A VARIATIONAL APPROACH FOR THE CALCULATION
OF RESONANCE ESCAPE PROBABILITIES
IN SLAB LATTICES,

by

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Abstract
NOMENCLATURE

A  absorption rate per unit area in the fuel region
A_s  hydrogen scattering term in the absorption rate
a  half-width of the fuel region
α  parameter related to the nuclear mass number of water
α_o  parameter related to the nuclear mass number of oxygen
b  half-width of the moderator region
β  parameter related to moderator properties
D  diffusion coefficient
Δ  oxygen scattering contribution to the absorption rate
ΔE  energy region over one resonance
δ  optical thickness of the fuel region
E_i  resonance energy
Γ  natural line width
Γ_Y  radiative line width
Γ_n  neutron line width
Γ_p  practical line width
ϕ(x,E,μ)  angular neutron flux
ϕ_e(x,E)  total flux
μ  cosine of the neutron scattering angle
P_i  resonance escape probability for resonance i
Q  symbol used for simplifying the neutron transport equation
Σ  total macroscopic cross section for the moderator
\[ \Sigma_a \] macroscopic absorption cross section for the fuel
\[ \Sigma_s \] macroscopic scattering cross section for water
\[ \Sigma_{so} \] macroscopic scattering cross section for oxygen
\[ \Sigma_s(E\rightarrow E) \] differential scattering cross section for water
\[ \Sigma_{so}(E\rightarrow E) \] differential scattering cross section for oxygen
\[ \sigma \] microscopic cross section
\[ \sigma_i \] microscopic peak absorption cross section for resonance i
\[ \theta \] angle neutron trajectory makes with x-axis
\[ \chi(E) \] average number of fission neutrons emitted at energy E
\[ V_F \] volume of the fuel region
\[ V_M \] volume of the moderator region
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Figure 1. Representation of a unit cell

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1. INTRODUCTION

The resonance absorption in uranium-238 in a heterogeneous fuel-moderator arrangement causes a loss of neutrons, which is significantly less than in a homogeneous system of the same overall composition. This is because the neutrons slow down in the moderator, which is physically separate from the fuel which contains the resonant absorber. For this same reason the calculation of the resonance absorption is much more complicated in heterogeneous media than in homogeneous media. The strong neutron absorption of the fuel at resonance energies produces a minimum in the neutron flux in the interior of the fuel at these energies. Thus an accurate prediction of resonance absorption requires a detailed knowledge of both the energy and spatial variation of the neutron flux.

In the past various approaches for the calculation of resonance escape probabilities and resonance integrals in heterogeneous media have been done. In the first theories, developed by Dancoff and Ginsburg (1), absorption is divided into separate contributions from the surface of the fuel and its volume. A fuel lattice is divided into cells. A correction, called the Dancoff correction, is introduced for including the interaction between adjacent cells.

Chernick and Vernon (2), and Dresner (3), use the rational approximation for determining collision probabilities. The general ideas behind this method come from Wigner (21). The collision probability method is summarized in a clear manner by Bell and Glasstone.
(12), Duderstadt and Hamilton (13), and Lamash (14). This method starts with a distinction between narrow and wide resonances, which gives widely different results in some cases. Chernick and Vernon introduced an iteration procedure which reduces the gap between the two approximations.

Goldstein and Cohen (4) have developed a variational principle for intermediate resonances for a homogeneous fuel-moderator mixture. A similar approach for heterogeneous media has been done by Goldstein and Seghal (5). The absorption for an intermediate resonance has a value between the wide and the narrow resonance approximation. The variational principle leads to an adjustable parameter, which can be considered merely as a weight factor for the results obtained by the wide and narrow resonance approximations.

Nordheim (7) developed a code for the calculation of resonance integrals for heterogeneous configurations, based on a direct solution of the integral equation for the average flux in the absorber.

All methods discussed above use Dancoff corrections. A simple method for evaluating Dancoff corrections has been established by Leslie, Hill and Jonsson (8). A method which uses Dancoff corrections tends to give difficulties for closed-packed lattices. A calculation for resonance escape probabilities for isolated resonances in a heterogeneous medium by solving the neutron slowing down equations has been done by Chiarella (9). Paviotti Corcuera and Solanilla (10) used operational expressions for deriving resonance integrals. Corngold (6) discussed neutron absorption in a slab lattice by using
directly the integral Boltzmann transport equation followed by flux expansion in Legendre polynomials. The interference between resonances in a slab lattice has been studied by Mannan and Zweifel (11). A thorough discussion of resonance absorption and slowing down theory is given by Dresner (3), Ferziger and Zweifel (15), and Williams (16).

The objective of this work is the development of basic ideas for an accurate calculation of resonance escape probabilities in fairly closed-packed lattices. Therefore the use of Dancoff corrections is avoided. For simplicity we limit ourselves to a slab geometry. Although Monte Carlo methods can be used, the computer time required would be far too long. A new method, which is based on the Boltzmann equation, will be explained. This method includes Doppler broadening and obviates the necessity of choosing between the narrow and the wide resonance approximations. The algorithm is set up for a light water moderator and one can therefore ignore interference scattering (20). The reaction rate in the fuel contains two contributions. The first term appears as an integral expression, which can be calculated numerically; the second term can be considered as a correction factor for oxygen scattering and is derived by using a variational principle. A computer code has been developed. Input data required are the resonance parameters, specification of temperature and the dimensions of fuel and moderator width. We assume no interference between resonances. Isotropic scattering is assumed. We further use a $1/E$ slowing down spectrum for hydrogen scattering and consider a non-moderating fuel and non-scattering absorber. The resonance escape
probability for various resonances of uranium-238 is evaluated and is in agreement with values obtained by Corngold (6). The variational principle used in this work is similar to Williams' approach (17). More about variational theory for reactor calculations can be found in Bell and Glasstone (12), Williams (18), or Stacey (19).
2. DERIVATION OF AN EXPRESSION FOR REACTION RATES IN SLABS

2.1 Problem Statement

We attempt to give a systematic scheme for the calculation of resonance escape probabilities in a one-dimensional heterogeneous system. This system is composed of alternating slabs of fuel and moderator. Our aim is to obtain formulas for resonance absorption that contain only geometrical parameters, fuel and moderator cross sections and the resonance parameters.

