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STUDY OF SLIGHTLY-ENRICHED URANIUM-WATER
LATTICES WITH HIGH CONVERSION RATIO

RESONANCE ABSORPTION IN WATER MODERATED LATTICES

Quarterly Progress Report, February 1 to April 30, 1960

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Combustion Engineering, Inc.
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Table of Contents

	<u>Page No.</u>
I. Summary	1
II. Review of Some Theoretical Descriptions of Resonance Capture	2
III. Geometrical Escape Probabilities for Lattices	10
IV. Calculation of Effective Absorption Cross Sections for Lattices with Metal Rods	15
V. Resonance Capture in Uranium Oxide Rod Lattices	17
VI. Calculation of the Effective Absorption Cross Section for the Unresolved Resonance Range	20
VII. Comparison of Calculations by the NR-NRIA Method with Monte Carlo Calculations	21
A. Lattices	21
B. Homogeneous Mixtures	24
C. Temperature Dependence	24
D. Resonance by Resonance Comparison with Monte Carlo	25
VIII. Comparison with Experiment	25
IX. Discussion	28
Appendix	29

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D. W. Drawbaugh

I. SUMMARY

In the past few years, there has been substantial progress made on the problem of calculating the resonance escape probability from the resonance parameters. This progress has been the result of many contributions both to the theory and to the experimental measurement of the resonance parameters. There also now exist a fair number of experimental measurements of lattice parameters which should allow a verification of theoretical calculations of resonance escape probabilities for lattices by experiment.

From the theoretical work on resonance escape, two methods of calculation have been chosen for the purpose of making a set of comparative calculations because of their immediate applicability in the form of computer programs. One method is the Monte Carlo method developed by R. D. Richtmyer, R. Van Norton and A. Wolfe⁽¹⁾. The second method is the Narrow Resonance and Narrow Resonance Infinite Mass

method which has been investigated by F. T. Adler, G. W. Hinman, and L. W. Nordheim⁽²⁾, who have published tabulated functions for applying the method. Both of these methods have been the subject of 1958 Geneva Conference papers, and, therefore, need not be described here in detail.

To apply the Adler-Hinman-Nordheim method to calculating resonance escape in a lattice it is necessary to make use of an equivalence between an isolated lump system and a lattice of lumps. Moreover, this equivalence must give an effective average chord length for the lumps in a lattice. Various ways of calculating such an effective average chord length have been suggested; several of these ways have been used and the results compared.

A computer program, QUERY⁽³⁾, for applying the Adler-Hinman-Nordheim method has been developed. The results of an extensive series of calculations of resonance integrals for uranium metal-water and uranium dioxide-water systems at various fuel temperatures using this program are given. Monte Carlo calculations for a variety of lattices have been made at room temperature. These results are compared with calculations using the QUERY program. Some Monte Carlo calculations at elevated temperatures have been made for comparison.

Finally, an attempt has been made to compare resonance escape calculations with experimental measurements of ratios of epithermal-to-thermal capture in U-238 in various lattices. Some of the problems involved in making such comparisons when enriched fuel elements are involved will be discussed.

II. REVIEW OF SOME THEORETICAL DESCRIPTIONS OF RESONANCE CAPTURE

The analytical approach to the heterogeneous resonance escape problem is concisely as well as exactly posed by the two coupled integral equations given by Chernick and Corngold⁽⁴⁾. These equations form the basis of most recent work on the heterogeneous resonance escape problem. The equations are conveniently written in the notation used by G. I. Bell⁽⁵⁾. Consider a periodic array of fuel lumps in a moderator. Let the fuel region be denoted by the subscript 0 and the moderator region be denoted by the subscript 1. The region 0 is made up of all the lumps and region 1 all the moderator. The space averaged flux in region i is ϕ_i . Let $P_i(E)$ be the probability that a neutron of energy E originating in region i makes its next collision in region i (possibly after traversing the other region). Then

$$\Sigma_{ot}(E)\phi_o(E) = P_o(E) \sum_{j=1}^J \frac{1}{1-a_j} \int_E^{E/a_j} N_{oj}\sigma_{sj}(E')\phi_o(E') \frac{dE'}{E'} + \quad (1a)$$

$$+ (1-P_1(E)) \frac{V_1}{V_o} \sum_{j=1}^J \frac{1}{1-a_j} \int_E^{E/a_j} N_{1j}\sigma_{sj}(E')\phi_1(E') \frac{dE'}{E'}$$

$$\Sigma_{1t}(E)\phi_1(E) = P_1(E) \sum_{j=1}^J \frac{1}{1-a_j} \int_E^{E/a_j} N_{1j}\sigma_{sj}(E')\phi_1(E') \frac{dE'}{E'} +$$

$$+ (1-P_o(E)) \frac{V_o}{V_1} \sum_{j=1}^J \frac{1}{1-a_j} \int_E^{E/a_j} N_{oj}\sigma_{sj}(E')\phi_o(E') \frac{dE'}{E'} \quad (1b)$$

where V_i = volume of region i , N_{ij} = density of j -th nuclide in region i ; $\sigma_{sj}(E)$ is the scattering cross section for nuclide j .

The first equation states that the collision density, $\Sigma_{ot}\phi_o(E)$, in the lump is equal to the density of neutrons in the lump slowing down to energy E multiplied by the probability that a neutron in a lump makes its next collision in a lump plus the number of neutrons per unit lump volume in the moderator arriving at energy E multiplied by the probability that a neutron in the moderator makes its next collision in the lump. The second equation has a similar interpretation with moderator and fuel roles interchanged.

If the distance between lumps is sufficiently large, a lump may be considered isolated. Then Equations (1a) and (1b) still hold if P_o and P_1 are interpreted as the collision probabilities for an isolated lump. These isolated lump collision probabilities will be denoted P_o^o, P_1^o .

The integral equations might be solved numerically or one might attempt to reduce the integral equations to differential equations by series expansion of the flux. On the other hand, the integrals in the equations may be approximated to reduce the integral equations to algebraic equations. Two types of approximations will be considered. These are called the narrow resonance approximation (NR), and the infinite mass approximation (IM). These approximations are based upon the practical width concept originally introduced by Wigner.

For a given scattering nuclide, each resonance can be classified as narrow or wide accordingly as the maximum energy change in a collision is greater or less than the practical width of the resonance Γ_p . The practical width for homogeneous mixtures is the energy range about the energy, E_o , of the resonance peak in which the resonance cross section

is greater than the total scattering cross section off resonance Σ_o . For the homogeneous case, Spinrad, Chernick and Corngold⁽⁴⁾ define a practical width as

$$\Gamma_p = \Gamma \left(\frac{\Sigma_{\max} + \Sigma_o}{\Sigma_o} \right)^{1/2} \quad (2)$$

where

$$\Sigma_o = \sum_{j=1}^J N_j (\sigma_j - \sigma_{\text{res } j})$$

the sum being over J isotopes, one of which has a resonance, the others have constant scattering cross sections but no resonances near the given resonance energy E_o . For the j -th isotope, a resonance will be narrow if $(1-a_j) E_o \gg \Gamma_p$; if $(1-a_j) E_o < \Gamma_p$ the resonance is wide. Bell has generalized the concept of practical width to the heterogeneous case. Let

Σ_{oo} = lump scattering cross section off resonance

Σ_{ot} = lump total cross section

$$\Sigma_{or} = \Sigma_{ot} - \Sigma_{oo}$$

Then

$$\frac{\Sigma_{or}(E)}{\Sigma_{ot}(E)} P_o(E)$$

is the probability that a neutron in the lump will make its next collision due to the cross section contributed by the resonance and within the lump. Bell then defines the practical width Γ_p as the energy interval about E_o over which

$$\frac{\Sigma_{or}(E)}{\Sigma_{ot}(E)} P_o(E) > \frac{1}{2}$$

Consider the integral

$$\frac{1}{1-a_j} \int_E^{E/a_j} N_j \sigma_{sj} \phi(E') \frac{dE'}{E'} \quad (3)$$

This represents the number of neutrons arriving at energy E in a given region. Above the resonance energy E_0 , it is a good assumption that $\phi = \bar{\phi}/E$, where $\bar{\phi}$ is a constant. Also, if the maximum energy loss at E_0 in a collision is large compared with the practical width, i. e., if $(1-a) E_0 \gg \Gamma_p$, then the resonance is narrow compared to energy losses in scattering. In this case, the dominant contribution to the above integral is in the range where $\phi(E) = \bar{\phi}/E$ and we therefore substitute $\phi(E) = \bar{\phi}/E$ into the integral, using the above approximation for ϕ over the whole range within the integral, to obtain

$$\frac{1}{1-a_j} \int_E^{E/a_j} N_j \sigma_{sj} \phi(E') \frac{dE'}{E'} = N_j \sigma_{sj} \frac{\bar{\phi}}{E} \quad (4)$$

in the NR approximation. We have assumed σ_{sj} constant over the range of integration; if the j -th material has a resonance, σ_{sj} is taken to be the constant potential scattering cross section, since this is the value of σ_{sj} in the dominant range of the integral.

