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THE DOPPLER EFFECT FOR A NON-UNIFORM TEMPERATURE DISTRIBUTION IN REACTOR FUEL ELEMENTS

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ABSTRACT

The Monte Carlo method is used in this work to investigate the temperature effects on the Doppler coefficient of reactivity and resonance capture probability due to a non-uniform temperature distribution in the fuel rods arrayed in a reactor lattice. Scattering is allowed in the fuel and moderator, and Doppler broadening of the resonances is taken into account.

This investigation begins with the Boltzmann equation describing the transport of neutrons in steady state. By transforming this equation into an integral equation, the solution can be expressed as a Neumann series, for which a convergence criterion is established. It is shown that the Neumann series can be used to obtain series equivalents for general reactor parameters and their derivatives which depend on the neutron collision density.

A Monte Carlo process that traces neutrons in spatial propagation and energy degradation through a reactor can be related to random walk chains governed by the source and kernel of the integral equation. Also, once the relationship between Monte Carlo histories and the Neumann series is established, one can determine the proper form for random variables which depend upon the paths of the neutron histories in order to evaluate reactor parameters and their derivatives by Monte Carlo. By application of this technique a new and direct method is devised for evaluating the Doppler coefficient.

As an example of this method a computer program was developed for a cylindrical cell and a fuel rod with arbitrary radial temperature dependence. Several cases for different fuel temperatures were investigated using water moderator and UO_2 fuel. Results illustrating temperature dependence of the Doppler coefficient of ractivity and the resonance capture probability are reported for uniform temperature and parabolic temperature distributions in the fuel.

The results indicate that this direct method of calculating the Doppler coefficient by Monte Carlo is practical, and allows more efficient use of computer time in comparison to empirical and finite difference approximations previously used. It is also concluded that the Doppler coefficient is more sensitive than the capture probability to a temperature distribution appropriate to power reactors. This Monte Carlo program also provides the means of investigating these same effects for temperature distributions appropriate to reactors in excursion conditions.

CHAPTER I

INTRODUCTION

A. BACKGROUND

Nuclear reactors may contain in the fuel certain nuclides, such as U-235, U-238, Pu-239, and Th-232, which have neutron resonances that lie within the neutron energy spectrum present in reactors. If the temperature of the resonance material were at absolute zero, then each resonance would have a shape, called 'natural line' shape, with very sharp peak and very narrow energy width. Because of the thermal motion of atoms at normal reactor temperatures, the relative energy distribution of the neutrons and target nuclei changes as the temperature of the material increases and causes the resonances to broaden and lower. This phenomenon is called 'Doppler broadening', and is named after Christian Doppler[1] who noticed similar effects in his original work with light waves. The Breit and Wigner[2] single level formula for neutron resonance cross sections is similar to that for the natural shape of an optical line. In 1937 Bethe and Placzek[3] discussed Doppler broadening of a neutron absorption resonance caused by the thermal agitation of the resonance atoms and derived expressions describing the temperature dependence of the cross sections.

The effect of the Doppler broadening of resonances on the neutron reaction rate is called the Doppler effect and the resulting influence on the reactivity of a nuclear reactor is called the Doppler temperature coefficient of reactivity. The dependence of the Doppler coefficient of

reactivity upon fuel temperature makes it important in reactor safety considerations because a decrease in reactivity with increasing fuel temperature helps to make a power excursion self-limiting. U-238 produces just such an effect whereas fissile resonance absorbers cause the opposite effect. Also the capture of neutrons in the resonances of U-238 and the ensuing conversion to Pu-239 is an important factor in long term temporal studies of reactor criticality.

It is reported[4] that as early as 1937, Meitner, Hahn and Strassmann first surmised that neutrons were absorbed in resonances of U-238, and that soon thereafter Fermi and Szilard recognized that resonance absorption could be decreased by mixing the fuel and moderator heterogeneously instead of homogeneously.

At Szilard's suggestion, Wigner, Creutz, Jupnik, and Snyder[5] performed experimental and theoretical studies in 1941 on resonance absorption of neutrons in heterogeneous fuel-moderator systems that included measurements of the temperature dependence in uranium dioxide (UO_2). Since that time many authors have reported extensive work, both of theoretical and experimental nature, that has contributed to the understanding and quantitative evaluation of the importance of the Doppler effect in the design and performance of nuclear reactors. The work for thermal reactors has been reviewed by Creutz, Jupnik, Snyder and Wigner[4] in 1955, by Wigner[6] in 1956, by Sampson and Chernick[7] in 1958, by Nordheim[8,9] in 1959 and 1961, and by Pearce[10] in 1961. The importance of the Doppler effect in fast reactors has been studied by Feshback, Goertzel and Yamanchi,[11] Frost, Kato and Butler,[12] and Nicholson.[13] The remainder of this discussion will deal exclusively with thermal reactors.