2.2 The Basic Equations

We more specifically consider water as moderator and uranium-238 as absorber in the fuel region. We furthermore assume a non-moderating fuel region with an energy-dependent absorption cross section (\(\Sigma_a\)), and a non-absorbing moderator with an energy-independent macroscopic total cross section (\(\Sigma\)). We assume isotropic scattering and ignore interference scattering. Note that the assumption of no slowing down in the fuel corresponds to making the mass of the absorber atoms infinite, which is a common approach for the calculation of resonance escape probabilities.

By describing the system of alternating slabs of fuel and moderator as being composed of a succession of unit cells, we can limit the study to one single unit cell. Such a unit cell is pictured in Fig. 1.
Figure 1. Representation of a unit cell.
The equations describing the neutron flux in the moderator and the fuel are

\[ \mu \frac{\partial \phi(x,E,\mu)}{\partial x} + \Sigma_f(x,E,\mu) = \frac{1}{2} \int_{0}^{\infty} dE' \Sigma_s(E' \rightarrow E) \phi_o(x,E') \]  

(1)

for the moderator, or for \(0 \leq x \leq 2b\), and

\[ \mu \frac{\partial \phi(x,E,\mu)}{\partial x} + \Sigma_f(E) \cdot \phi(x,E,\mu) = \frac{x(E)}{2} \int_{0}^{\infty} dE' \nu(E') \Sigma_f(E') \cdot \phi_o(x,E') \]  

(2)

for the fuel region, or for \(-2a \leq x \leq 0\).

In the equations above we have defined

\[ \phi_o(x,E') = \int_{-1}^{1} \mu \phi(x,E,\mu). \]

\(\Sigma_s(E' \rightarrow E)\) is the differential scattering cross section for the moderator. The right-hand side of Eq. 2 represents the fission source. Owing to the symmetry of the system, the flux depends only on one spatial co-ordinate and one angular co-ordinate, \(\mu = \cos \theta\), \(\theta\) being the angle the neutron trajectory makes with the \(x\)-axis.

Since we are only interested in the resonance region, the fission source in the fuel can be neglected. For constructing a variational principle similar to Williams (17), we consider the scattering term in the moderator equation as being composed of a continuous slowing down source due to the scattering of hydrogen, \(\Sigma(E)\), and a scattering contribution from oxygen. We will represent the differential scattering cross section for oxygen by \(\Sigma_{so}(E' \rightarrow E)\) and the slowing
down source in hydrogen by the well known approximation (13)

\[ S(E) = S_0 / E. \]

With the above assumptions, Eqs. 1 and 2 reduce to

\[
\frac{\partial \phi(x, E, \mu)}{\partial x} + \Sigma \phi(x, E, \mu) = \frac{1}{2} \int_0^\infty dE' \Sigma_{SO}(E' \rightarrow E) \phi(x, E') + \frac{1}{2} S(E) \tag{3}
\]

and

\[
\frac{\partial \phi(x, E, \mu)}{\partial x} + \Sigma_a(E) \phi(x, E, \mu) = 0. \tag{4}
\]

2.3 Integral Equation for \( \phi_0(x, E) \)

The variational approach used is based on an integral equation for \( \phi_0(x, E) \). This integral equation is suited for a variational treatment because it is nearly self-adjoint (almost symmetric kernel).

We denote the right hand side of Eq. 3 by \( \frac{1}{2} Q(x, E) \) and treat the equation as a first order one in the \( x \)-variable. After integrating and introducing the periodicity condition \( \phi(2b, E, \mu) = \phi(0, E, \mu) \), the moderator equation becomes

\[
\phi_0(x, E) = \int_0^1 \phi(0, E, \mu) \cdot \left\{ \exp(-\Sigma x / \mu) + \exp(-\Sigma(2b-x) / \mu) \right\} d\mu \\
+ \frac{1}{2} \int_0^{2b} Q(x', E) \ E_1(\Sigma |x-x'|) dx'. \tag{5}
\]

Here \( E_1 \) stands for an exponential integral of the first order.
If we introduce the optical thickness of the fuel, \( \delta(E) \), we get
after integrating Eq. 3 over the fuel region,

\[
\phi(0,E,\mu) = \phi(0,E,-\mu) \exp(-2a\Sigma_a/\mu)
\]
or,

\[
\phi(0,E,\mu) = \phi(0,E,-\mu) \exp(-\delta(E)/\mu).
\]  

(6)

Insertion of this expression into Eq. 5 together with the relations
(which come from integrating Eq. 3 over the moderator region and
periodicity)

\[
\phi(0,E,-\mu) = \exp(-\beta/\mu)\phi(2b,E,\mu) + \frac{1}{2} \int_0^{2b} Q(x',E) \exp(-\Sigma x'/\mu) dx'/\mu,
\]  

(7)

where \( \beta = 2b\Sigma \),
and \( \phi(2b,E,-\mu) = \phi(0,E,\mu) \),

(8)

leads to

\[
\phi_0(x,E) = \frac{1}{2} \int_0^{2b} Q(x',E) \cdot \left\{ f_1(x,x',\beta,\delta(E)) + E_1(\Sigma |x-x'|) \right\} dx'.
\]  

