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WAPD-TM-1468

DOE Research and Development Report

A Successive Collision Calculation of Resonance Absorption

(AWBA Development Program)

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July 1980

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Prepared for the
U.S. Department of Energy
By Westinghouse Electric Corporation
Under Contract No. DE-AC11-76-PN00014

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Printed in the United States of America
Available from the
National Technical Information Service
U. S. Department of Commerce
5285 Port Royal Road
Springfield, Virginia 22151

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NOTICE

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ABSTRACT

The successive collision method for calculating resonance absorption solves numerically the neutron slowing down problem in reactor lattices. A discrete energy mesh is used with cross sections taken from a Monte Carlo library. The major physical approximations used are isotropic scattering in both the laboratory and center-of-mass systems. This procedure is intended for day-to-day **analysis** calculations and has been incorporated into the current version of MUFT. The calculational model used for the analysis of the nuclear performance of LWBR includes this resonance absorption procedure. Test comparisons of results with RCP01 give very good agreement.

FOREWORD

The Shippingport Atomic Power Station located in Shippingport, Pennsylvania was the first large-scale, central-station nuclear power plant in the United States and the first plant of such size in the world operated solely to produce electric power. This program was started in 1953 to confirm the practical application of nuclear power for large-scale electric power generation. It has provided much of the technology being used for design and operation of the commercial, central-station nuclear power plants now in use.

Subsequent to development and successful operation of the Pressurized Water Reactor in the Atomic Energy Commission (now Department of Energy, DOE) owned reactor plant at the Shippingport Atomic Power Station, the Atomic Energy Commission in 1965 undertook a research and development program to design and build a Light Water Breeder Reactor core for operation in the Shippingport Station.

The objective of the Light Water Breeder Reactor (LWBR) program has been to develop a technology that would significantly improve the utilization of the nation's nuclear fuel resources employing the well-established water reactor technology. To achieve this objective, work has been directed toward analysis, design, component tests, and fabrication of a water-cooled, thorium oxide-uranium oxide fuel cycle breeder reactor for installation and operation at the Shippingport Station. The LWBR core started operation in the Shippingport Station in the Fall of 1977 and is expected to be operated for about 4 to 5 years. At the end of this period, the core will be removed and the spent fuel shipped to the Naval Reactors Expended Core Facility for a detailed examination to verify core performance including an evaluation of breeding characteristics.

In 1976, with fabrication of the Shippingport LWBR core nearing completion, the Energy Research and Development Administration, now DOE, established the Advanced Water Breeder Applications (AWBA) program to develop and disseminate technical information which would assist U. S. industry in evaluating the LWBR concept for commercial-scale applications. The program is exploring some of the problems that would be faced by industry in adapting technology confirmed in the LWBR program. Information being developed includes concepts for commercial-scale prebreeder cores which would produce uranium-233 for light water breeder cores while producing electric power, improvements for breeder cores based on the technology developed to fabricate and operate the Shippingport LWBR core, and other information and technology to aid in evaluating commercial-scale application of the LWBR concept.

All three development programs (Pressurized Water Reactor, Light Water Breeder Reactor, and Advanced Water Breeder Applications) are under the technical direction of the Division of Naval Reactors of DOE. They have the goal of developing practical improvements in the utilization of nuclear fuel resources for generation of electrical energy using water-cooled nuclear reactors.

Technical information developed under the Shippingport, LWBR, and AWBA programs has been and will continue to be published in technical memoranda, one of which is this present report.

Revised 1-17-80

A SUCCESSIVE COLLISION CALCULATION OF RESONANCE ABSORPTION

E. Schmidt
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INTRODUCTION AND MOTIVATION

Deterministic procedures to estimate epithermal neutron resonance absorption in day to day nuclear analysis calculations evolved during the 1954-1960 period. The limitations of computer speed and architecture of that period certainly influenced what was reasonable to compute. These procedures were incorporated into MUFT(1,12), which is a multigroup slowing down spectrum program.

Resonance absorption in MUFT is based on a resonance escape model with the resonance absorption rate in MUFT multigroup m being given by $q^{m-1}(1-\rho^m)$ where q^{m-1} is the slowing down density at the top of group m and ρ^m the resonance escape probability for group m. ρ^m is in turn given by $e^{-RI^m_{hom}}$ where RI^m_{hom} is the resonance integral in group m with subscript hom referring to the homogeneous value. Finally RI^m_{hom} can be constructed from microscopic data in the MUFT library which lists resonance integrals for each resonance in group m.

This is certainly a simple model for computational purposes. However many simplifying assumptions are contained in this model. Some of the more significant simplifications are: no resonance overlap, no heterogeneous effects, the library data is not Doppler broadened, and only hydrogen moderation is permitted. In recognition of the effect of these simplifying assumptions, the

MUFT program provides for correction in the form of an L factor which can be applied as a multiplier on the RI_{hom} for each nuclide. For most applications the usefulness of MUFT depended on the analyst's ability to determine these L factors such that ρ^m accurately gave the desired relation to q^{m-1}. Both analytic(2) and later Monte Carlo(13) programs were used to determine effective L factors.

Later, a spatially dependent slab cell capability was incorporated into MUFT. This model, provided by Candelore and Gast(3), was designed to calculate L factors which accounted for resonance overlap, Doppler Broadening, and slab lattice heterogeneity. This corrects many of the assumptions in the MUFT calculation that result from the use of the RI_{hom}. The principal remaining difficulties were then: restriction to hydrogenous moderation only and an overly restricted heterogeneous capability which excluded rod lattices. The computed L factors were averaged over energy ranges including many MUFT multigroups.