When $(1-a_j) E_0 < \Gamma_p$, that is, the maximum energy loss by scattering is less than the practical width, the resonance is called wide. Then the energy loss in scattering may be neglected. This means, let the max $A \rightarrow \infty$, so $a = (A-1/A+1)^2 \rightarrow 1$, and find

$$\lim_{a \rightarrow 1} \frac{1}{1-a_j} \int_E^{E/a_j} N_j \sigma_{sj} (E') \phi(E') \frac{dE'}{E'} = N_j \sigma_{sj} \phi(E) \quad (5)$$

in the IM approximation.

Whether an integral is to be approximated by the NR or IM approximation depends both on the resonance and the scattering material. Thus, the designation IM for infinite scatterer mass

is also called the wide resonance approximation. A given scatterer is, in general, IM for some resonances and NR for others. In the unresolved range, all resonances are NR.

If the moderator scattering is primarily NR, then $\phi_1 = \bar{\phi}/E$ for all energies. In this case, all integrals over ϕ_1 may be approximated by the NR expression. For NR scattering, as noted above, the off resonance scattering cross section, Σ_{oo}^{NR} , in the lump is used; and for IM scattering, Σ_{os}^{IM} , the full scattering cross section in the lump is used. With this notation, (1a) and (1b) become

$$\Sigma_{ot}\phi_o(E) = P_o(E) \left[\Sigma_{oo}^{NR} \frac{\bar{\phi}}{E} + \Sigma_{os}^{IM}(E) \phi_o(E) \right] + (1-P_1(E)) \frac{V_1}{V_o} \Sigma_1 \frac{\bar{\phi}}{E} \quad (6a)$$

$$\Sigma_{1t}(E) \phi_1(E) = P_1(E) \Sigma_1 \frac{\bar{\phi}}{E} + (1-P_o(E)) \frac{V_o}{V_1} \left[\Sigma_{oo}^{NR} \frac{\bar{\phi}}{E} + \Sigma_{os}^{IM} \phi_o(E) \right] \quad (6b)$$

Solving for $\phi_o(E)$:

$$\phi_o(E) = \frac{P_o(E) \Sigma_{oo}^{NR} + (1-P_1(E)) \frac{V_1}{V_o} \Sigma_1}{\left[1 - P_o(E) \frac{\Sigma_{os}^{IM}(E)}{\Sigma_{ot}(E)} \right] \Sigma_{ot}} \cdot \frac{\bar{\phi}}{E} \quad (7)$$

and

$$\begin{aligned} \phi_1(E) = & \frac{P_1(E) \Sigma_1 \bar{\phi}}{\Sigma_{1t}(E) E} + \\ & + (1-P_o(E)) \frac{V_o}{V_1} \left[\Sigma_{oo}^{NR} + \frac{\Sigma_{os}^{IM} \left\{ P_o \Sigma_{oo}^{NR} + (1-P_1(E)) \frac{V_1}{V_o} \Sigma_1 \right\}}{\left(1 - P_o(E) \frac{\Sigma_{os}^{IM}(E)}{\Sigma_{ot}(E)} \right) \Sigma_{ot}} \right] \frac{\bar{\phi}}{E \Sigma_{1t}} \quad (8) \end{aligned}$$

Assume $(1-P_0) V_0/V_1$ is small (this is a good assumption for isolated lumps), and $P_1 \approx 1$, so for a moderator without absorption $\phi_1(E) \approx \bar{\phi}/E$.

We define the effective absorption cross section by

$$\sigma_{a, \text{eff}} = \int \sigma_a \phi_0 dE \quad (9)$$

with $\bar{\phi} = 1/\xi \Sigma_s$, where

$$\xi \Sigma_s = \frac{1}{V_0} \left[V_0 \xi_0 \Sigma_{p0} + V_1 \xi_1 \Sigma_{s1} \right] \quad (10)$$

to normalize the asymptotic flux to unit source.

The connection between the resonance escape probability p and $\sigma_{a, \text{eff}}$ is taken to be

$$p = \exp \left[- \frac{N_0}{\xi \Sigma_s} \sigma_{a, \text{eff}} \right] \quad (11)$$

Using the reciprocity relation

$$(1-P_1) V_1 \Sigma_1 = (1-P_0) V_0 \Sigma_0 \quad (12)$$

to obtain P_1 , and substituting in Equation (9) gives

$$\sigma_{a, \text{eff}} = \int \frac{1-P_0(E) \left[1 - \frac{\Sigma_{00}^{\text{NR}}}{\Sigma_{0t}} \right]}{1-P_0(E) \frac{\Sigma_{0s}^{\text{IM}}}{\Sigma_{0t}}} \sigma_{a0} \frac{dE}{E} \quad (13)$$

So for NR scattering, putting $\Sigma_{0s}^{\text{IM}} = 0$, gives

$$\sigma_{a, \text{eff}} = \int \left\{ 1 - P_0(E) \left[1 - \frac{\Sigma_{00}^{\text{NR}}}{\Sigma_{0t}} \right] \right\} \sigma_{ao} \frac{dE}{E} ,$$

(14)

$$= \int \frac{\sigma_{ao}}{\sigma_t} \left[\sigma_t (1 - P_0) + P_0 \sigma_p \right] \frac{dE}{E} .$$

The first term in the integral represents absorptions in the lump due to neutrons whose last collision was in the moderator. The second term represents absorption in the lump due to neutrons whose last collision is in the lump. A direct derivation of the above formula on this basis is given by Dresner in his thesis⁽⁶⁾. The separation of terms can also be made to correspond to a surface absorption and volume absorption term in the manner originally introduced by Wigner⁽⁷⁾. The last equation may be written:

$$\sigma_{a, \text{eff}} = \int \left[\frac{\sigma_{ao} \sigma_p + \sigma_{ao} (\sigma_t - \sigma_p) (1 - P_0)}{\sigma_t} \right] \frac{dE}{E} . \quad (15)$$

Let

$$A_v = \int \frac{\sigma_{ao} \sigma_p}{\sigma_t} \frac{dE}{E} \quad (16)$$

and

$$A_s = \int \frac{\sigma_{ao} (\sigma_t - \sigma_p)}{\sigma_t} (1 - P_0) \frac{dE}{E} . \quad (17)$$

Then

$$\sigma_{a, \text{eff}} = A_v + A_s . \quad (18)$$

The first term, A_v , corresponds to Wigner's volume absorption term, while the second term, A_s , roughly corresponds to the surface absorption term of Wigner's. However, the surface term is no longer simply proportional to S/M , the surface-to-mass ratio of the lump, since $1 - P_0$ depends on the lump geometry.

The analysis of the infinite mass case is not quite as straightforward. Recalling Equation (13) and setting $\Sigma_{00}^{NR} = 0$ in that equation gives

$$\sigma_{a, eff} = \int \left[\frac{1 - P_0(E)}{1 - P_0(E) \frac{\Sigma_{0s}^{IM}}{\Sigma_{0t}}} \right] \sigma_{ao} \frac{dE}{E} . \quad (19)$$

This approximation has been discussed by Bell⁽⁵⁾ among others. The QUERY program follows the infinite mass approximation formulation of Adler, Hinman and Nordheim which follows.

If the infinite mass scattering in the lump is small compared with Σ_{0t} , then

$$\sigma_{a, eff} \approx \int (1 - P_0) \sigma_{ao} \frac{dE}{E} . \quad (20)$$

This approximation means that only the contribution of neutrons originating in the moderator region has been taken into account. For metal rods there is still a small contribution due to slowing down of neutrons in the lump. In the lump, the asymptotic slowing down density is $\xi_0 \sigma_{po}$ and for heavy elements $\xi_0 = 2/A$. If it is assumed that all these neutrons are absorbed, the volume absorption term is $2\sigma_{po}/A$ so

$$I_{eff} = A_v + A_s$$

with

$$A_s = \int (1 - P_0) \sigma_{ao} \frac{dE}{E} \quad (21)$$

and

$$A_v = \frac{2}{A} \sigma_{po} . \quad (22)$$

This last equation can be given somewhat more theoretical justification than our derivation indicates. However, the detailed numerical comparisons given by Bell⁽⁵⁾ are perhaps the best justification of this form of the infinite mass approximation.

III. GEOMETRICAL ESCAPE PROBABILITIES FOR LATTICES

For isolated lumps and a constant isotropic flux in the lump, the collision probability $P_0(E)$ has been calculated exactly and tabulated in the work of Case, Placzek and deHoffman⁽⁸⁾. The tables of integrals for computing the effective resonance integral for isolated lumps prepared by Adler, Hinman and Nordheim make use of these exact collision probabilities.