(9)

where,

\[
f_1(x,x',\beta,\delta(E)) = \int_0^1 \frac{\exp\left\{-[\Sigma (x+x') + \delta(E)]/\mu\right\} + \exp\left\{-[\Sigma (x'-x) + \beta + \delta(E)]/\mu\right\} d\mu}{1 - \exp\{-\beta/\mu\}}.
\]  

(10)

By replacing \( Q(x,E) \) by the full expression, Eq. 9 becomes

\[
\phi_0(x,E) = \frac{1}{2} \int_0^{2b} \int_0^{2b} dx'\Sigma_\text{so}(E' \rightarrow E) \phi_0(x',E') \{ f_1(x,x',\beta,\delta) + E_1(\Sigma |x-x'|) \}
\]

\[
+ \frac{1}{2} \int_0^{2b} dx' S(E) \{ f_1(x,x',\beta,\delta) + E_1(\Sigma |x-x'|) \}.
\]  

(11)
This is an integral equation for the flux in the moderator under conditions of periodicity. When the moderator width becomes infinite we have the same geometry as Williams (17). As will be shown in appendix A, this equation reduces to Williams' Eq. 5 when $\beta$ approaches infinity.

2.4 Derivation of an Expression for the Absorption Rate in the Fuel over a Particular Resonance

The partially averaged flux in the fuel region, $\bar{\phi}(E)$, is directly related to the angular distribution incident on it. By conservation arguments we obtain

$$\int_0^1 \delta(E) \cdot \bar{\phi}(E) = \int_0^1 \mu \{ \phi(0,E,-\mu) - \phi(-2a,E,-\mu) \}.$$  

Since,

$$\phi(-2a,E,\mu) = \phi(0,E,-\mu) \exp\{-\delta(E)/\mu\},$$

the above equation reduces to

$$\bar{\phi}(E) = \frac{2}{\delta(E)} \int_0^1 \mu \{1-\exp\{-\delta/\mu\}\} \phi(0,E,-\mu) d\mu.$$  

Using Eqs. 7 and 8 we have,

$$\bar{\phi}(E) = \frac{1}{\delta(E)} \int_0^{2b} dx' \int_0^\infty dE' \Sigma_{so}(E'\rightarrow E) \phi_o(x',E') f_2(x',\beta,\delta(E)).$$
\[ + \frac{1}{\delta(E)} \int_0^b S(E) f_2(x', \beta, \delta(E)) \, dx', \quad (13) \]

where

\[ f_2(x, \beta, \delta(E)) = \int_0^1 \exp(-\Sigma x/\mu) \frac{1-\exp(-\delta(E)/\mu)}{1-\exp(-(\delta+\beta)/\mu)} \, d\mu. \quad (14) \]

This expression reduces to the same form as Williams (17) Eq. 11 when \( \beta \) approaches infinity (see appendix A).

The absorption rate in the fuel over a particular resonance is given by

\[ A = \int_{V_F} \int_{\Delta E} dV_F \, dE \Sigma_a(E) \phi_o(x, E), \]

or per unit area,

\[ A = \int_{\Delta E} \int_{-2\delta}^{0} dE \Sigma_a(E) \phi_o(x, E), \]

or,

\[ A = \int_{\Delta E} dE \delta(E) \bar{\phi}(E). \quad (15) \]

Using Eq. 13 the absorption rate becomes
\[ A = \int_{\Delta E} \int_{0}^{2b} \int_{0}^{2b} dE' \Sigma_{so}(E' \rightarrow E) \phi_0(x', E') \xi_2(x', \beta, \delta(E)) + \int_{\Delta E} \int_{0}^{2b} dE' S(E) \xi_2(x', \beta, \delta(E)). \] (16)

We denote the first term of Eq. 16 as \( \Delta \), and the second term as \( A_s \).
Then we can write the absorption rate in the fuel per unit area as

\[ A = \Delta + A_s. \] (17)

2.5 The Variational Principle

If we multiply Eq. 11 by \( \Sigma_{so}(E \rightarrow E'') \) and integrate over \( E \), then by replacing \( E \) by \( E' \) and \( E'' \) by \( E \) and defining

\[ \Lambda(E, x) = \int_{0}^{2b} dE' \Sigma_{so}(E' \rightarrow E) \phi_0(x, E), \] (18)

\[ K(E, x, x') = \xi_1(x, x', \beta, \delta(E)) + E_1(\Sigma|x-x'|) \] (19)

and

\[ S(E, x) = \frac{1}{2} \int_{0}^{2b} dE' \int_{0}^{2b} dE' \Sigma_{so}(E' \rightarrow E) S(E) K(E', x, x') , \] (20)

we get

\[ \Lambda(E, x) = \frac{1}{2} \int_{0}^{2b} dE' \int_{0}^{2b} dx' \Sigma_{so}(E' \rightarrow E) \Lambda(E', x) K(E', x, x') + S(E, x) , \] (21)
an integral equation for $\Lambda(E,x)$. The equation adjoint to Eq. 21 is

$$\Lambda^+(E,x) = S^+(E,x) + \frac{1}{2} \int_0^a \int_0^{2b} dE' \int dx' \Sigma_{SO} (E\rightarrow E') \Lambda^+(E',x') K(E,x,x'). \quad (22)$$

The reason why Eq. 22 is not self-adjoint to Eq. 21 lies in the fact that we have $K(E,x,x')$, instead of $K(E',x,x')$ in Eq. 22.