Methods that rely on using this L factor type of correction can become quite complex. If correct resonance absorption rates are to be preserved for each multigroup using the relation,

$$RI_{het} \equiv L\ RI_{hom} \tag{1}$$

then each isotope requires an L factor for each multigroup. In addition the homogeneous resonance integrals must be subdivided among the multigroups to properly localize the absorption. Current practice isolates the homogeneous integral to the multigroup containing the resonance peak energy E_i.

The method described in this report departs from previous procedures since the use of L-factors is abandoned entirely for repeating lattice arrays. Instead a direct computation is made of a proper resonance escape probability per nuclide per MUFT group by using a space-energy shielded flux shape computed over the entire resonance energy range (5.531 keV down to 0.625 eV by MUFT convention) and, as input, a true Doppler broadened line shape profile generated by whatever formalism is appropriate to the particular resonance nuclides of interest. An excellent source for such profiles is a Monte Carlo library, such as generated by RCPL1(15). The spatial heterogeneities are treated within the confines of integral transport theory assuming infinite lattice arrays. This method offers various refinements over similar earlier generation methods used in the computer programs ZUT and TUZ(4) as well as WIMS(5) and RABBLE(6). The major modelling assumptions are:

(a) scattering is isotropic in both the laboratory and center of mass systems,

(b) all scattering and slowing down sources are spatially flat within distinct lattice zones, and

(c) all elements contribute to neutron moderation.

The programs referred to above are primarily analysis tools to be used for special calculations as the limitations of their computation systems permit. The method presented here is intended for use in day to day calculations on current computers.

Assumption b, commonly referred to as the flat flux approximation is the most significant assumption remaining for systems in which the spatial flux undergoes large variation. The flat flux approximation causes a redistribution of neutrons in a strongly space-shielded zone away from the surface areas where most of the actual scattering occurs. This results in an overestimate of the reaction rates for such absorbers. In principle this error can be made as small as desired by subdividing such zones. Initial experience with this model indicates that it generates quite accurate results. Typical errors in practical lattice design problems are less than 1% in resonance reaction rate for saturated absorbers and substantially less for the others. The method is currently included in the LWBR calculational model. Extensive comparisons of resonance reaction rates calculated for LWBR lattices with Monte Carlo, RCP01$^{(13)}$ and PAX, a program containing an updated version of MUFT along with this resonance model, are presented in an LWBR report (Ref. 14).

THE DISCRETE METHOD FOR THE SUCCESSIVE COLLISION CALCULATION

Briefly, the successive collision calculation solves for the space-energy fluxes in a reactor lattice throughout the energy range of interest. The energy dependent integral Boltzmann equation is solved for this purpose under the simplifying physical assumptions a-c mentioned above. A discrete numerical flux solution is obtained at discrete energy and spatial mesh points. The spatial mesh consists of zones in the lattice. The reaction rates for each isotope are determined from these space-energy fluxes. A useful feature of this method is that it divides naturally into three independent subdivisions. These are the library and energy mesh, the slowing down model, and the first collision transfer probability model. Each of these subdivisions can be improved either in physics modelling or numerically without having to change the other two. A more detailed description of these subdivisions will now be given.

THE ENERGY MESH

The energy mesh to be used is derived from the energy mesh in the Monte Carlo library. It is assumed implicitly that the Monte Carlo mesh is adequate for our purposes in both representing resonance line shapes and for slowing down integral calculations. The obvious choice of mesh for this discrete calculation is to use the full Monte Carlo mesh. However, if this results in excessive computing times, some reduction of mesh is desirable. A uniform reduction would not be satisfactory since essential detail in line shapes could be lost. An algorithm has been devised that evaluates the relative importance of each mesh point and retains or rejects that point accordingly. Such a reduced mesh is thus tailored to the specific isotopes present in the library and in this sense would be part of the library since its use might not extend to other isotopes not in the library.

The selection process proceeds by selecting some isotope in the library and constructing its accumulative resonance integral to each point E_n in the Monte Carlo energy mesh

$$I_n = \int_{E_n}^{E_1} \frac{\sigma_a \, dE}{E} \qquad (2)$$

using in this case trapezoidal rule with the starting point E_1. The integral due to omitting points starting with E_2 is now determined. When the relative difference between the fine and coarse integral exceeds some accuracy criterion the last point E_k omitted is selected for the reduced mesh. This procedure is now repeated by omitting E_{k+1} and measuring the integrals from E_k. Such a process can be seen to control the local truncation error in the resonance integral over the reduced mesh for the particular isotope. The accuracy criterion is further modified to reflect the relative contribution of the coarse mesh interval to the total resonance integral. In this way the mesh is more concentrated where significant absorption occurs. So as not to skip minor resonances completely, all maximum and minimum points from the original mesh are retained. After the mesh is determined for a given isotope the next isotope is examined in a similar manner except that all points already accepted are now automatically retained. This results in filling in only the gaps as necessary to adequately represent this isotope. This process is continued until all isotopes have been processed. The final mesh is actually a function of the order in which the isotopes are processed and not the union of the meshes from each isotope determined independently. Finally, points are added that are convenient for editing purposes and for filling any gaps left that would be too large to properly represent scattering integrals for the heaviest isotope in the library.