For lattices with a low moderator-to-metal volume ratio, there will be a large interaction between fuel rods. A correction of the resonance integral for this effect is usually made by the Dancoff-Ginsburg method. Recently, G. I. Bell and W. Rothenstein have independently developed more accurate methods of calculating effective cross sections for lattices which take account of the interaction. The method due to Bell will be briefly reviewed here.

Bell has shown how the method of calculating effective absorption cross sections for isolated lumps can be generalized to lattices with closely spaced lumps. He obtained the simple result that the effective resonance absorption cross section for a lattice may be obtained from an isolated lump expression by replacing s_0 , the inverse average chord length in the lump, by a new quantity τ_0 where

$$\tau_0 = \frac{s_0 \Sigma_1}{\Sigma_1 + s_0 \frac{V_0}{V_1}} \quad (23)$$

The inverse average chord length $s_0 = S/4V_0$, where S is the surface area of the lump and V_0 is the volume of the lump. Σ_1 is the total cross section in the moderator region and V_1/V_0 is the moderator volume per unit lump volume. The quantity τ_0 may be interpreted as an effective cross section representing leakage from a lump. On the other hand,

$$\frac{1}{\tau_0} = \frac{1}{s_0} + \frac{V_0}{V_1} \cdot \frac{1}{\Sigma_1} \quad (24)$$

so $1/\tau_0$ may be interpreted as an average chord length equal to the average chord length in an isolated lump plus the fuel-to-moderator volume ratio multiplied by the mean free path in the moderator.

Bell's derivation of the above expression for τ_0 makes use of the so-called Wigner approximation to the neutron escape probability from a lump. The usual isolated lump formulas also depend upon this approximation. More exact expressions for the effective resonance absorption cross section for isolated lumps use the analytical expressions and tables⁽⁸⁾ for the lump escape probability. The more exact isolated lump formulas can be used to obtain the effective resonance absorption cross section for a lattice by replacing s_0 in these formulas by the τ_0 given in Equation (23). The resulting expression for the lattice appears to be a much better approximation than Bell's derivation of Equation (23) by the Wigner approximation would at first glance seem to imply.

Bell derived the following expression for the escape probability $(1-P_0)$ for a lump in a lattice

$$1-P_0 = (1-P_0^0) \frac{G_1}{1 - (1-G_1)(1-G_0)} \quad (25)$$

where P_i is the probability that a neutron originating uniformly in region i of a lattice makes its next collision in the same region (possibly after traversing the other region). The fuel region, $i = 0$, is made up of all the fuel lumps. It is not a connected region. The moderator region corresponds to $i = 1$. The P_i^0 are the corresponding probabilities for an isolated lump. Bell defines G_i as the probability that a neutron incident on region i makes a collision in region i before leaving. Bell's derivation of Equation (25) makes no use of the Wigner approximation to the quantities P_i and G_i .

Bell next shows that $1-P_0$ may be approximated by $\tau_0(\Sigma_0 + \tau_0)^{-1}$ with τ_0 as given by Equation (23) if one approximates $(1-P_0^0)$, $(1-G_0)$, and $(1-G_1)$ by the Wigner approximation, namely

$$(1-P_0^0) = \frac{s_0}{\Sigma_0 + s_0} \quad 26-a$$

$$(1-G_0) = \frac{s_0}{\Sigma_0 + s_0} \quad 26-b \quad (26)$$

$$(1-G_1) = \frac{s_1}{\Sigma_1 + s_1} \quad 26-c$$

with $s_1 = S/4V_1 = s_0 V_0/V_1$, since Equation (26) substituted into Equation (25) gives

$$(1-P_0) \text{Wigner approximation} = \tau_0/(\Sigma_0 + \tau_0) \quad (27)$$

Instead of using Equation (27), $1-P_0$ may be approximated by $1-P_c(\Sigma_0/2\tau_0)$. Here, and throughout this note, P_c denotes the "exact" geometrical capture probability for a slab, cylinder, or sphere (as the case may be) given analytically and tabulated in Reference 8. The motivation for this is two-fold. First, one might conjecture that $1-P_c(\Sigma_0/2\tau_0)$ is a better approximation to the escape probability of a lump in a lattice than the Wigner approximation just as $1-P_c(\Sigma_0/2s_0)$ is a better approximation than the Wigner approximation for an isolated lump. Secondly, the function $1-P_c(t)$ appears under the integral in the isolated lump expressions which have been tabulated⁽²⁾ with t as a parameter. Thus, the use of this form for the escape probability for a lattice allows the use of these tables for lumps in a lattice.

To test the above conjecture, Equation (25) has been evaluated for cylinders in a hexagonal lattice approximating G_1 by

$$G_1 = (1-6C) \quad (28)$$

with $(1-6C)$ the usual Dancoff expression⁽⁹⁾ with $n = 6$, and

$$G_0 = \left[1-P_c\left(\frac{\Sigma_0}{2s_0}\right) \right] \frac{\Sigma_0}{s_0} \quad (29)$$

and

$$P_o^0 = P_c \left(\frac{\Sigma_o}{2s_o} \right). \quad (30)$$

With these substitutions, Equation (25) becomes

$$1 - P_o = \left[1 - P_c \left(\frac{\Sigma_o}{2s_o} \right) \right] \frac{1 - 6C}{1 - 6C \left(1 - \left[1 - P_c \left(\frac{\Sigma_o}{2s_o} \right) \right] \frac{\Sigma_o}{s_o} \right)}. \quad (31)$$

The value of C in Equation (28) was computed from the curves given in Reference 9.

In Figure 1, $[1 - P_o]$, (Wigner approximation) given by Equation (27) and $1 - P_c(\Sigma_o/2\tau_o)$ are compared with $1 - P_o$ as given by Equation (31) for three different moderator-to-fuel volume ratios. For all three volume ratios, it is evident that $1 - P_c(\Sigma_o/2\tau_o)$ is the better approximation to Equation (31). The results of a Monte Carlo calculation made at Brookhaven are also shown for the 1/4" rod and for a .600" rod.

Bell's method gives the correct homogeneous limit, i. e., when $S/4V_o \rightarrow \infty$. The modified Bell method does not give the exact homogeneous limit. In the isolated rod limit, when $(V_1 \rightarrow \infty)$, $\tau_o \rightarrow s_o$, Bell's method gives the Wigner approximation for an isolated rod while the modified Bell method gives the exact isolated rod collision probability.

The above "modification of Bell's method" can be interpreted in the following way⁽¹⁰⁾: the quantity $1 - nC = 1 - T$, where nC is the usual Dancoff correction, is the probability that a neutron entering the moderator makes a collision in the moderator. Thus, T is the moderator escape probability. Using the Wigner rational approximation

$$T \approx \frac{1}{1 + \frac{\Sigma_1}{s_1}},$$

where

$$s_1 = \frac{S}{4V_1}$$

is the inverse chord length in the moderator. Or, writing

$$s_0 = \frac{S}{4V_0}$$

$$T \approx \frac{s_0 \frac{V_0}{V_1}}{\Sigma_1 + s_1 \frac{V_0}{V_1}} \frac{V_1}{V_0} \frac{1}{\Sigma_1} \tau_0$$

$$T \approx \frac{V_1}{V_0} \frac{1}{\Sigma_1} \tau_0$$

So the "modified Bell method" amounts to using the exact isolated rod escape probability function with an effective chord length determined by a Wigner rational approximation to the Dancoff correction.

Another approximation for P_0 , the collision probability for lumps in lattices, has been proposed by Bakshi⁽¹¹⁾, and independently by Nordheim⁽¹⁰⁾.

$$P_0 = P_c \left(\frac{1}{2} \frac{\Sigma_0}{s_0 [1-T]} \right) \text{ (Bakshi)}$$

with $T = \sum_i c_i$ the Dancoff correction for neighboring rods.

Putting $\bar{r} = 1/\tau$ and $\bar{r}_0 = 1/s_0$

$$P_0 = P_c \left(\frac{1}{2} \frac{\bar{r}_0 \Sigma_0}{[1-T]} \right) \text{ (Bakshi)}$$

So

$$\bar{r}_{\text{eff}} = \frac{\bar{r}_0}{1-T}$$

is the effective chord length by Bakshi's method. The Dancoff correction is calculated on the assumption that the rods are black, i. e., that $\Sigma_0 \rightarrow \infty$. Thus, Bakshi's approximation has the correct "black limit" ($\Sigma_0 \rightarrow \infty$).