In operator notation we can write Eqs. 21 and 22 as

$$\Lambda = Q\Lambda + S,$$

and

$$\Lambda^+ = Q^+\Lambda^+ + S^+.$$

Consider the functional

$$F\{\Lambda, \Lambda^+\} = \frac{(\Lambda, S^+)(\Lambda^+, S)}{(\Lambda^+, \Lambda - Q\Lambda)} \quad , \quad (23)$$

where $(A,B)$ means

$$(A,B) = \int_{\Delta E} dE \int_0^{2b} dx A(E,x) B(E,x).$$

The above functional is called the "schwinger functional". It can be proved that this functional is stationary with respect to small variations of $\Lambda$ and $\Lambda^+$ about the solutions $\Lambda$ and $\Lambda^+$ of Eqs. 21 and 22 (18). Furthermore,

$$F\{\Lambda, \Lambda^+\} = (\Lambda, S^+) = (\Lambda^+, S)$$
By choosing $S^+(E,x) = f_2(x,\beta,\delta(E))$, $F$ becomes a stationary expression for $\Delta$.

Since $\Theta$ is not self-adjoint, it is not guaranteed that trial functions which satisfy Eqs. 21 and 22 will maximize $F$. Nevertheless the error in $\Delta$ will be small compared with the error in the trial functions (17).

With the above variational principle the expression for the absorption rate in the fuel per unit area becomes

$$A = A_s + \frac{I_1 I_2}{I_3},$$  \hspace{1cm} (25)

where,

$$I_1 = \int_{\Delta E} dE \int_0^{2b} dx' \Lambda(E,x) S(E,x),$$  \hspace{1cm} (26)

$$I_2 = \frac{1}{2} \int_{\Delta E} dE \int_0^{2b} dx' \Lambda'(E,x) S(E,x),$$  \hspace{1cm} (27)

$$I_3 = \int_{\Delta E} dE \int_0^{2b} dx' \Lambda'(E,x) \{ \Lambda(E,x) - \frac{1}{2} \int_{\Delta E} dE' \int_0^{2b} dx' \Sigma_S(E \rightarrow E) \Lambda(E',x) K(E',x,x') \},$$  \hspace{1cm} (28)

and

$$A_s = \int_{\Delta E} dE \int_0^{2b} dx f_2(x,\beta,\delta(E)) S(E).$$  \hspace{1cm} (29)

2.6 Derivation of an Expression for the Resonance Escape probability

Normalizing $1/2.S(E) = 1/E$, the total number of neutrons absorbed per second in the whole lump for a particular resonance at energy $E_1$ is
\[ V_F \int_{\Delta t} \Sigma_a(E)\phi(E) \, dE , \]
where \( V_F \) represents the fuel volume.

When \( V_M \) stands for the moderator volume, there are \( V_M \) neutrons "produced" by hydrogen scattering in the cell per second. It therefore follows that the escape probability for a particular resonance is

\[ p_i = 1 - \frac{V_F}{V_M} \int_{\Delta t} \Sigma_a(E)\phi(E) \, dE , \]

or in terms of the reaction rate per unit area we have

\[ p_i = 1 - \frac{A}{2b} . \]

Due to the normalization procedure for \( S(E) \), the resonance escape probability will be dimensionless, as physically required.

### 2.7 Trial Expressions for \( A \) and \( A^† \)

In diffusion theory, Eq. 1 can be approximated as

\[ -D \frac{\partial^2 \phi_o(x,E)}{\partial x^2} + \Sigma_f(x,E) = \int_{\theta}^{\sigma} \Sigma_s(E' \rightarrow E)\phi_o(x,E') \, dE' , \]

where \( D \) is the diffusion constant for the moderator.

When we assume \( \phi_o(x,E) = \phi_o(x)/E \), which is a common approach for the energy dependence of the flux in slowing down problems, and assume isotropic scattering, or
\[ \Sigma_s(E' \rightarrow E) = \begin{cases} \frac{\Sigma_s}{(1-\alpha)E'} & \text{for } E' > E > \alpha E' \\ 0 & \text{otherwise} \end{cases} \]

it can be shown that \( \phi_0(x) \) satisfies the one-speed diffusion equation

\[ -\frac{d^2 \phi_0(x)}{dx^2} + \Sigma_a(E) \phi_0(x) = 0. \]

Using Eq. 18, the definition for \( \Lambda(E,x) \), we have

\[ \Lambda(E,x) = \Sigma_s \phi_0(x)/E. \]

Solving the one-speed diffusion equation for \( \phi_0(x) \) and using the condition that \( \phi_0(x) \) has to reach its maximum value in the center of the moderator region, we get

\[ \Lambda(E,x) = \frac{1}{E} \left\{ \exp \left[ \frac{(2b-x)}{L} \right] + \exp \left[ \frac{x}{L} \right] \right\}, \]

where \( L \) is the diffusion length of the moderator and \( B \) a constant factor.
Since the trial functions for a Schwinger functional can be multiplied by an arbitrary constant without changing its value, an appropriate expression for \( \Lambda(E,x) \) will be
\[ \Lambda(E, x) = \frac{1}{E} \{ \exp \left[ \frac{(2b-x)}{L} \right] + \exp \left( \frac{x}{L} \right) \} . \]  

The equation adjoint to Eq. 31 will be

\[ -D \frac{\partial^2 \phi_o \dagger(x, E)}{\partial x^2} + \Sigma \phi_o \dagger(x, E) = \int_0^\infty dE' \Sigma_s(E' \rightarrow E) \phi_o \dagger(x, E') . \]  

Assuming \( \phi_o \dagger(x, E) = E \phi_o \dagger(x) \)

and

\[ \Sigma_s(E \rightarrow E') = \begin{cases} \frac{\Sigma_s}{(1-\alpha)E}, & \text{for } E > E' \geq \alpha E \\ 0, & \text{otherwise} \end{cases} \]

It can be shown that \( \phi_o \dagger(x) \) satisfies the energy independent equation

\[ -D \frac{d^2 \phi_o \dagger(x)}{dx^2} + \left[ \Sigma - \Sigma_s(1-\alpha)/2 \right] \phi_o \dagger(x) = 0 . \]

Note that if \( \alpha = 1 \) (infinite mass moderator atoms), the equations for \( \phi_o \dagger(x) \) and \( \phi_o(x) \) become self-adjoint, as is well known for one speed diffusion theory.