If the Monte Carlo library contains a representation for unresolved resonances a corresponding method for reducing the mesh must be determined. The Monte Carlo library contains a cross section value at each point that is randomly selected from the unresolved distributions. There are no continuous profiles for such a distribution although trapezoidal integrals are still meaningful. Any subset of this distribution is acceptable if the reduced set is renormalized so as to retain the resonance integral of the fine mesh values.

In practice a uniform subset is selected and, when more than one isotope is treated as unresolved, the same subset is used for all. A more formal description of this algorithm is given in the appendix. The RCPL1 program generates this file for PAX which is used in conjunction with the XAP(15) library for smooth cross sections.

While the final mesh is tailored to the RCPL1 library, it is not equivalently tailored to the actual problem. This is so because the effective resonance profile, averaged over a lattice reflects saturation effects, which flattens the strong absorption peaks. This has the effect of accentuating the resonance wings where a broader mesh was selected. When saturation effects are anticipated it is advisable to calculate at least once with the full Monte Carlo mesh for the purpose of evaluating any effects due to mesh reduction.

THE SLOWING DOWN CALCULATION

The method for treating neutron moderation is based on the initial assumption of isotropic scattering in the center of mass system. The normalized kernel for this type of scattering is

$$P(E \rightarrow E') = \begin{cases} \dfrac{1}{(1-\alpha)E} & E \geq E' \geq \alpha E \\ 0 & E < E' \text{ or } E' < \alpha E \end{cases} \qquad (3)$$

with $\alpha \equiv \left(\frac{M-n}{M+n} \right)^2$ where M is the target mass and n the neutron mass. A useful property of this kernel is that the outscattering probability per unit energy is constant over the range allowed. This permits the source levels due to neutron scattering to be stored in an accumulative manner for each spatial zone in the lattice. In order to further describe this technique it is first necessary to describe the method adopted for energy integrations. Reaction rate calculations are carried out at the discrete points of the energy mesh. However, the source levels for these calculations are integrals over precisely defined energy ranges whose end points will not correspond exactly with this discrete mesh. Since the final results of this calculation are the integrated absorption rates for all isotopes, the integration scheme for scattering integrals is effectively defined by the absorption rate integrations. The trapezoidal rule was chosen for this purpose. This is equivalent to adopting a group scheme with cut points that lie between the entries of the discrete mesh. The contribution to a scattering integral from a given mesh point thus becomes proportional to the fraction of the group that lies within the energy range of integration. The outscatter distribution from the initial energy point is defined in this manner using the normalized integral. The source levels are constant for those energy "point groups" below the initial energy point that lie entirely within the allowed range from E_i to αE_i. The point group in which αE_i falls is reduced fractionally. Also that fraction of the initial group below E_i is accounted for by treating it as in-group scattering. This numerical kernel is neutron conservative which is a necessary constraint to this method.

The accumulative source is determined by the ensuing prescription. Let S_i be the scattering collision density due to some given element at E_i. As part of this calculation the "in-group" scattering cross section

$$\sigma_{ss} = \frac{\sigma_s(E_i)}{(1-\alpha)E_i} \left(\frac{E_i - E_{i+1}}{2} \right) \tag{4}$$

is used for this element. The source at E_{i+1} is incremented by

$$\Delta q_{i+1} = \frac{S_i(E_{i-1} - E_{i+1})}{2(1-\alpha)E_i} . \tag{5}$$

This contribution is left in the source until group point k is reached where k is the group containing αE_i. The k^{th} point source is incremented by the negative value

$$\Delta q_k = \frac{-S_i}{(1-\alpha)E_i} \left[\alpha E_i - \frac{(E_{k+1} + E_k)}{2} \right] . \tag{6}$$

Finally the k+1 source is incremented negatively by Δq_{k+1} where

$$\Delta q_{i+1} + \Delta q_k + \Delta q_{k+1} = 0 \tag{7}$$

and the source at E_{k+1} has no contribution left from initial energy E_i. This procedure requires an addition to the library of $\sigma_{ss}(E_i)$, k, and $\Delta q_k / S_i$ which can be either precomputed or determined as needed. While this method is used in actual calculations it should be noted that the in-group scattering and the end point corrections have no great physical significance. They are merely functions of the energy mesh and quadrature scheme used. An interesting alternative would be to use both degrees of freedom available here to retain an additional physical property; that of neutron conservation. An obvious choice would be to maintain the correct asymptotic flux solution for the given elemental scattering kernel. Under the initial isotropic scattering assumption the asymptotic flux is $1/E\ \Sigma_s(E)$. The in-group scattering and end point fraction are determined simultaneously to preserve both neutron balance and the correct asymptotic flux for an infinite medium containing only the specified scatterer. This method was found to be feasible but was not incorporated into these calculations since the simpler and faster trapezoidal method proved adequate.