IV. CALCULATION OF EFFECTIVE ABSORPTION CROSS SECTIONS FOR LATTICES WITH METAL RODS

An IBM-704 computer program called QUERY⁽³⁾ has been developed to facilitate the calculations. For metal fuel, the program is based upon Equations (16, 17, 21, and 22). To include the effect of Doppler broadening of the resonances, the Doppler line shape ψ is used so:

$$\sigma_a = \frac{\Gamma_Y}{\Gamma} \sigma_0 \psi(\xi, x) \quad (32)$$

$$\sigma_{rs} = \frac{\Gamma_R}{\Gamma} \sigma_0 \psi(\xi, x) \quad (33)$$

with

$$\psi(\xi, x) = \frac{\xi}{\sqrt{4\pi}} \int_{-\infty}^{\infty} \frac{\exp \left[- (\xi^{2/4})(x-y)^2 \right]}{1+y^2} dy \quad (34)$$

where

$$x = \frac{2(E-E_i)}{\Gamma} \quad (35)$$

and

$$\xi = \frac{\Gamma}{\left(\frac{4E_i kT}{A+1} \right)^{1/2}} \quad (36)$$

$$\sigma_o = \frac{2.6 \times 10^6}{E_i} \frac{\Gamma_n}{\Gamma} \quad (37)$$

With these substitutions, Equations (16) and (17) become:

$$\text{NR} \quad \left\{ \begin{array}{l} A_{v,i} = \frac{\sigma_p \Gamma_Y}{E_i} J(\xi, \beta) \end{array} \right. \quad (38)$$

$$\text{NR} \quad \left\{ \begin{array}{l} A_{s,i} = \frac{\sigma_o \Gamma_Y}{E_i} L(t, \xi, \beta) \end{array} \right. \quad (39)$$

$$\text{NR} \quad \left\{ \begin{array}{l} \text{with } t = N_o \sigma_p \frac{1}{\tau_o}, \beta = \frac{\sigma_p}{\sigma_o} \end{array} \right. \quad (40)$$

and Equations (21) and (22) become:

$$\text{IM} \quad \left\{ \begin{array}{l} A_{v,i} = \frac{2\sigma_{po}}{A} \end{array} \right. \quad (41)$$

$$\text{IM} \quad \left\{ \begin{array}{l} A_{s,i} = \frac{\sigma_o \Gamma_Y}{E_i} L'(t'', \xi) \end{array} \right. \quad (42)$$

$$\text{IM} \quad \left\{ \begin{array}{l} \text{with } t'' = N \sigma_{ao} \frac{1}{\tau_o} \end{array} \right. \quad (43)$$

The functions J, L and L' above are defined by

$$J(\xi, k) = \int_0^\infty \frac{\psi(\xi, x)}{\psi(\xi, x) + \beta} dx \quad (44)$$

$$L(\xi, k, t) = \int_0^\infty P_o \left\{ t \left(\frac{\psi(\xi, x)}{\beta} + 1 \right) \right\} \frac{[\psi(\xi, x)]^2}{\psi(\xi, x) + \beta} dx \quad (45)$$

$$L', (\xi, j) = \int_0^\infty P_o \left\{ t'' \psi(\xi, x) \right\} \psi(\xi, x) dx \quad (46)$$

In the above:

σ_p = the off-resonance scattering cross section in the lump
(potential scattering)

$\sigma_{ao} = \frac{\Gamma_Y}{\Gamma} \sigma_o$, where σ_o is the total resonance cross
section at the resonance peak,

and j is defined by $t''/2 = 2^{-j} \times 10^4$. The functions J , L and L' have been computed and tabulated over a range of their parameters by Adler, Hinman, and Nordheim⁽²⁾. The part of the QUERY computer program for the resolved resonance range is essentially an interpolation routine for using these tables.

The classification of resonances as NR or IM was taken to be the same as the classification for homogeneous mixtures. The resonance parameters were taken from the 1955 edition of BNL-325 in order to compare with Monte Carlo calculations which use these parameters. The resonances at 6.68, 21, 36.9, 66.3, 103.5, 192 ev were taken to be IM with respect to U-238 scattering; all others were considered to be NR.

V. RESONANCE CAPTURE IN URANIUM OXIDE ROD LATTICES

From Equations (16, 17, and 18) above, the effective absorption cross section in the NR approximation was given by

$$\sigma_{a, eff} = A_v + A_s$$

with

$$A_v = \int \frac{\sigma_{ao}\sigma_p}{\sigma_t} \frac{dE}{E}$$

and

$$A_s = \int \frac{\sigma_{ao}(\sigma_t - \sigma_p)}{\sigma_t} (1-P_o) \frac{dE}{E} .$$

For the $P_o(E)$ the exact isolated rod escape function $P_o(\Sigma_{ot}/2\tau_o)$ is used. As in the metal rod case, τ_o is the inverse effective chord length. When the absorption cross section with Doppler broadening is substituted into these equations, A_v and A_s may be written

$$A_{v,i} = \frac{\sigma_p \Gamma_\gamma}{E_i} J(\xi, \beta) \quad (47)$$

$$A_{s,i} = \frac{\sigma_p \Gamma_\gamma}{E_i} L(t, \xi, \beta) \quad (48)$$

with

$$t = N_o \sigma_p \frac{1}{\tau_o} \quad (49)$$

and

$$\beta = \frac{\sigma_p}{\sigma_o} \quad (50)$$

In Section I above, Equation (13), the effective absorption cross section for both NR and IM scattering was given by

$$\sigma_{a, eff} = \int \frac{1 - P_o(E) \left[1 - \frac{\Sigma_{oo}^{NR}}{\Sigma_{ot}} \right] \sigma_{ao}}{1 - P_o(E) \frac{\Sigma_{os}^{IM}}{\Sigma_{ot}}} \frac{dE}{E} \quad (13)$$

If the infinite mass approximation is made for the U-238 in the oxide rod and the NR approximation made for the oxygen in the oxide, then Σ_{oo}^{NR} should be set equal to Σ_m , the total cross section of the oxygen in the oxide. The last equation may now be written

$$\sigma_{a, eff} = \int \frac{\Sigma_m \sigma_{ao}}{\Sigma_{ot} - P_o \Sigma_{os}^{IM}} \frac{dE}{E} + \int \frac{\{\Sigma_{ot} - P_o(E) [\Sigma_{ot} - \Sigma_m] - \Sigma_m\} \sigma_{ao}}{\Sigma_{ot} - P_o \Sigma_{os}^{IM}} \frac{dE}{E} \quad (51)$$

and since $\Sigma_{ot} - \Sigma_m = \Sigma_{ao}$,

$$\sigma_{a, eff} = \int \frac{\Sigma_m \sigma_{ao}}{\Sigma_{ot} - P_o \Sigma_{os}^{IM}} \frac{dE}{E} + \int \frac{\Sigma_{ao}(1 - P_o(E)) \sigma_{ao}}{\Sigma_{ot} - P_o \Sigma_{os}^{IM}} \frac{dE}{E} . \quad (52)$$

Since $\Sigma_{os}^{IM} \ll \Sigma_{ot}$ the last equation may be approximated by

$$\sigma_{a, eff} = \int \frac{\Sigma_m \sigma_{ao}}{\Sigma_{ot}} \frac{dE}{E} + \int \frac{\Sigma_{ao}(1 - P_o(E)) \sigma_{ao}}{\Sigma_{ot}} \frac{dE}{E} . \quad (53)$$

For $P_o(E)$ one may use the exact isolated rod function P_c for the collision probability with the inverse effective chord length τ_o . For the oxide fuel rods in the IM approximation, the argument of P_c should be $\Sigma_{ao}/2\tau_o$ in place of $\Sigma_{ot}/2\tau_o$ as for the NR case. This is because in the IM approximation, a collision with the fuel no longer removes the neutron from the resonance region.

Substituting the Doppler broadened cross sections gives

$$\sigma_{a, eff} = A_{vi} + A_{si}$$

with

$$A_{vi} = \frac{\sigma_m \Gamma}{E_i} J(\xi, \beta') \quad (54)$$

and

$$A_{si} = \frac{\sigma_m \Gamma}{\beta'} \frac{1}{E_i} L(t', \xi, \beta') \quad (55)$$

oxide IM

where

$$\beta' = \frac{\sigma_m \Gamma}{\sigma_o \Gamma_\gamma} \quad \text{and} \quad t' = \frac{N \sigma_m}{\tau_o} . \quad (56)$$