By defining \( L \dagger \) as

\[ L \dagger = \left\{ \frac{\Sigma - \Sigma_s(1-\alpha)/2}{D} \right\} ^{-0.5} , \]

and taking a similar approach for the derivation of \( \Lambda(E, x) \), an
appropriate trial expression for $\Lambda^+(E, x)$ will be:

$$\Lambda^+(E, x) = E\{\exp\left[\frac{(2b-x)}{L^+}\right] + \exp\left(\frac{x}{L^+}\right)\}.$$  \hfill (34)
3. NUMERICAL RESULTS

3.1 Explicit formula For the Absorption Rate in the Fuel

Inserting the trial expressions for $\Lambda(E,x)$ and $\Lambda^{+}(E,x)$ into Eqs. 26,27 and 28, and working out the integrals analytically as far as possible gives the expressions for $I_1$, $I_2$ and $I_3$ below.

$$I_1 = \int_{-\Delta E}^{\Delta E} \frac{dE}{E} \int_{0}^{1} d\mu \left[ \frac{1 - \exp(-\delta/\mu)}{1 - \exp(-\delta/\mu)} \right]$$

$$\cdot \left[ \frac{L_{\mu}}{\mu + \Sigma L} \{ \exp(2b/L) - \exp(-2b\Sigma/\mu) \} \right.$$  

$$+ \frac{L_{\mu}}{\mu - \Sigma L} \{ \exp \left( \frac{2b(\mu - \Sigma L)}{L\mu} \right) - 1 \} \right]. \quad (35)$$

The integrals over the resonance region will be approximated by the integral over the interval $(E_i - \Gamma_p/2, E_i + \Gamma_p/2)$. $E_i$ and $\Gamma_p$ are the symbols for the resonance energy and the practical resonance width. The latter is defined by Duderstadt and Hamilton (13).

$$I_2 = I_{21} + I_{22},$$

where,
\[ I_{21} = \frac{8 \Sigma_S \exp(b/Lt)}{(1-\alpha_0)} \int \Delta F \cdot E \int E' \int_0^{E' \cdot \alpha_0} \mu \cdot \frac{\sinh(\theta b/\mu)}{\exp((\theta + \delta)/\mu) - 1} \]

\[ \cdot \left[ \frac{\mu \cdot \sinh(b(\mu + \Sigma L^\top))}{\mu + \Sigma L^\top} + \frac{\mu \cdot \sinh(b(\Sigma L^\top - \mu))}{\Sigma L^\top - \mu} \right], \quad (36) \]

and

\[ I_{22} = \frac{2 \Sigma_S \exp(b/Lt \cdot \mu)}{\mu} \int_{-b}^{b} \cosh(x/Lt) \cdot \left[ 2 - E_2 \left\{ (x+b) - E_2 \left\{ (b-x) \right\} \right\} \right] dx. \quad (37) \]

\[ I_3 = I_{31} + I_{321} + I_{322} + I_{3222}. \]

\[ I_{31} = 4 \mu \exp(b/Lt + b/L) \left[ \frac{L \cdot \Sigma L^\top \sinh(b(L + \Sigma L^\top))}{L + \Sigma L^\top} + \frac{L \cdot \Sigma L^\top \sinh(b(L - \Sigma L^\top))}{L - \Sigma L^\top} \right]. \quad (38) \]

\[ I_{321} = - \frac{4 \Sigma_S \exp(b/Lt)}{(1-\alpha_0)} \int \Delta F \cdot \int_0^{E \cdot \alpha_0} \mu \cdot \int G_1 \cdot G_2 \cdot G_3 \cdot \frac{E'}{E^\prime \cdot \alpha_0} \cdot \cdot \cdot \quad (39) \]

where,

\[ G_1 = \frac{\mu L}{\mu + \Sigma L} \sinh(b(\mu + \Sigma L)) + \frac{\mu L}{\Sigma L - \mu} \sinh(b(\Sigma L - \mu)) \]

\[ G_2 = \frac{L \cdot \Sigma L^\top}{\Sigma L^\top + \mu} \sinh(b(\mu + \Sigma L^\top)) + \frac{L^\top \cdot \Sigma L^\top}{\Sigma L^\top - \mu} \sinh(b(\Sigma L^\top - \mu)) \]
and,

\[ G_3 = \exp\left(\frac{\gamma + \delta(E)}{\mu}\right) - 1. \]

\[ I_{3221} = \frac{2 \Gamma_p \Sigma_0 \exp\left(\frac{(b/L_1) + (b/L)}{\mu}\right)}{E} \int_{x}^{b} dx \cosh(x/L_1) G_4, \quad (40) \]

where,

\[ G_4 = \cosh\left(\frac{b}{L \mu}\right) \left\{ \cosh\left(\frac{b}{L}\right) \left[ E_2\left\{ E(x+b) \right\} + E_2\left\{ E(b-x) \right\} \right] - 2 \cosh\left(\frac{x}{L}\right) \right\}. \]

\[ I_{3222} = \frac{2 \Gamma_p \Sigma_0 \exp\left(\frac{(b/L_1) + (b/L)}{\mu}\right)}{E} \int_{-b}^{b} dx \cosh(x/L_1) \]

\[ \cdot \left[ - \frac{1}{E} \int_{x}^{0} E_2(\gamma) \sinh\left(\frac{E(x-\gamma)}{L}\right) d\gamma - \frac{1}{E} \int_{0}^{\frac{b-x}{E}} E_2(\gamma) \sinh\left(\frac{E(x-\gamma)}{L}\right) d\gamma \right]. \quad (41) \]

Equation 29 reduces to

\[ A_s = 2 \int_{a}^{b} \frac{dE}{E} \int_{d}^{d_{\mu}} \left(1 - \exp\left(\frac{-2bE}{\mu}\right)\right) \cdot \left[ \frac{1 - \exp\left(\frac{-\gamma}{\mu}\right)}{1 - \exp\left(\frac{-\gamma + b}{\mu}\right)} \right]. \quad (42) \]

The symbol \( E_2 \) in Eq. 41 represents an exponential integral of the second order.