The entire epithermal energy range is not in fact a true slowing down range. At the lower energies some upscattering due to thermal molecular motion and molecular binding is observed. Many resonance absorbers have effective cross sections that are high enough in energy to ignore upscattering effects. However, important 1/v cross sections, such as hydrogen and Boron as well as fuel materials with low energy resonances, are more sensitive. In order to include this effect, a modification to the slowing down equations was made for hydrogenous moderators only. This modification is approximated as follows. At epithermal energies the bound hydrogen outscattering approximates a distribution exhibiting a sharp elastic peak plus a slowing down shape of the form Erf $\left(\sqrt{\frac{E}{T^*}}\right)$ where T^* is a known kernel parameter called the effective temperature. For H_2O, T^* is about

0.12 eV and the error function is essentially unity for epithermal energies. The approximation is to regard the elastic peak as a delta function (or in this approximation as in-group scattering) and the remainder as regular slowing down. The infinite medium flux from such a kernel can be found from the balance equation with $\alpha = 0$ (since $M = n$).

$$\sigma_s{\downarrow}(E)\varphi_\infty(E) = \sigma_{fp}\int_E^\infty \frac{\mathrm{Erf}\left(\sqrt{\frac{E}{T^*}}\right)\varphi_\infty(E')}{E'}\,dE' \tag{8}$$

Here $\sigma_s{\downarrow}(E)$ is the slowing down part of the cross section

$$\sigma_s{\downarrow}(E) = \frac{\sigma_{fp}}{E}\int_0^E \mathrm{Erf}\left(\sqrt{\frac{E'}{T^*}}\right)dE' \simeq \sigma_{fp}\left(1 - \frac{T^*}{2E}\right) \tag{9}$$

where σ_{fp} is the free particle cross section which is energy independent. The approximation in equation 9 assumes $T^* \ll E$. If one uses the approximate $\sigma_s{\downarrow}(E)$ and lets $\mathrm{Erf}\left(\sqrt{\frac{E}{T^*}}\right)$ equal unity the balance equation becomes

$$\left(1 - \frac{T^*}{2E}\right)\varphi_\infty(E) = \int_E^\infty \frac{\varphi_\infty(E')dE'}{E'}\,. \tag{10}$$

This has for a solution $\varphi_\infty(E) = \frac{1}{E}\left(1 - \frac{T^*}{2E}\right)^{-2}$. Using typical values for an H_2O kernel, this solution is accurate to about 1% at 0.625 eV when compared to the correct solution for the original kernel(7). The actual computation uses a library value for hydrogen scattering and the above analysis requires that the library values have been modified to account for upscattering. A corresponding modification of the total scattering cross section is $\sigma_{fp}\left(1 + \frac{T^*}{2E}\right)$.

The same isotropic slowing down kernel also is used to determine the initial source levels and distributions. The initial source is from neutrons scattered last at energies above the top resonance energy considered. Asymptotic conditions are assumed to hold at these energies and the absorption free flux is proportional to 1/E and flat spatially. The resulting slowing down neutron sources at resonance energies are computed and used to initiate the accumulative source calculation process.

THE FIRST COLLISION TRANSFER MATRIX CALCULATION

The methods for determining the first collision transfer probability matrices over the lattice spatial zones are based on the initial assumptions that all neutron sources are isotropic in the laboratory system and uniform spatially in the originating zone. The transfer probability from one of the type I zones to all of the type J zones can be written symbolically.

$$P_{IJ} = \frac{1}{V_I} \int_{V_I} dr' \sum_{i=1}^{\infty} \int_{V_J(i)} K(r' \rightarrow r) dr \qquad (11)$$

where $K(r' \rightarrow r)$ is the isotropic first collision transport kernel. This kernel could be very complex even in a simple rod lattice. If a periodic lattice or infinite array of cells can be defined, then by using cell or periodic boundary conditions through the use of periodic boundary conditions, the sum in P_{IJ} can be eliminated. This will always be the case for these computations. If the lattice element contains n zones, then there are $\frac{n(n-1)}{2}$ independent P_{IJ} values. This follows from neutron reciprocity and balance conditions.

$$(\Sigma V)_I \; P_{IJ} = (\Sigma V)_J \; P_{JI} \tag{12}$$

$$\sum_{J=1}^{n} P_{IJ} = 1 \tag{13}$$

where Σ is the total cross section and V the zone volume.

P_{IJ} has been evaluated for four distinct types of lattices. Three of these are rod lattices and the fourth a slab lattice. The first two rod lattices are made up of 4 zones consisting of a central rod, a possible void gap, a clad zone, and a moderator zone. Although rod, clad, and moderator are referred to for convenience, this does not restrict the material content of these zones as the procedure treats all zones equivalently. The zone boundaries are circular cylinders except for the lattice boundary which is either a symmetric hexagon or a square. The third rod lattice is actually a Wigner-Seitz cell with up to 8 concentric cylindrical zones. The Wigner-Seitz cell method replaces a geometrically complicated cell with a much simpler one preserving volumes. In this case the outer hexagonal or square cell boundary is replaced with a cylindrical one with the same volume. A white boundary condition is assumed which can be visualized as a one-for-one neutron exchange with an external isotropic infinite neutron bath. The slab lattice is straight forward with up to 8 zones.

The hexagonal and square rod lattices are too complex to attempt to evaluate the P_{IJ} integrals directly. A common approach here is to use Monte Carlo for this purpose. The Monte Carlo method is used but with systematic instead of random sampling. This is similar to the method used in the THERMOS(8) program. The Monte Carlo approach for such a problem would be to select starters randomly on the surface of the source zone and a random exiting direction Ω drawn from an isotropic Ω distribution. An initial weight is calculated based on the chord length in the source zone in the -Ω direction. This is called a surface source technique which can be used whenever the internal source spatial and angular distributions are known which of course is the case here. The particle is tracked through the lattice and the weights deposited in each zone contributed to the desired P_{IJ} values. The tracking is terminated when the particle weight has fallen below some specified small value. This can easily be sampled systematically by using a uniformly distributed set of Ω_i and a uniform set of surface points. The latter distribution is required since these lattices do not have cylindrical symmetry. This method was incorporated into the system by using modified tracking routines from the Monte Carlo program RESQ2$^{(1)}$ which treated similar geometries. However this method is too laborious to execute for each point in the energy mesh. Instead, tables were prepared over a discrete set of input cross ections in each zone which must span the range of cross section values encountered in the specific problem. Thus the calculation is carried out a few hundred times to prepare tables rather than a few thousand times which would be required for each energy point. The tracking routines in RESQ2 were limited to three nonvoid zones. This, plus potentially large computer storage requirements, is the reason for limiting the number of zones in these lattices.