VI. CALCULATION OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR THE UNRESOLVED RESONANCE RANGE

In the unresolved resonance range, all resonances are narrow and the NR approximation is used. An effective absorption cross section for an energy range from E_1 to E_2 is obtained by integrating the expressions for $(\sigma_a)_{\text{eff}}$ in the NR approximation over the energy range and dividing by the average distance between resonances D . Before this integration is performed, an integration of the effective absorption cross section for a resonance with peak at energy E over a Porter-Thomas distribution of neutron widths is performed. The Porter-Thomas distribution of neutron widths is given by:

$$P(y)dy = (2\pi y)^{-1/2} \exp(-y/2) dy \quad (57)$$

where

$$y = \frac{\Gamma_n^0}{\langle \Gamma_n^0 \rangle}, \quad (58)$$

and $\langle \Gamma_n^0 \rangle$ is the average reduced neutron width. The I/β or J functions defined above are averaged over the Porter-Thomas distribution to give:

$$\bar{J}(E) = \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{e^{-y/2}}{\sqrt{y}} J(\xi, \beta) dy \quad (59)$$

$$\left(\frac{\bar{L}}{\beta} \right) \frac{1}{\sqrt{2\pi}} \int_0^\infty \frac{e^{-y/2}}{\sqrt{y}} \frac{L(\xi, \beta, z)}{\beta} dy \quad (60)$$

where

$$\xi = \frac{1}{2} \sqrt{\frac{A}{kT}} \left(\langle \Gamma_n^0 \rangle y + \frac{\Gamma_\gamma}{E} \right) \quad (61)$$

$$\beta = \frac{\sigma_p}{2.6 \times 10^6} \left(E + \frac{\Gamma_\gamma \sqrt{E}}{y \langle \Gamma_n^0 \rangle} \right) \quad (62)$$

and

$$z = \frac{1}{2} N \sigma_p \bar{r} \quad (63)$$

Then integrating over an unresolved energy range gives

$$A_v = \frac{\sigma_p \Gamma_\gamma}{D} \int_{E_1}^{E_2} \frac{\bar{J}(E)}{E} dE \quad (64)$$

and

$$A_s = \frac{\sigma_p \Gamma_\gamma}{D} \int_{E_1}^{E_2} \left(\frac{\bar{L}(E)}{\beta(E)} \right) \frac{dE}{E} \quad (65)$$

as the volume and surface contributions to the effective absorption cross section.

VII. COMPARISON OF CALCULATIONS BY THE NR-NRIA METHOD WITH MONTE CARLO CALCULATIONS

A. Lattices

As mentioned in the introduction, two of the most useful methods of calculating resonance escape are the narrow resonance approximation and the Monte Carlo method. (The term "narrow resonance method" will be used in the following to denote a calculation made using the NR approximation for all resonances except the six broad resonances of U-238 named above; for the latter, the NRIA approximation is always used.)

The Monte Carlo method is inherently capable of giving much more accurate results since it can be made as accurate a model of the slowing down process as the cross section measurements allow. However, it is extravagant with computer time if results with a high degree of statistical confidence are desired. The narrow resonance approximation has been shown to give surprisingly good agreement with isolated lump experiments^{(10), (12)} at least for U-238 systems. The equivalences and appropriate equivalences between homogeneous, isolated lump and lattice resonance integrals developed with the narrow resonance approximation by Dresner⁽⁶⁾, Bakshi⁽¹¹⁾, and Bell⁽⁵⁾ and others is also a useful means of correlating measurements made on different systems. It thus appears useful to compare calculations made by these two methods.

Calculations have been made by both methods for a range of water moderated lattices both with U-238 metal and UO_2 rods of circular cross sections. The calculations of effective absorption cross sections were made using the same set of 18 resolved resonances given in the 1955 edition of BNL-325. The choice of the old cross sections is of no consequence for this comparison. The Monte Carlo calculations were all made using the NYU computer code⁽¹⁾.

Using either the modified Bell method or the Bakshi method, the effective absorption cross section is a function of an inverse effective chord length τ divided by the fuel density ρ . Thus, using either of these effective chord length methods, a single curve gives the effective absorption cross section for isolated rods and for all lattices with a given fuel type but with different water-to-fuel volume ratios and fuel rod sizes. In particular, the curve for $(\sigma_a)_{\text{eff}}$ is plotted as a function of $2\sqrt{\tau_0/\rho}$, which is an effective $\sqrt{S/M}$. In using these curves, the τ for a given lattice may be calculated either by the modified Bell method or by Bakshi's method.

In Figures 2 and 3, the Monte Carlo results are plotted for the τ corresponding to the lattice using the modified Bell method to compute τ . In Figures 4 and 5, each Monte Carlo result is plotted at three different abscissae, corresponding to three different ways used to compute τ for each lattice. A Monte Carlo point plotted at τ' calculated by the Bakshi method using six nearest neighbors has a stroke / through the point. When τ is calculated by the Bakshi method using 18 neighbors, it is denoted τ'' and the Monte Carlo point has a stroke \ through it. When τ is calculated by the modified Bell method it is denoted simply τ and the Monte Carlo point is plotted with no stroke through the symbol. Table I gives the computed τ , τ' , τ'' . The Monte Carlo calculations, also for rods in a hexagonal lattice, are shown in Table II.

It is very difficult to obtain Dancoff Corrections by interpolation of the curves given in the original Dancoff-Ginsburg report⁽⁹⁾. Instead, the Dancoff corrections have been obtained from the curves given in a paper by Namias⁽¹³⁾. The calculations have been checked using the curves in CP-2157 and agree as well as interpolation and extrapolation of the latter curves allow.

The comparison of inverse effective chord length, τ , calculated by the Bell method and by use of Dancoff corrections (Bakshi method) is shown graphically in Figure 6 and in Table I. In Figure 6 the abscissa is τ calculated by the Bell method and the solid line is τ

(by the Bell method). The points with a stroke / are inverse effective chord lengths calculated using the Dancoff corrections due to the six nearest neighbors in a hexagonal lattice. Points with a stroke \ through the point are inverse effective chord lengths calculated using the Dancoff corrections due to the 18 nearest neighbors. (This is essentially the correction due to the twelve nearest neighbors.) No account is taken of the screening of next nearest neighbors by nearest neighbors. The "proper" Dancoff corrected τ presumably lies somewhere between a pair of points / and \ having the same abscissa.

At a water-to-fuel volume ratio of 4, there should be little screening effect on the next-to-nearest neighbors. Thus, the points marked ∇ should have nearly the corrected Dancoff corrections due to 12 nearest neighbors.

The 4 to 1 volume ratio points marked ∇ lie very nearly on a straight line which passes through the origin. This line has been drawn on Figure 6 and labelled τ''' . The deviation of a point marked \ from this straight line should give a measure of the screening of next nearest neighbors by nearest neighbors. This deviation is especially apparent on a very dry lattice with small rods. For example; the point marked \ with abscissa 0.5077 which corresponds to a lattice with rods of radius .3175 cm (= .25 inches diameter) and a water-to-fuel volume ratio equal to 0.5. The indication is that for this lattice, the next-to-nearest neighbors are completely screened by the nearest neighbors, and that the proper Dancoff correction should take account of the six nearest neighbors only. The curved line in Figure 6 is drawn through points with constant rod size = .3175 cm radius. Similar curves can be drawn for other rod sizes.

The conclusions which may be drawn from this comparative analysis are:

1. For lattices with water-to-fuel ratios of unity or less, the calculation of effective chord lengths by the Dancoff method involves uncertainties which make it difficult to apply.
2. The Bell method of calculating effective chord lengths ($1/\tau$) and thus effective surface-to-mass ratios, $(S/M)_{\text{eff}} = 4\tau/\rho$, gives good agreement with corresponding Monte Carlo calculations over a wide range of lattice parameters (rod sizes and water-to-metal ratios) for both oxide and metal fuel rods.

The inverse effective chord length τ may also be obtained from a series of one-speed transport calculations of capture probabilities for different fuel region absorption cross sections followed by a fitting of the resulting curve (as a function of rod absorption cross section) to the exact isolated rod escape probability curve by a suitable choice of τ .

A comparison has been made of escape probabilities for cylinders in a lattice as a function of absorber cross section calculated by the Legendre polynomial P-3 approximation, by the double Legendre polynomial P-1 approximation for cylinders (dP_1)⁽¹⁴⁾, by diffusion theory, by the Bell method, by the modified Bell method and by the Monte Carlo method (the latter calculations were done at the Brookhaven National Laboratory) by W. Rothenstein⁽¹⁵⁾. The results are shown in Table III.

The P-3 calculations were performed by a P-3 cylinder transport code for the IBM-704 developed at Combustion Engineering, Inc.⁽¹⁶⁾. The double P-1 calculations were made using a modification of the above code to solve the double P-1 equations.

B. Homogeneous Mixtures

The QUERY code has been used to calculate effective absorption cross sections for homogeneous mixtures of uranium oxide and water with water-to-oxide ratios equal .5, 1, and 2. Corresponding Monte Carlo results were obtained by running two region problems with the same mixture in each region. The results are shown in Table IV-A. Similar results for homogeneous metal-water mixtures are shown in Table IV-B.

