + (1 - P_e)^2 q^2 + \dots] \\ = \frac{P_e}{1 - q(1 - P_e)} \quad (87)$$

This expression was previously derived by Dyos and Pomraning⁸ and others. Substituting for P_e from Eq. (44) in Eq. (87), we obtain

$$P_{e,s} = \frac{1}{1 + \frac{\Sigma_a \bar{c}_0}{a}} \quad (88)$$

where $\Sigma_a = \Sigma_0 - \Sigma_{s,0}$ is the macroscopic absorption cross section in the grain.

The above restriction of q being independent of energy implies that the scatterer is infinitely heavy so that no change in the neutron energy takes place through scattering. In the multigroup cross section approximation it is, therefore, reasonable to replace $\Sigma_{s,0}$ by $\Sigma_{ss,0}$, the self-scattering cross section of the groups(s) in which resolved resonances fall. Hence, $P_{e,s}$ can be written as

$$P_{e,s} = \frac{1}{1 + \frac{\Sigma_{out,0} \bar{c}_0}{a}} \quad (89)$$

where $\Sigma_{out,0}$ is the out-scatter cross section in a particular group. Accordingly, one can now write

$$P_{e,s} = \frac{1}{1 + \frac{\Sigma_0 \bar{c}_0}{a}} \quad (90)$$

where

$$a^* = \frac{a}{1 - \frac{\sum_{ss,0}}{\sum_0}} \quad (91)$$

Thus a^* becomes energy dependent.

If one is interested in broad-group cross sections for use in transport calculations, all ^{232}Th resonances for an HTGR calculation are lumped in one or few groups. Quantity a^* then becomes a group constant and can still be used to replace a in Eq. (73).

D. Application of the Method and Conclusions

The method discussed above was applied to the generation of few group cross sections to be used for neutronics calculations of a large HTGR system. The results based on this method were compared with results supplied on magnetic tapes by General Atomic to Los Alamos Scientific Laboratory for the same reactor system and were calculated by the General Atomic code MICROX.⁴ They were also compared with LASL calculated cross sections based on the more elaborate grain shielding method of Wälti, apparently incorporated in the MICROX code. It should be pointed out that the Wälti method operates on pointwise cross sections and its applicability depends upon accessibility to such cross section in a multi-grouping code. At LASL, the Wälti grain shielding method calculations were performed at the pointwise level by a specially written code PETOPES operating on PENDF cross sections (pointwise cross sections in ENDF/B format) generated by the MINX code.³⁹ Application of the new method discussed in this report does not require such sophistication and can be directly incorporated in most epithermal collapsing codes, starting from fine-group cross sections. The code used at LASL was IDX (Ref. 33) which has the built-in capability of accepting the Bondarenko formalism provided by the MINX code.

Detailed comparisons of results based on the various methods will be reported elsewhere. However, an illustration of the quality of results obtained with the method described in this report is given below.

Few group cross sections in an energy structure given in Table I were calculated at several temperatures by the above method and by the Wälti grain shielding method. Also, results from General Atomic,

calculated with the MICROX code, were provided to LASL for the same reactor system and the same few-group energy structure. All ^{232}Th resolved resonances in this energy structure are incorporated in above-thermal group 3 having boundaries at 96.0 and 17.6 eV. Table II shows a comparison of the ^{232}Th group 3 absorption (capture) cross sections for three temperatures, 300, 800, and 1200°K, as calculated by MINX and IDX incorporating the present method (P.M.), as calculated by MINX (including the Wälti pointwise grain shielding method) and IDX (MINX/IDX), and as supplied by General Atomic (MICROX). Methods I and II used basic ENDF/B-III cross sections as initial input data.

TABLE I
FEW-GROUP EPITHERMAL ENERGY STRUCTURE

Group No	Energy Boundaries
1	10 MeV - 183 keV
2	183 keV - 961 eV
3	961 eV - 17.6 eV
4	17.6 eV - 3.95 eV
5	3.95 eV - 2.38 eV
6	2.38 eV - 0.414 eV

TABLE II
RESOLVED-RESONANCE-GROUP ABSORPTION
CROSS SECTION IN ^{232}Th (barns)

Temperature (°K)	Method I M(P.M.)	Method II (MINX/IDX)	Method III (MICROX)
300	6.64	6.58	6.76
800	7.94	7.82	8.12
1200	8.56	8.42	8.78

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