The Wigner-Seitz cell can be calculated more directly using techniques similar to those in the PIJ$^{(10)}$ and RABBLE$^{(6)}$ programs. Here the transport line source kernel is used to determine the first collision probabilities for all neutrons traveling in a given vertical plane. These planar probabilities can be expressed using the K_{i3} function for which accurate rational polynomial approximations are available$^{(11)}$. The plane is then integrated numerically as it traverses the cell along some radius. This process also sweeps out all possible orientations because of the cylindrical symmetry and the P_{IJ} matrices follow directly. The procedure is carried out as if the cell were isolated and the probability of exiting through the boundary surface S is also recorded. The white boundary condition selected admits a surface to volume reciprocity relation of the form

$$(\Sigma V)_I \; P_{IB} = \frac{S}{4} \, P_{BI} \tag{14}$$

which determines the probability of neutrons entering from the external bath colliding in zone I. In equation 14, S is the surface area of the external zone B. This permits the determination of a matrix P^*_{IJ} that includes the effect of the white boundary and effectively converts the P_{IJ} matrix for an isolated nest to that of an infinite lattice within, of course, the Wigner-Seitz cell approximation.

$$P^*_{IJ} = \frac{P_{IJ} \; P_{IB} \; P_{BJ}}{1 - P_{BB}} \tag{15}$$

The slab lattice calculation can be done directly from the integral definition. The resulting P_{IJ} values can be expressed in terms of the two parameter function

$$F(y,x) = \int_1^\infty \frac{\left[1-e^{-(y-x)t}\right]\left[1-e^{-xt}\right]}{1-e^{-yt}} \, \frac{dt}{t^3} \qquad x \leq y \tag{16}$$

Let the optical thickness of slab zone I = τ_I. Then we define τ_A as the optical thickness of the zones between I and J and τ_B the optical thickness of the zones in the lattice element but external to I and J. The thickness of the entire lattice element Δ is then

$$\Delta = \tau_I + \tau_J + \tau_A + \tau_B \qquad (17)$$

and we have

$$P_{IJ} = \frac{1}{2\tau_I}\left[F(\Delta, \tau_A+\tau_I) + F(\Delta, \tau_A+\tau_J) - F(\Delta, \tau_A) - F(\Delta, \tau_B)\right] . \qquad (18)$$

The function F(y,x) can be expressed in two convenient forms

$$F(y,x) = \frac{1}{2} - E_3(x) + \sum_{n=1}^{\infty}\left[2\ E_3(ny) - E_3(ny+x) - E_3(ny-x)\right] \qquad (19)$$

or

$$F(y,x) = x^2\left[\frac{1}{2}\ \ell n\left(\frac{2\pi x}{y}\right) - \frac{3}{4}\right] - \sum_{n=1}^{\infty}\left[\frac{B_n x^2}{2n(2n+2)!}\left(\frac{2\pi x}{y}\right)^{2n} - \frac{2y^{2n-1}}{(2n-3)!(2n)!}\ \varphi_{2n}\left(\frac{x}{y}\right)\right] \quad y<2\pi \qquad (20)$$

In the latter form B_n are Bernoulli numbers and $\varphi_{2n}(x)$ is defined

$$\varphi_{2n}(x) = x^{2n} - nx^{2n-1} + \binom{2n}{2} B_1 x^{2n-2} - \binom{2n}{4} B_2 x^{2n-4} + \ldots \qquad (21)$$

where $\varphi_{2n}(x)$ ends in x or x^2. The first series is useful for large y and the latter series for small y. If desired for more rapid computation, F(y,x) could be tabulated as it is a universal function that is problem independent.

MUFT USABLE RESULTS

The resonance integral method produces space-energy fluxes $\Phi(\underset{\sim}{x},E)$ for $E_B < E < E_T$ using the approximations previously discussed. This statement is totally independent of any MUFT formalism. If it is assumed for simplicity that the source of neutrons, q_T, slowing down past energy E_T is precisely unity, then all reaction rates are directly interpretable as probabilities of interaction.

Let $(AR)^m$ and $(AS)^m$ be the resonance and smooth macroscopic absorption probabilities for MUFT group m.