C. Temperature Dependence

Calculations using the QUERY code have been made for a range of temperatures for both metal and oxide cylindrical fuel rod lattices with circular cross sections. The results are shown in Figures 7 and 8. By reading $(\sigma_a)_{eff}$ at the various temperatures for a constant $2\sqrt{\tau_0/\rho}$ on Figure 7 or 8 then plotting the results on Figure 9 or 10 as a smooth curve, the $(\sigma_a)_{eff}$ for any effective surface-to-mass ratio ($=4\tau_0/\rho$) and any combination of moderator and rod temperatures may be obtained. In these calculations, the 54 resolved resonances of U-238 given in Reference 17 were used. The interval 1 kev to 30 kev was chosen for the unresolved range. The absorption due to s-wave scattering was calculated for this range using the QUERY code as indicated above. The average spacing between levels, D , was taken as average from Reference 17.

Additional average barns were added to account for p-wave absorption in the range 1 to 30 kev as calculated by Rothenstein⁽¹⁵⁾. Finally, again following Reference 15, one barn was added to account for absorption above 30 kev.

Two Monte Carlo results at 3,000°K have been compared with corresponding QUERY calculations for lattices with metal rods. The results are summarized in Table V-A. Two similar comparisons for lattices with oxide rods are shown in Table V-B.

In their 1958 Geneva Conference paper, Richtmyer, Van Norton and Wolfe⁽¹⁾ give the results of Monte Carlo calculations of the resonance escape probability for a lattice at three different temperatures. Calculations covering the same temperature range have been made using the QUERY program. A comparison of the results is shown in Figure 11. The original Monte Carlo calculation included the unresolved range from 1 to 10 kev. The additional absorption from 10 kev up as calculated using the QUERY code has been added to the original result for the purpose of comparison.

D. Resonance by Resonance Comparison with Monte Carlo

A comparison of QUERY with Monte Carlo calculations resonance by resonance is shown in Figures 12 to 15. The symbols on the graphs have the same meaning as in Figure 13. The Monte Carlo code edit gives the absorption in an energy range. For U-238 using the first 18 resonances and the 1955 parameters, an energy range includes only a single resonance for the first 15 resonances. The highest energy range includes three resonances, when the upper energy cut-off is at 438 ev. Thus, there is only an approximate between the NR or NRIA calculated absorption for a single resonance (or small group of resonances) and the Monte Carlo calculated absorption in the neighborhood of the peak energy. Nevertheless, the comparison shows fair agreement between the NR and NRIA calculation and the Monte Carlo. Large fluctuations in the Monte Carlo for a single resonance are apparent especially in resonances with small absorption.

VIII. COMPARISON WITH EXPERIMENT

The resonance escape probability between the energies E_1 and E_2 may be defined as the ratio of the slowing down density at energy E_1 to the slowing down density at E_2 .

$$p(E_1, E_2) = \frac{q(E_2)}{q(E_1)} \quad (66)$$

or

$$p(E_1, E_2) = \frac{q(E_2)}{q(E_2) + \text{capture in } (E_1, E_2)} \quad (67)$$

Considering U-238 as the only absorber present, one can then define the resonance escape probability for a U-238 lattice by:

$$p = \frac{q_c}{q_c + \Sigma_{ar}^{28} \phi_r} \quad (68)$$

as is done by Klein et al⁽¹⁸⁾, for example. In the above expression, q_c is the density of neutrons slowing down part of the cadmium cut-off energy E_{Cd} per second; $\Sigma_{ar}^{28} \phi_r$ is the epicadmium radiative capture in U-238 and is equal to

$$\int_{E_{Cd}}^{\infty} \Sigma_a^{28}(E) \phi(E) dE \quad (69)$$

Transforming the equation for p gives:

$$\frac{1-p}{p} = \frac{\Sigma_{ar}^{28} \phi_r}{(q)_c} = pfR \quad (70)$$

where

$$\rho = \frac{\text{radiative capture in U-238 above cadmium cut-off energy}}{\text{radiative capture in U-238 below cadmium cut-off energy}}$$

f = thermal utilization

R = ratio of radiative capture in U-238 in the thermal neutron region to total thermal neutron capture in the fuel.

An experimental p is defined by the last equation when R is determined from cross section values, while ρ and f are determined from experiment. From an experimentally derived resonance escape probability p an experimental effective absorption cross section can be defined by:

$$(\sigma_a)_{\text{eff}}^{\text{exp}} = - \overline{\xi \sigma_s} \ell_{\text{np exp}} \quad (71)$$

When the uranium fuel is slightly enriched with U-235, the measured ratio p is not the same as it would be if only U-238 were present because of the competition between U-238 and U-235 epithermal capture. To compare experimental results with calculation of the resonance escape probability which does not include the effect of U-235 absorption, the experimental determination of p by the above formula may be approximately corrected to what it would be in the absence of U-235.

Results obtained by several different experimental groups have been compared with theoretical calculations using the modified Bell method. The measurements on metal-water lattices were done at the Brookhaven National Laboratory⁽¹⁹⁾ and at the Westinghouse Bettis Plant⁽¹⁸⁾. The uranium oxide-water results are from Bettis experiments on TRX lattices, and Westinghouse experiments on Yankee lattice and BR-3 lattices⁽²⁰⁾. The results obtained from Brookhaven had already been corrected for enrichment and leakage effects. The method of correction is described in Reference 21. The other experimental results had not been corrected for enrichment or leakage effects. An enrichment effect correction was made on these experimental values as follows. The theoretical resonance escape probability for the given lattice was used in two slowing down calculations using the MUFT-IV slowing down code⁽²²⁾. One calculation was made with no U-235 present. The second calculation was made with U-235 in the amount present in the experimental lattice. The MUFT code treats U-235 as having a smooth cross section, and to that extent gives the effect on the neutron energy spectrum of competitive absorption by U-238 and U-235. From the two calculations, a percent change in p^{28} due to the presence of U-235 was calculated. This percent effect was used to "correct" the experimental values of p^{28} to zero enrichment. No correction for leakage effects was made.

The comparison of the corrected experimental results with theory is shown in Figures 16 and 17. In both figures, vertical dashed lines connect points corresponding to lattices which were the same except for U-235 enrichment.

IX. DISCUSSION

The deviation between calculations of the resonance escape probability in U-238 water lattices by different theoretical methods is smaller than the deviations that exist between calculations and experimental determinations of resonance escape. Indeed there is considerable scatter in the experimental results themselves.

In all of the above analysis, the fuel rod cladding has been treated as a void. H. Kouts⁽²³⁾ has suggested that a more careful analysis of the effect of the cladding may improve the agreement of experiment and theory especially for the drier metal lattices with 1/4" fuel rods. In general, as suggested by J. Chernick⁽²⁴⁾, it would appear that a more refined analysis of experimental results will be necessary to obtain agreement with theoretical calculations of resonance escape.

Appendix

For the convenience of those who prefer to use the 1955 resonance parameters of U-238, curves similar to Figures 7 and 8 but using the 1955 parameters are given in Figures 18 and 19.

The component parts of the absorption curves plotted in Figures 7 and 8 are shown in Figures 20 to 25. In the latter figures, the following notation is used:

- *1. contribution of the first 21 resolved resonances
- 2. contribution of the 22nd to 54th resolved resonance
- 3. contribution of $\ell = 0$ unresolved resonances in the range 1,000 to 30,000 ev
- 4. unresolved resonances above 30,000 ev .8 barns
p-wave scattering in 1,000 to 30,000 ev range .83 barns
1.63 barns

The data contained in Figure 8 for oxide lattices including the resolved and unresolved range using the 1958 parameters has been plotted somewhat differently in Figure 26 to show the Doppler temperature coefficient.

*Observe that 1. covers the same energy range using the new parameters as Figures 7 and 8 cover using the 1955 parameters.

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Table I

Effective Inverse Chord Lengths

$\frac{V_w}{V_f}$	Rod Radius	τ	$6C_1$	$6C_2$	$6C_3$	τ'	τ''
.5	.3175 cm	.5077	.64857	.11672	.06868	.55343	.26146
	.762003	.3498	.43026	.014496	.005154	.37385	.36095
	2	.1874	.108708	0	0	.22282	.22282
1.0	.3175	.7678	.416844	.06868	.046968	.91835	.73623
	.762003	.4563	.198768	.005154	.008784	.52574	.51660
	2	.2143	.020565	0	0	.24486	.24486
2.0	.3175	1.0323	.234000	.05088	.03207	1.206	1.0757
	.762003	.5383	.067806	.006016	.002268	.61168	.60624
	2	.2307	.00228	0	0	.24943	.24943
3.0	.3175	1.166	.14625	.03207	.02001	1.3445	1.2625
	.762003	.5726	.02334	.002268	.001215	.64086	.63857
	2	.2368	0	0	0	.25	.25
4.0	.3175	1.247	.09675	.02274	.016824	1.4224	1.3601
	.762003	.5914	.009054	.001248	.000228	.65023	.64926
	2	.2400	0	0	0	.25	.25

Note:

C_1 is the Dancoff correction due to a nearest neighbor at distance d_1 .

C_2 is the Dancoff correction due to a next-to-nearest neighbor at distance $\sqrt{3}d_1$.