The expressions for \( I_1, I_2, I_3 \) and \( A_s \) were evaluated numerically using Gauss quadrature formulas. Therefore, all the intervals have been transformed to the interval \((-1,1)\).

A computer code has been developed. The number of Gauss quadrature points is an input parameter in the program. The Gauss quadrature parameters are tabulated by Abramowitz and Stegun (22), and by Stroud
and Secrest (23). No potential scattering interference (11) between resonances is assumed. The Doppler-broadened Breit-Wigner formula has been used for calculating the absorption cross section of the fuel. The algorithm for doing these calculations is the second method described by Beynon and Grant (24) and is based on a series expansion for the Doppler broadening function introduced by Bethe (27).

For checking the accuracy of this method, table I from reference 24 has been reproduced. The results agree with those obtained from the first method (24) up to four significant digits in most of the cases and up to two significant digits for all other cases. The accuracy for the results obtained by Beynon and Grant is partly determined by the empirical formula they use for calculating \(\exp(a^2)\{1 - E_2(a)\}\). By evaluating this function more accurately, slightly better results for \(\Sigma_a(E)\) can be obtained.

The macroscopic cross sections for water are calculated from the microscopic cross sections of oxygen and hydrogen. Although we assume an absolute temperature of 279 K in the program, the code can easily be modified for other temperatures. The parameters used for calculating \(\Sigma_a(E)\) are the resonance energy \((E_i)\), the maximum microscopic cross section for the resonance region \((\sigma_{\lambda})\), the temperature, the practical resonance width \((\Gamma_p)\), the total line width \((\Gamma)\), the radiative line width \((\Gamma_r)\) and the neutron line width \((\Gamma_n)\).
3.2 Numerical Data used in the Program

3.2.1 The Resonance Parameters

The resonance parameters for uranium-238 are tabulated in reference 13. Typical values are:

- \( \sigma_i = 2.16 \times 10^5 \) b
- \( E_i = 6.67 \) eV
- \( \Gamma_Y = 0.026 \) eV
- \( \Gamma_n = 0.02752 \) eV
- \( \Gamma_p = 1.26 \) eV
- \( T = 279 \) K

3.2.2 The Cross sections and Atom densities

The cross sections used are the total, absorption, scattering and transport microscopic cross sections for oxygen and hydrogen. Those cross sections are fairly constant with respect to energy in the resonance region. The atom densities needed are the atom density for water and uranium-238. Those data can be found in BNL 325 (25). We used:

- \( \sigma_{to} = 3.7 \) b
- \( \sigma_{ao} = 0.0 \) b
- \( \sigma_{tro} = 3.55 \) b
- \( \sigma_{so} = 3.7 \) b
\[ \sigma_{tH} = 21 \text{ b} \]
\[ \sigma_{aH} = 0.65 \text{ b} \]
\[ \sigma_{trH} = 7.1 \text{ b} \]
\[ \sigma_{sH} = 20.4 \text{ b} \]
\[ N_{U-238} = 0.0478 \times 10^{24} \text{ atoms per cubic cm} \]
\[ N_{H_2O} = 0.0355 \times 10^{24} \text{ atoms per cubic cm} \]

The first subscript of the microscopic cross sections, \( \sigma \), refers to the kind of cross section (total, absorption, transport or scattering), the second subscript refers to the kind of atom (oxygen or hydrogen).

3.2.3 Other Data used in the Program

Other input data required in the program are the fuel width (2a), the moderator width (2b) and the number of points used for the Gauss quadrature integration (N). Typical values are:
\[ a = 0.25 \text{ cm} \]
\[ b = 0.1 \text{ cm} \]
\[ N = 8 \]

3.3 Results

As a check for the computer code, a homogeneous mixture of water and uranium-238 has been simulated by making the fuel and the moderator region very small. The fuel-moderator volume ratio is 1:1.
We assume a fuel width of 0.508 cm (0.2 inches). The resonance escape probabilities have been calculated for the resonances at 6.67, 20.9, 36.8, 66.6, 102.5, 116.85, 165.27 and 208.7 eV.

In all the Gauss quadrature integrations, 8 points were used. The results with 20 points for the Gauss quadrature integration are the same for the first two significant digits and require 90 seconds computing time for a particular resonance. The time for one resonance with 8 points takes 5 seconds. The program has not been optimized with respect to computing time. The results for a homogeneous mixture are given in table I. We compared our results with those obtained by Chernick and Vernon (2), and Spinney (26). Those authors assume a 1:1 homogeneous atomic mixture of uranium-238 with hydrogen. Since we have a 1:1 volume ratio of uranium-238 with water we would expect our results for the resonance absorption to be slightly less. This expectation holds for resonances under 100 eV. Note also that there is a serious discrepancy between the absorption probabilities calculated by Chernick and Vernon, and by Spinney.

In table II we compare resonance absorption probabilities, calculated with the variational method, with those obtained by Corngold (6). Following Corngold we also assume 0.508 cm thick fuel plates of uranium-238, separated by slabs of water. The fuel-moderator volume ratio is 1:1.