Thus,

$$(AR)^m = \int_X \int_{E_m}^{E_{m-1}} \Sigma_{a_{res}} (E,\underset{\sim}{x}) \; \Phi \; (E,\underset{\sim}{x}) \; dEd\underset{\sim}{x} \tag{22}$$

and

$$(AS)^m = \int_X \int_{E_m}^{E_{m-1}} \Sigma^m_{a_{sm}} (E,\underset{\sim}{x}) \; \Phi \; (E,\underset{\sim}{x}) \; dEd\underset{\sim}{x} \tag{23}$$

Then with $q_T = 1$,

$$q_m = q_{m-1} - (AR)^m - (AS)^m \quad . \tag{24}$$

The resonance absorption ρ is defined as

$$\rho^m = Exp(-RI^m_{het,a}) \tag{25}$$

and

$$RI^{m}_{het,a} = \ln(1-(AR)^{m}/q_{m-1}) \tag{26}$$

The isotopic distribution of the ρ's or alternatively the RI_{het}'s, are obtained from:

$$RI^{m,i}_{het,a} = \frac{(AR)^{m}_{i}}{(AR)^{m}} RI^{m}_{het,a} \tag{27}$$

where

$$(AR)^{m}_{i} = \int_{X} \int_{E_m}^{E_{m-1}} N_i(\underset{\sim}{x})\sigma_{a_{res}}(E)\ \Phi\ (E,\underset{\sim}{x})\ dE d\underset{\sim}{x} \tag{28}$$

However, if a particular lattice is very heterogenous then there exists a nontrivial amount of spatial shielding of the smooth cross sections also.

This resonance integral treatment computes the isotopes' resonance absorption and fission for the actual heterogenous lattice cells. This implicitly contains the effects of the space energy shielding of the smooth cross sections to within the accuracy of the integral transport used. This data would then be cast away by MUFT since it only accepts resonance escape information per nuclide per multigroup. However, if the "resonance escape" ρ were redefined to include all absorption and then the MUFT absorption $\Sigma^{m}_{a_{sm}}$ set to 0.0, MUFT would then preserve the slowing down density distribution as computed by the heterogenous resonance integral treatment exactly. Consequently, the following alternative treatment is possible. In the MUFT calculation set $\sigma^{i,m}_{a_{sm}}$ and $\sigma^{i,m}_{f_{sm}}$ equal to 0.0 for all multigroups and isotopes in the MUFT resonance range that is being explicitly computed by the new resonance treatment (usually 5.531 keV down to 0.625 eV). In the editing portion of the resonance integral calculation, trigger an option so that ρ is defined as the total absorption escape probability as follows:

$$\rho^{m} = \mathrm{Exp}\,(-RI^{*m}_{het,a}) \tag{29}$$

but

$$RI^{*m}_{het,a} = \ln(1 - [(AR)^{m} + (AS)^{m}]/q_{o}^{m-1}) \tag{30}$$

as opposed to

$$RI^{m}_{het,a} = \ln(1-(AR)^{m}/q_{o}^{m-1}). \tag{31}$$

Thus, the MUFT calculation will preserve the isotropic slowing down density q_o in the resonance range as calculated by the heterogenous resonance integral treatment. The version of MUFT contained in PAX will do either method; however, one slight difference will appear. The basic MUFT method does not include the concept of a scattering resonance shape; also, the infinite mass scattering has no effect on the MUFT computed flux Γ_o^m. The isotropic MUFT slowing down equation below the inelastic scattering energy range for the case of no buckling is given by

$$(\Sigma^{sma} + \Xi_{o})^{m}\,\frac{\Gamma_{o}^{m}}{\Delta^{m}} = \frac{-(1-\rho^{a,m})}{\Delta^{m}}\,q_{o}^{m-1} + \sum_{i}\,(K_{o})_{i}^{m}\,(q_{o})_{i}^{m-1} \tag{32}$$

but

$$(\Sigma^{sma})^m = 0.0 \text{ for this model} \tag{33}$$

and

$$(K_o)^m_i = \frac{2}{\Delta^m} \to \sum_i (K_o)^m_i \, (q_o)^{m-1}_i = \frac{2}{\Delta^m} \, q_o^{m-1} \, . \tag{34}$$

Thus

$$(\Xi_o)^m \, \Gamma^m_o = (1 + \rho^{a,m}) \, q_o^{m-1} \tag{35}$$

where

$$(\Xi_o)^m = \frac{2}{\Delta^m} \sum_{i \epsilon Iso} \overline{N}_i \, (\xi_o)^m_i \tag{36}$$

and

$\overline{N}_i$ is the homogenized cell number density and $(\xi_o)^m_i$ is the isotropic Grueling-Goertzel slowing down power.

A NUMERICAL EXAMPLE

As a test of the applicability of this discrete method, we give the following numerical example is given using LWBR seed and blanket rod lattices. The essential features of these calculations are given below. The Monte Carlo library contained six isotopes with resolved resonance shape cross section profiles. There were in all 386 resonances in the calculational range of 5531.0 to 0.625 electron volts. The Monte Carlo mesh contained 29,000 points. **Using an algorithm of the type described in tne appendix, this mesn was reduced to** about 5400 points. The LWBR rod lattice is hexagonal and was divided into **rod, clad, and moderator** zones. P_{IJ} tables were constructed for 162 points over the zone cross section sets. The systematically sampled Monte Carlo was carried out using 72 surface points around the zone perimeters and an angular mesh with 360 Ω_i. Resonance reaction rates were determined for the profile part of the cross section with this discrete method and with Monte Carlo for comparison purposes. The discrete method took 1.7 minutes and the Monte Carlo 60 minutes on the CDC 7600 computer. Table 1 gives the ratios of discrete to Monte Carlo reaction rates for each isotope. The figure in parentheses is the Monte Carlo 95% confidence interval in units of the last digit.