C_3 is the correction due to a neighbor at distance $2d_1$.

τ is by Bell's method.

τ' is by Dancoff using 6 neighbors.

τ'' is by Dancoff using 18 neighbors.

value 570

Table II-A

Resonance Escape Probability
for 18 Resolved Resonances
for Metal U-238 Lattices
from Monte Carlo

<u>V_{H_2O}/V_U</u>	<u>0.5</u>		<u>1.0</u>	
Rod Radius	Monte Carlo		Monte Carlo	
	<u>p</u>	<u>PE of p*</u>	<u>p</u>	<u>PE of p*</u>
.318 cm	.6001	.004	.7318	.0035
.762	.6417	.004	.7769	.003
2.0	.7172	.0035	.8319	.003

<u>V_{H_2O}/V_U</u>	<u>2.0</u>		<u>3.0</u>	
Rod Radius	Monte Carlo		Monte Carlo	
	<u>p</u>	<u>PE of p*</u>	<u>p</u>	<u>PE of p*</u>
.318 cm	.8253	.003	.8714	.003
.762	.8689	.003	.9076	.002
2.0	.9124	.002	.9402	.002

<u>V_{H_2O}/V_U</u>	<u>4.0</u>			
Rod Radius	Monte Carlo			
	<u>p</u>	<u>PE of p*</u>		
.318 cm	.8969	.0025		
.762	.9341	.002		
2.0	.9545	.002		

*PE of p denotes the probable error in the Monte Carlo calculation.

Table II-B

Resonance Escape Probability
for 18 Resolved Resonances
for Oxide Lattices
from Monte Carlo Results

<u>V_{H_2O}/V_{UO_2}</u>	<u>0.5</u>		<u>1.0</u>		<u>2.0</u>	
Rod Radius	Monte Carlo		Monte Carlo		Monte Carlo	
	<u>p</u>	<u>PE of p*</u>	<u>p</u>	<u>PE of p*</u>	<u>p</u>	<u>PE of p*</u>
.318	.683	.004	.793	.003	.872	.003
.762	.710	.004	.821	.003	.901	.003
2.0	.763	.004	.865	.003	.927	.002

*PE of p is the probable error of p.

Table III-A

Escape Probabilities for Cylinders in Water
(Hexagonal Lattice)
Rod Diameter 0.25"; vol. of water/vol. of fuel = 1

<u>$\Sigma_0 l_0$</u>	<u>P_1</u>	<u>P_3</u>	<u>dP_1</u>	<u>Bell</u>	<u>Modified Bell</u>	<u>Bakshi</u>	<u>Monte Carlo</u>
0.5	.636	.616	.605	.493	.578	.614	.572 + .004
1.0	.456	.432	.426	.327	.400	.427	.397 + .003
1.5	.351	.327	.325	.245	.295	.319	.304 + .003
2.0	.283	.261	.260	.196	.231	.251	.248 + .002
3.0	.201	.184	.184	.140	.159	.174	.173 + .002
4.0	.155	.141	.141	.108	.120	.132	.133 + .002
6.0	.105	.096	.095	.075	.080	.089	.088 + .002

Table III-B

Escape Probabilities for Cylinders in Water
(Hexagonal Lattice)
Rod Diameter 0.60"; vol. of water/vol. of fuel = 1

<u>$\Sigma_0 l_0$</u>	<u>Bell</u>	<u>Modified Bell</u>	<u>Bakshi</u>	<u>Monte Carlo</u>
0.5	.581	.676	.706	.691 + .004
1.0	.410	.498	.535	.522 + .004
1.458	.316	.394	.430	.422 + .003
2.0	.258	.312	.344	.346 + .003
3.0	.188	.221	.248	.250 + .002
4.0	.145	.170	.192	.194 + .002
6.0	.104	.115	.130	.133 + .002
8.0	.080	.086	.098	.100 + .002

Reduce 84%

Table IV-A

Comparison of Analytical and Monte Carlo Results
for Homogeneous Uranium Oxide-Water Mixtures
at 68°F (18 resolved resonances)

	<u>V_{H_2O}/V_{UO_2}</u>		
	<u>.5</u>	<u>1</u>	<u>2</u>
Analytical p	.644	.737	.805
Monte Carlo p	.652	.743	.803
Monte Carlo probable error of p	.004	.004	.0035
Analytical $(\sigma_a)_{eff}$	13.56	18.51	26.18
Monte Carlo $(\sigma_a)_{eff}$	13.19	18.06	26.44

Table IV-B

Comparison of Analytical and Monte Carlo Results
for Homogeneous Uranium Metal-Water Mixtures
at 68°F (18 resolved resonances)

	<u>.5</u>	<u>1</u>	<u>2</u>	<u>3</u>	<u>4</u>
<u>V_{H_2O}/V_U</u>					
Analytical p	.5520	.6559	.7383	.7778	.8021
Monte Carlo p	.5533	.6654	.7461	.7818	.8054
Monte Carlo probable error of p	.004	.004	.004	.004	.0035
Analytical $(\sigma_a)_{eff}$	8.71	12.36	17.79	22.09	25.85
Monte Carlo $(\sigma_a)_{eff}$	8.67	11.94	17.17	21.64	25.37

Table V-A

Effect of Doppler Broadening on
Resolved Resonances
Metal-Water Lattices

volume water/volume U-238 = .5; rod radius = .762 cm

	<u>p at 293°K</u>	<u>p at 3,000°K</u>
Monte Carlo	.6417	.6091
Probable Error of Monte Carlo	.004	.004
QUERY	.6454	.6110

Monte Carlo $\frac{\Delta p}{p_{293^{\circ}}} \cdot \frac{1}{\Delta T} = -1.88 \times 10^{-5}/^{\circ}\text{C}$, probable error = $.33 \times 10^{-5}$

QUERY $\frac{\Delta p}{p_{293^{\circ}}} \cdot \frac{1}{\Delta T} = -1.97 \times 10^{-5}/^{\circ}\text{C}$

volume water/volume U-238 = 4; rod radius = .762 cm

	<u>p at 293°K</u>	<u>p at 3,000°K</u>
Monte Carlo	.9341	.9212
Probable Error of Monte Carlo	.002	.002
QUERY	.9316	.9216

Monte Carlo $\frac{\Delta p}{p_{293^{\circ}}} \cdot \frac{1}{\Delta T} = -.510 \times 10^{-5}/^{\circ}\text{C}$, probable error = $.11 \times 10^{-5}$

QUERY $\frac{\Delta p}{p_{293^{\circ}}} \cdot \frac{1}{\Delta T} = -.401 \times 10^{-5}$

Table V-B

Effect of Doppler Broadening on
Resolved Resonances
Oxide-Water Lattices

volume water/volume of $\text{UO}_2 = 1.0$; rod radius = .762 cm

	<u>p at 293°K</u>	<u>p at 3,000°K</u>
Monte Carlo	.8208	.7796
Probable Error of Monte Carlo	.003	.0035
QUERY	.8197	.7810

$$\text{Monte Carlo } \frac{\Delta p}{p_{293^\circ}} \cdot \frac{1}{\Delta T} = -1.85 \times 10^{-5}/^\circ\text{C}, \text{ probable error} = .27 \times 10^{-5}$$

$$\text{QUERY } \frac{\Delta p}{p_{293^\circ}} \cdot \frac{1}{\Delta T} = -1.74 \times 10^{-5}/^\circ\text{C}$$

volume water/volume of $\text{UO}_2 = 2.0$; rod radius = .762 cm

	<u>p at 293°K</u>	<u>p at 3,000°K</u>
Monte Carlo	.9014	.8830
Probable Error of Monte Carlo	.0025	.003
QUERY	.9044	.8742

$$\text{Monte Carlo } \frac{\Delta p}{p_{293^\circ}} \times \frac{1}{\Delta T} = -.7541 \times 10^{-5}/^\circ\text{C}, \text{ probable error} = .21 \times 10^{-5}$$

$$\text{QUERY } \frac{\Delta p}{p_{293^\circ}} \times \frac{1}{\Delta T} = -1.23 \times 10^{-5}/^\circ\text{C}$$

Table VI

"1958 Resonance Parameters"
for U-238

The resonance parameters for U-238 used in all calculations described as using "1958 parameters" are listed below together with the approximation used (i. e., either NR or IM). A constant $\Gamma_V = 2.46 \times 10^{-2}$ ev is used for each resonance.