When we compare our results with those obtained by Corngold, four of them agree within 5% accuracy. However for the four other
Table I. Comparison of the resonance absorption probability for a homogeneous mixture of fuel and moderator between the results obtained in this work and those obtained by Chernick and Vernon (2), and Spinney (26).

<table>
<thead>
<tr>
<th>Resonance energy</th>
<th>Resonance escape probability (this work)</th>
<th>Resonance absorption probability (this work)</th>
<th>Resonance absorption probability (Chernick)</th>
<th>Resonance absorption probability (Spinney)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_i$ (eV)</td>
<td>$p_i$</td>
<td>$1 - p_i$</td>
<td>$1 - p_i$</td>
<td>$1 - p_i$</td>
</tr>
<tr>
<td>6.67</td>
<td>0.8215</td>
<td>0.1785</td>
<td></td>
<td>0.1963</td>
</tr>
<tr>
<td>20.90</td>
<td>0.9405</td>
<td>0.05951</td>
<td></td>
<td>0.06755</td>
</tr>
<tr>
<td>36.8</td>
<td>0.9477</td>
<td>0.05230</td>
<td></td>
<td>0.05820</td>
</tr>
<tr>
<td>66.54</td>
<td>0.9797</td>
<td>0.02030</td>
<td>0.0253</td>
<td></td>
</tr>
<tr>
<td>81.3</td>
<td>0.9925</td>
<td>0.007495</td>
<td>0.00627</td>
<td>0.009596</td>
</tr>
<tr>
<td>90</td>
<td>0.9987</td>
<td>0.001252</td>
<td>0.00113</td>
<td>0.001104</td>
</tr>
<tr>
<td>102.47</td>
<td>0.9804</td>
<td>0.01965</td>
<td></td>
<td></td>
</tr>
<tr>
<td>116.85</td>
<td>0.9904</td>
<td>0.009602</td>
<td>0.0202</td>
<td>0.009170</td>
</tr>
<tr>
<td>165.27</td>
<td>0.9959</td>
<td>0.004104</td>
<td>0.00294</td>
<td></td>
</tr>
<tr>
<td>192</td>
<td>0.9884</td>
<td>0.01160</td>
<td>0.01043</td>
<td>0.007119</td>
</tr>
<tr>
<td>208.46</td>
<td>0.9933</td>
<td>0.006714</td>
<td></td>
<td>0.005021</td>
</tr>
</tbody>
</table>
Table II. Comparison of resonance absorption probabilities calculated in this work and obtained by Corngold (6) for a heterogeneous slab with a 1:1 uranium-238/water volume ratio and a fuel width of 0.508 cm at 300 K.

<table>
<thead>
<tr>
<th>Resonance energy (eV)</th>
<th>Resonance absorption probability (this work)</th>
<th>Resonance absorption probability (Corngold)</th>
<th>Relative difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>E₁</td>
<td>p₁</td>
<td>p₁</td>
<td>%</td>
</tr>
<tr>
<td>6.67</td>
<td>0.1146</td>
<td>0.1138</td>
<td>- 0.7</td>
</tr>
<tr>
<td>20.90</td>
<td>0.04215</td>
<td>0.05116</td>
<td>+ 21.4</td>
</tr>
<tr>
<td>36.8</td>
<td>0.03889</td>
<td>0.04671</td>
<td>+ 20.1</td>
</tr>
<tr>
<td>66.54</td>
<td>0.01395</td>
<td>0.01453</td>
<td>+ 4.1</td>
</tr>
<tr>
<td>81.30</td>
<td>0.005225</td>
<td>0.00437</td>
<td>- 16.3</td>
</tr>
<tr>
<td>90</td>
<td>0.0008951</td>
<td>0.001078</td>
<td>+ 20.4</td>
</tr>
<tr>
<td>102.47</td>
<td>0.01404</td>
<td>0.01410</td>
<td>+ 0.4</td>
</tr>
<tr>
<td>116.85</td>
<td>0.006311</td>
<td>0.006152</td>
<td>- 2.5</td>
</tr>
<tr>
<td>165.27</td>
<td>0.003067</td>
<td></td>
<td></td>
</tr>
<tr>
<td>208.46</td>
<td>0.004670</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
resonances, we find a large discrepancy (20% difference); this might be due to a different value for the input parameter $T_p$ (practical resonance width). The changing sign of the relative difference indicates that no serious systematic errors are present.

Resonance escape probabilities for various resonances and different lattice parameters are represented in table III. From table III we conclude that an increase in the moderator-fuel volume ratio, with a constant fuel volume, causes an increase in the resonance escape probability, as would be expected from physical considerations. Furthermore we see that the more homogeneous the fuel-moderator mixture becomes, the less the resonance escape probability will be. The fact that lumping gives a lower resonance absorption is well known.
### Table III. Resonance escape probabilities for a heterogeneous slab for different slab geometries.