TABLE I

Resonance Reaction Rate Ratios in LWBR Seed and Blanket Lattices

	Seed		Blanket	
	$\frac{\text{Discrete}}{\text{Monte Carlo}}$			
Isotope				
U^{233}	0.9974	(46)	0.9977	(43)
U^{234}	1.0181	(346)	0.9785	(305)
U^{235}	0.9936	(114)	1.0061	(61)
Th^{232}	1.0110	(65)	1.0085	(61)
Zr	0.9982	(357)	0.9977	(252)
Pa^{233}	--		1.0042	(101)

It is to be noted that only the thorium ratios differ from unity by more than the 95% confidence intervals. This is due to the flat flux approximation together with the highly saturated nature of the thorium resonances in LWBR rods. The behavior of the ratios in Table I are typical of the experience with this method. The computational times for the discrete method are short enough to justify its use in conjunction with MUFT or MUFT type cross section programs without having to resort to separate resonance shielding calculations.

REFERENCES

1. R. L. Hellens, "Neutron Slowing Down in Group Diffusion Theory," WAPD-114 (1956).
2. S. Stein, "Resonance Capture in Heterogeneous Systems," WAPD-139 (1955).
3. N. R. Candelore and R. C. Gast, "Doppler-Broadened Resonance Absorption in Heterogeneous Systems Containing Several Resonance Materials for a Number of Slab and Particle Geometries in Water," p. 1, WAPD-BT-26 (1962).
4. G. Kuncir, "A Program for the Calculation of Resonance Integrals," GA-2525 (1961).
5. Proceedings of the Conference on the Application of Computing Methods to Reactor Problems, p. 51, ANL-7050 (1965).
6. P. H. Kier and A. A. Robba, "RABBLE, A Program for Computation of Resonance Absorption in Multiregion Reactor Cells," ANL-7326 (1967).
7. N. Corngold, "Chemical Binding Effects in the Thermalization of Neutrons," Annals of Physics <u>11</u>, 338 (1960).
8. H. C. Honeck, "THERMOS, A Thermalization Transport Theory Code for Reactor Lattice Calculations," BNL-5826 (1962).
9. B. L. Anderson, E. M. Gelbard, and J. Spanier, "RESQ2, A Combined Analytic Monte Carlo Calculation of Resonance Absorption Based on Super Position," WAPD-TM-665 (1967).
10. Proceedings of the Conference on the Application of Computing Methods to Reactor Problems, p. 93, ANL-7050 (1965).
11. I. Gargantini, T. Pomentale, "Rational Chebyshev Approximations to Bessel Function Integrals," Comm. ACM, Vol. 7, p. 727 (1964).

REFERENCES (Cont'd)

12. H. Bohl Jr., and A. P. Hemphill, "MUFT-5 - A Fast Neutron Spectrum Program for the Philco 2000," WAPD-TM-218 (1961).

13. N. R. Candelore, R. C. Gast, and L. A. Ondis II, "RCP01 - A Monte Carlo Program for Solving Neutron and Photon Transport Problems in Three-Dimensional Geometry with Detailed Energy Description," WAPD-TM-1267 (1978).

14. L. B. Freeman, editor, "The Calculational Model Used in the Analysis of Nuclear Performance of the Light Water Breeder Reactor (LWBR)," WAPD-TM-1314 (1978).

15. A. V. Dralle, N. R. Candelore, and R. C. Gast, "RCPL1 - A Program to Prepare Neutron and Photon Cross-Section Libraries for RCP01," WAPD-TM-1268 (1978).

APPENDIX

Formation of a Reduced Energy Mesh from a Given RCPL1 Library

I. REDUCED MESH FOR ONE ISOTOPE IN THE RESOLVED RESONANCE RANGE

The resolved profile is given by a set of pairs (E_i, σ_i) for $i = N_1, \ldots, N_2$ where E_{N_1} is the highest resolved energy, and E_{N_2} is the lowest. Let R_i be the infinitely dilute resonance integral $\int_{E_i}^{E_{N_1}} [\sigma(E)/E]dE$, then R_i is given recursively by $R_{N_1} = 0$

and

$$R_i = R_{i-1} + \left[\frac{\sigma_i}{E_i} + \frac{\sigma_{i-1}}{E_{i-1}} \right] \frac{(E_{i-1} - E_i)}{2} \qquad i = N_1+1, \ldots, N_2$$

This is, in fact, the trapezoidal approximation to the actual integrals. This is assumed adequate since RCPL1 also uses the trapezoidal rule for its edited integrals. Also define the following two quantities:

$$RI_\infty = R_{N_2}$$

and

$$\bar{\sigma} = RI_\infty / \ln(E_{N_1}/E_{N_2})$$

Let a prescribed criterion ϵ contained in $(0,1)$ and a constant c contained in $[0,1]$ be input. Then the following algorithm will insure all local maxima and minima will be retained as well as points where either the distribution has much curvature or is absolutely quite large.

(a) select E_{N_1} as a mesh point

(b) let i be the last accepted mesh point and set $j = i+2$

(c) if E_{j-1} has already been selected for a previously considered nuclide, then go back to step (b) after setting i to j-1

(d) if $(\sigma_{j-1}-\sigma_{j-2})(\sigma_j-\sigma_{j-1}) < 0$, then select E_{j-1} and return to Step (b)

(e) let $T_1 = c(R_j-R_i) + (1-c)\,\bar{\sigma}\,\ln(E_i/E_j)$

and $T_2 = \left|\left(\frac{\sigma_j}{E_j} + \frac{\sigma_i}{E_i}\right)\left(\frac{E_i-E_j}{2}\right) - (R_j-R_i)\right|$

if $T_2 \geq \epsilon T_1$, then E_{j-1} is selected and return to Step (b); otherwise, $j = j+1$ and go to Step (c).