<u>Resonance No.</u>	<u>Approximation</u>	<u>E₀ in ev</u>	<u>Γ_n in ev</u>
1	IM	6.7000	1.5200(-3)
2	IM	2.1000(1)	8.9000(-3)
3	IM	3.6900(1)	3.2500(-2)
4	IM	6.6300(1)	2.5000(-2)
5	NR	8.1300(1)	2.1000(-3)
6	NR	9.0000(1)	9.0000(-5)
7	IM	1.0250(2)	6.5000(-2)
8	NR	1.1650(2)	1.5000(-2)
9	NR	1.4560(2)	8.0000(-4)
10	NR	1.6520(2)	3.5000(-3)
11	IM	1.8960(2)	1.3500(-1)
12	NR	2.0850(2)	5.5000(-2)
13	NR	2.3750(2)	3.2000(-2)
14	NR	2.6450(2)	2.3000(-4)
15	NR	2.7400(2)	2.7000(-2)
16	NR	2.9100(2)	1.9000(-2)
17	NR	3.1150(2)	10.0000(-4)
18	NR	3.4800(2)	4.5000(-2)
19	NR	3.7700(2)	1.5000(-3)
20	NR	3.9850(2)	10.0000(-3)
21	NR	4.1100(2)	1.7000(-2)
22	NR	4.3500(2)	1.4000(-2)
23	NR	4.5500(2)	7.0000(-4)
24	NR	4.6400(2)	7.0000(-3)
25	NR	4.7900(2)	4.5000(-3)
26	NR	4.9000(2)	10.0000(-4)
27	NR	5.1900(2)	3.7000(-2)
28	NR	5.3600(2)	5.4000(-2)
29	NR	5.5700(2)	10.0000(-4)
30	NR	5.8100(2)	4.2000(-2)

Table VI
(Continued)

<u>Resonance No.</u>	<u>Approximation</u>	<u>E₀ in ev</u>	<u>Γ_n in ev</u>
31	NR	5.9600(2)	6.6000(-2)
32	NR	6.0500(2)	6.0000(-4)
33	NR	6.2100(2)	3.9000(-2)
34	NR	6.2900(2)	9.0000(-3)
35	NR	6.6200(2)	1.2500(-1)
36	NR	6.8000(2)	1.3000(-3)
37	NR	6.9500(2)	5.3000(-2)
38	NR	7.1000(2)	1.7000(-2)
39	NR	7.2300(2)	1.4700(-2)
40	NR	7.3200(2)	4.2500(-3)
41	NR	7.6600(2)	9.0000(-3)
42	NR	7.8200(2)	3.0000(-3)
43	NR	7.9200(2)	1.1000(-2)
44	NR	8.2500(2)	6.0000(-2)
45	NR	8.5500(2)	1.3000(-1)
46	NR	8.5900(2)	6.0000(-2)
47	NR	8.6700(2)	2.2000(-3)
48	NR	8.9600(2)	1.3000(-3)
49	NR	9.0900(2)	9.0000(-2)
50	NR	9.2800(2)	3.7000(-2)
51	NR	9.4000(2)	1.9500(-1)
52	NR	9.6000(2)	1.9500(-1)
53	NR	9.8300(2)	10.0000(-4)
54	NR	9.9500(2)	4.0000(-1)

Table VII

Comparison of τ Calculated by Bell Method
and by Curve Fitting

τ_B is by Bell Method; τ by fitting using two largest values of Σ_0/s_0 ;
 τ' using all chosen values of Σ_0/s_0 .

<u>Transport Approximation</u>	<u>$\frac{v_{\text{water}}}{v_{\text{fuel}}}$</u>	<u>Rod Radius. (cm)</u>	<u>τ</u>	<u>τ'</u>	<u>τ_B</u>
DOBLP	0.5	.3175	.4782	.4890	.5077
CEPTR	0.5	.3175	.4965	.5051	.5077
DOBLP	1.0	.3175	.8244	.83542	.7678
CEPTR	1.0	.3175	.8660	.8724	.7678
DOBLP	4.0	.3175	1.7525	1.7203	1.247
CEPTR	4.0	.3175	1.7547	1.643	1.247
DOBLP	0.5	2.0	.2124		.1874
CEPTR	0.5	2.0	.2285		.1874
DOBLP	1.0	2.0	.2450		.2143
CEPTR	1.0	2.0	.2567		.2143
DOBLP	4.0	2.0	.2742		.2400
CEPTR	4.0	2.0	.2540		.2400
CEPTR	0.5	.762	.4032	.4050	.3498
CEPTR	1.0	.762	.5675	.5656	.4563
CEPTR	4.0	.762	.7273	.7236	.5914

GEOMETRICAL ESCAPE PROBABILITIES

FIG. 1-a

43

reduce 590

GEOMETRICAL ESCAPE PROBABILITIES

FIG. I-b

44

reduce 5%

GEOMETRICAL ESCAPE PROBABILITIES

FIG. 1-c

45

Reference 5-7

GEOMETRICAL ESCAPE PROBABILITIES

FIG. 1-d

46

Figure 1-d

47
reduce 1070

FIG. II. METAL RODS AT 20° C

Fig. 2. - $(\sigma_a)_{eff}$ FOR U-238 METAL, WATER LATTICES AT 20° C

Fig. 3.- $(\sigma_a)_{eff}$ FOR UO_2 , WATER LATTICES AT $20^\circ C$

Fig. 4 — $(\sigma_a)_{eff}$ FOR U-238 METAL WATER LATTICES AS FUNCTIONS OF τ_0, τ', τ''

Fig. 5— $(\sigma_a)_{eff}$ FOR UO_2 WATER LATTICES AS FUNCTIONS OF τ_0, τ', τ''

Fig. 6- τ_0, τ', τ'' AS A FUNCTION OF τ_0

Fig. 7— $(\sigma_a)_{eff}$ FOR U-238 METAL WATER LATTICES INCLUDING RESOLVED AND UNRESOLVED RESONANCES USING THE 1958 RESONANCE PARAMETERS

52

Reduce 570

822 51

Fig. 8— $(\sigma_d)_{\text{eff}}$ FOR UO_2 WATER LATTICES INCLUDING RESOLVED AND UNRESOLVED RESONANCES USING THE 1958 RESONANCE PARAMETERS

53

reduce 570

622 58

Fig. 9— $(\sigma_a)_{eff}$ AS A FUNCTION OF TEMPERATURE FOR U-238 METAL, WATER LATTICES (SAME DATA AS IN Fig. 7)

54

Volume 570

622 59

Fig. 10— $(\sigma_d)_{eff}$ AS A FUNCTION OF TEMPERATURE FOR UO_2 , WATER LATTICES (SAME DATA AS IN FIG. 8)

Fig. II - COMPARISON OF NR-NRIA RESONANCE INTEGRAL WITH
RICHTMYER MONTE CARLO AT VARIOUS TEMPERATURES

Fig. 12 COMPARISON OF QUERY CALCULATIONS WITH MONTE CARLO FOR INDIVIDUAL RESONANCES FOR VARIOUS UO_2 , WATER LATTICES

Fig. 13 COMPARISON OF QUERY CALCULATIONS WITH MONTE CARLO FOR INDIVIDUAL RESONANCES FOR VARIOUS UO_2 , WATER LATTICES

Fig. 14 COMPARISON OF QUERY CALCULATIONS WITH MONTE CARLO FOR INDIVIDUAL RESONANCES FOR VARIOUS UO_2 , WATER LATTICES

Fig. 15 COMPARISON OF QUERY CALCULATIONS WITH MONTE CARLO FOR INDIVIDUAL RESONANCES FOR VARIOUS UO_2 , WATER LATTICES

61
Fig.16- RESONANCE INTEGRAL FOR URANIUM METAL, WATER LATTICES;
COMPARISON WITH EXPERIMENT

Fig. 17-RESONANCE INTEGRAL FOR UO_2 , WATER LATTICES;
COMPARISON WITH EXPERIMENT

62

value 10^4

Fig. 18 - THE EFFECTIVE ABSORPTION CROSS SECTION FOR U-238 METAL, WATER LATTICES (18 RESOLVED RESONANCES OF U-238 IN BNL-325, 1955)

63

value 570

622 68

Fig.19— THE EFFECTIVE ABSORPTION CROSS SECTION FOR UO_2 , WATER LATTICES (18 RESOLVED RESONANCES OF U-238 IN BNL-325, 1955)

64

reference 590

622 69

Fig.20— THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR U-238 METAL, WATER LATTICES

65-

reduce 5%

622

70

Fig.21 - THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR U-238 METAL, WATER LATTICES

66

Adams 590

622 71

Fig.22 —THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR U-238 METAL, WATER LATTICES

Fig.23 — THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR UO_2 , WATER LATTICES

68

reduce 5%

622 73

Fig. 24— THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR UO_2 , WATER LATTICES

69

reduce 570

622 74

Fig.25 — THE COMPONENT PARTS OF THE EFFECTIVE ABSORPTION CROSS SECTION FOR UO_2 , WATER LATTICES

170

reduce 570

622 75

11

Value 540

622 75

Fig. 26 — THE DOPPLER TEMPERATURE
COEFFICIENT FOR VARIOUS
UO₂, WATER LATTICES