<table>
<thead>
<tr>
<th>Resonance energy $E_1$ (eV)</th>
<th>Fuel width $2a$ (cm)</th>
<th>Moderator width $2b$ (cm)</th>
<th>Res. Esc. Prob. $P_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.67</td>
<td>0.508</td>
<td>0.508</td>
<td>0.8854</td>
</tr>
<tr>
<td>20.90</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9578</td>
</tr>
<tr>
<td>36.80</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9611</td>
</tr>
<tr>
<td>66.54</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9860</td>
</tr>
<tr>
<td>102.47</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9850</td>
</tr>
<tr>
<td>116.85</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9937</td>
</tr>
<tr>
<td>165.27</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9969</td>
</tr>
<tr>
<td>208.46</td>
<td>0.508</td>
<td>0.508</td>
<td>0.9953</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.010</td>
<td>0.8122</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.020</td>
<td>0.8140</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.200</td>
<td>0.8464</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.300</td>
<td>0.8611</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.400</td>
<td>0.8737</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.500</td>
<td>0.8848</td>
</tr>
<tr>
<td>6.67</td>
<td>0.500</td>
<td>0.600</td>
<td>0.8941</td>
</tr>
<tr>
<td>20.90</td>
<td>0.200</td>
<td>0.200</td>
<td>0.9480</td>
</tr>
<tr>
<td>20.90</td>
<td>0.500</td>
<td>0.500</td>
<td>0.9576</td>
</tr>
</tbody>
</table>
4. CONCLUSIONS AND RECOMMENDATIONS

The method developed in this work is new with respect to the separate treatment of oxygen and hydrogen scattering, with an entirely different mathematical approach for each contribution.

The resonance absorption rate contains two terms. One term is related to the hydrogen scattering, and is derived directly by rearranging the Boltzmann equation. The second term includes the oxygen scattering, and can be considered as a correction term to the first one. The second term is calculated by using a variational principle.

The numerical results obtained are encouraging and in agreement with physical expectations. For the resonance absorption probabilities for a homogeneous mixture above 100 eV it is not sure that the discrepancy between our results and those obtained by Chernick an Vernon (2), or Spinney (26) is due to an error in the variational method (this work) or to an inaccuracy present in the method of Chernick and Vernon, or Spinney. A comparison with a Monte Carlo method or another more accurate code or experiment would provide the answer.

The resonance absorption probabilities for a heterogeneous slab are in good agreement (less than 5% difference) with those obtained by Corngold (6) for four resonances. For the other four resonances there is ± 20% difference. A comparison with another method would help to answer which of the two methods is the better one.
The computer time required by our code can be drastically decreased by using less points in the Gauss quadrature evaluation for the integrals in the calculation of $\Delta$ without affecting the accuracy seriously. We estimate that a decrease in computing time by a factor of five can be achieved easily.

Since we do not use a flat flux approximation with respect to space in the fuel region, the method developed in this work has a potential advantage above most of the other methods used for resonance absorption calculations. The assumption of a $1/E$ spectrum above the resonance energy is not a very good approximation for closed-packed lattices. The error introduced by this approximation can be reduced by assuming a more accurate energy dependence for the source term in the calculation of $A_s$.

It would require a serious effort to extend the variational method to anisotropic scattering or to other geometries. However, since the variational term in the resonance absorption, which is mathematically the most complicated one, can be considered as a correction term for oxygen scattering, crude approximations are allowed for the calculation of that part of the resonance escape probability.

The method established in this work (variational method) has the potential for being extended with high accuracy for cylindrical or hexagonal geometries. If simple approximate expressions for the factors in the variational term can be derived, it might be worth a try.
5. REFERENCES


Appendix A

The case of an infinite moderator region

When the moderator region becomes infinite we have exactly the same case as Williams (17). We will show that Eqs. 11 and 13 reduce to Williams' Eqs. 5 and 11.

If we take the limit for \( S \) going to infinity of \( f_1(x,x',\beta,\delta) \), we find from Eq. 10,

\[
f_1(x,x',\infty,\delta) = \int_0^1 \exp \left[ -\left( \Sigma(x+x')+\delta \right)/\mu \right] \frac{d\mu}{\mu}
\]

or,

\[
f_1(x,x',\infty,\delta) = E_1[\Sigma(x+x') + \delta] \quad (43)
\]

So that with Eq. 43, Eq. 11 will reduce to exactly the same expression as Williams' Eq. 5.

Similarly we find for \( f_2(x',\infty,\delta) \) from Eq. 14,

\[
f_2(x',\infty,\delta) = \int_0^1 \left[ \exp(-\Sigma x/\mu) - \exp\left(-\left(\delta + \Sigma x'\right)/\mu\right) \right] d\mu
\]

By noting that
\[ \int_0^\infty dx' f_2(x', \omega, \delta) = \frac{1}{2} - \sum \int_0^1 \mu d\mu \exp(-\delta/\mu) \]

\[ = \frac{1}{2} - E_3(\delta) \]

we can see that the second term of our Eq. 13 reduces to the first term of Williams' Eq. 11.

One can demonstrate the equality of the remaining term in each of both expressions.
input: microscopic cross sections for hydrogen and oxygen
# Gauss quadrature points, # cases
Gauss quadrature parameters
resonance parameters

calculation of cross sections and constants for the moderator
calculation of the optical thickness of the fuel region as a function of energy

calculation of $I_1, I_2, I_3, \text{ and } A_s$ with Gauss quadrature integration

calculation of the resonance escape probability
The vita has been removed from the scanned document
A VARIATIONAL APPROACH FOR THE CALCULATION
OF RESONANCE ESCAPE PROBABILITIES
IN SLAB LATTICES

by

Mark Julien Embrechts

(ABSTRACT)

A New method for calculating isolated resonance escape probabilities for slab lattices has been developed. It is based on the Boltzmann equation. The method avoids the use of Dancoff corrections and obviates the necessity of choosing between the wide and the narrow resonance approximations. The knowledge of the spatial dependence of the flux in the fuel region is not required.

Isotropic scattering and a 1/E spectrum above the resonance are assumed. The method is set up for a pure non-scattering uranium-238 absorber and a non-absorbing water moderator region.

The reaction rate in the fuel region contains two contributions, the first term appears as an integral expression, which can be integrated numerically, the second term can be considered as a correction factor for oxygen scattering and is derived by using a variational approach.

A computer code for calculating resonance escape probabilities in slab lattices has been developed. The results are in agreement with those obtained by Corngold.