(f) select E_{N_2} as a mesh point.

Thus, the "important" points of the resolved distribution have been chosen. Here "important" means all maxima and minima of the resolved distribution as well as sufficient strategically placed points to ensure that the error ΔRI_∞ satisfies

$$|\Delta RI_\infty| \leq \epsilon RI_\infty$$

To see that the above relationship is valid regardless of c requires some algebra. It can be seen that T_2 is the error in the RI_∞

integral due to compacting of the mesh between E_j and E_i. Let the set $\mathcal{S} = \left\{ E_\ell : \; E_{N_2} \leq E_\ell \leq E_{N_1} \right\}$ be the mesh selected by the above process. Thus,

$$\Delta RI_\infty = \sum_\ell \left\{ \left(\frac{\sigma_\ell}{E_\ell} + \frac{\sigma_{\ell-1}}{E_{\ell-1}} \right) \left(\frac{E_{\ell-1} - E_\ell}{2} \right) - \left(R_\ell - R_{\ell-1} \right) \right\}$$

$$|\Delta RI_\infty| \leq \sum_\ell T_2^\ell$$

Now, sum the T_1^ℓ's over the set $\mathcal{S}$

$$\sum_\ell T_1^\ell = \sum_\ell \left\{ c \left(R_\ell - R_{\ell-1} \right) + (1-c)\bar{\sigma} \ln \left(E_{\ell-1}/E_\ell \right) \right\}$$

$$\sum_\ell T_1^\ell = c \sum_\ell \left(R_\ell - R_{\ell-1} \right) + (1-c)\bar{\sigma} \sum_\ell \ln \left(E_{\ell-1}/E_\ell \right)$$

$$\sum_\ell T_1^\ell = cR_{N_2} - cR_{N_1} + (1-c)\bar{\sigma} \ln \left(E_{N_1}/E_{N_2} \right)$$

However, from the defining relations at the beginning of this section

$$\sum_\ell T_1^\ell = cRI_\infty + (1-c)\, RI_\infty = RI_\infty$$

Combining all results,

$$|\Delta RI_\infty| \leq \sum_\ell T_2^\ell \leq \epsilon \sum_\ell T_1^\ell = \epsilon RI_\infty$$

Large values of c tend to emphasize regions of high curvature in σ, while small values of c emphasize regions where σ is relatively large.

II. REDUCED MESH FOR THE UNRESOLVED RANGE

A frequency K will be used over the energy ranges where the nuclides have unresolved resonances. Nominally, for such ranges, the cross sections generated by RCPL1 at every K^{th} energy will be chosen. When, however, other nuclides have resolved data in such ranges, only sufficient additional energy mesh points will be selected to assure that no mesh gaps larger than K original points remain. Due to the arbitrariness of samples from the statistical distribution computed by RCPL1, it is possible to perturb significantly the RI_∞ over the unresolved range. In the unresolved range, the RI_∞ is slightly differently defined. Let N_3 and N_4 be the endpoints of the unresolved regime within a single RCP group, then

$$RI_\infty = \int_{E_{N_4}}^{E_{N_3}} \sigma(E)\,\frac{dE}{E} = \sum_{i=N_3+1}^{N_4-1} \sigma_i \left(\frac{E_{i-1}-E_{i+1}}{2E_i}\right) + \sigma_{N_3}\left(\frac{E_{N_3}-E_{N_3+1}}{2E_{N_3}}\right) + \sigma_{N_4}\left(\frac{E_{N_4-1}-E_{N_4}}{2E_{N_4}}\right)$$

Consequently, after the selection of the final mesh, RI_∞ (for each isotope's unresolved range) should be calculated for both the new reduced mesh and also the original RCPL1 mesh. The ratios of the integrals should then be used to normalize this discrepancy.

III. CONSTRUCTION OF THE FINAL MESH $\mathcal{F}$

By the techniques given in Sections I and II, it is possible to piece together an unresolved mesh and a resolved mesh for a given isotope i from the original RCPL1 mesh denoted by $\mathcal{E}$. Let this mesh be called $\mathcal{M}^i$. Let I be the set of all isotopes. Now form $\mathcal{M}$ by the following set-theoretical union

$$\mathcal{M} = \bigcup_{i \in I} \mathcal{M}^{i} \subseteq \mathcal{E}$$

and order the elements of $\mathcal{M}$ by decreasing energy value.

The mesh $\mathcal{M}$ may still lack sufficient points for an accurate representation of slowing down of very heavy isotopes. In order to obviate this possibility, let another input constant d (default value d = 0.01) be given. Then check the elements E_j and $E_{j+1} \in \mathcal{M}$ for all j. If $(E_j - E_{j+1}) > d\, E_j$, then pick an additional energy point (or points) from the set $\mathcal{E}$ until $(E_j - E_{j+1}) \leq d\, E_j$ is satisfied.

Given the point $E_j \in \mathcal{M}$ find $E_i \in \mathcal{E}$ such that the following relation is valid

$$E_{i+1} < (1-d)E_j \leq E_i \qquad \text{for } E_i, E_{i+1} \in \mathcal{E}$$

Then make E_i the new E_{j+1} and increase the index of all ensuing $E_j \in \mathcal{M}$. Also, if the energy E_j is in the unresolved range for at least one nuclide then we must also add sufficient points to $\mathcal{M}$ to insure sampling at least each K^{th} energy of the original mesh $\mathcal{E}$. This is then the final set $\mathcal{F}$.