The temperature dependence of the Doppler effect has also been investigated with Monte Carlo techniques by Morton,[14] and Arnold and Dannels.[15] The latter authors used the REP code developed by Richtmyer, Van Norton and Wolfe,[16] which treats the slowing down of neutrons from a "1/E" source in a rectangular cell with cylindrical fuel rod. The code allows use of the Breit-Wigner single level formula for the resonances. Pearce[10] and Hellstrand, Blomberg, and Hörner[17] have indicated that the discrepancy among experimental and theoretical methods in evaluating temperature dependence of the resonance integral of uranium metal, uranium dioxide, thorium metal and thorium dioxide lies outside the limits of experimental error. However, recently Nordheim[18] has discussed a new method of calculating the resonance integral which assumes isolation of the individual resonances and involves numerical integration to determine average collision densities in the fuel and moderator regions. He has obtained quantitative agreement of the resonance integrals for uranium metal and uranium dioxide and their temperature dependence with the experimental results of Hellstrand, Blomberg and Hörner.[17]

In the references on thermal reactors cited above, the Doppler coefficient is defined as

$$\alpha = \frac{1}{(RI)} \frac{\partial (RI)}{\partial T} \qquad (1-1)$$

where T is the fuel temperature, and (RI) is the effective resonance integral, which is related to the resonance escape probability, p, by the

following expression:

$$p = e^{-(RI)/\overline{\xi\sigma_s}} \qquad (1-2)$$

where $\overline{\xi\sigma_s}$ is the average slowing down power per resonance atom. Since

the temperature coefficient of reactivity is given by $(1/k)\ \partial k/\partial T$ where

k is the multiplication constant of the reactor, then the contribution

to the temperature coefficient due to Doppler broadening of the resonances

is given by

$$\frac{1}{p}\frac{\partial p}{\partial T} = \alpha\ \ell n\ p \qquad (1-3)$$

and is called the Doppler coefficient of reactivity in order to make the

verbal distinction between Eq. (1-1) and (1-3). In theoretical studies

in the past it has been the practice to obtain the Doppler coefficient by

approximating the differential in Eq. (1-1) or (1-3) as a finite differ-

ence or by fitting the temperature dependence of the resonance integral

by an empirical curve functionally dependent on $T^{1/2}$.

Monte Carlo has also been used in conjunction with other calculational

methods in reactor analysis in order to obtain more accurate design infor-

mation and knowledge of temporal behavior. Ritsi and Minton[19] have used

Monte Carlo to treat the slowing down of neutrons through the resonance

energy region and thence to provide energy group constants for the Muft

and Sufocate codes, which are multigroup codes for the epi-thermal and

thermal energy regions, respectively. In addition, Leshan, Burr, Temme,

Morrison, Thompson and Triplett[20] have combined Monte Carlo with diffusion

theory and kinetic equations for fuel life-time studies.

All of the works mentioned previously have considered only a uniform

temperature in the fuel, however in operating power reactors the temper-

ature distributions are non-uniform. In fact Belle[21] gives evidence that

the ratio of the peak to surface fuel temperature (absolute temperature

scale) for uranium dioxide could be greater than three depending on power

density and size of fuel rods. Under certain cases he reports temperatures

of about 2740°C and 400°C, respectively, in a simulation of an operating

power reactor with uranium dioxide fuel. There has been very little pub-

lished work discussing the effects of a non-uniform temperature distribu-

tion. The case of a 1 cm slab of uranium metal with surfaces at 0°K and

mid-plane at 900°K was studied by Keane[22] who used a simplified model of

the U-238 resonance structure and assumed neutrons to be normally incident

on the slab. In addition, Dresner[23] performed a similar study for a sin-

gle resonance on an isolated cylindrical fuel rod with maximum temperature

ratio of two, using resonance parameters typical of U-238 resonances.

Both authors conjectured that the resonance capture probability for a

parabolic temperature distribution can be approximated by that of a uni-

form temperature at the mean temperature, however both authors neglected

scattering and neither discussed the validity of the approximation in ob-

taining the Doppler coefficient of reactivity.

The neglect of scattering could be a serious error since the neutron

width is comparable or greater than the capture width for at least half

of the resolved resonances of U-238 and the expected value of the neutron
width is greater than the capture width for the unresolved resonances.
Furthermore the absolute zero temperature used by Keane does not have
physical significance for metal or oxide fuels as noted by Lamb.[24] The
Monte Carlo method is an attractive alternative to the analysis of Keane
and Dresner, since the problem of a non-uniform fuel temperature can be
solved by Monte Carlo for a realistic reactor simulation without making
the assumptions and approximations introduced by them.

For our purpose, Monte Carlo can be thought of as a mathematical ex-
periment, involving the use of random sampling procedures, for simulating
and studying a physical process or solving a deterministic mathematical
problem. The physical process that we are studying is the slowing down
of neutrons through the resonances of fuel in a heterogeneous reactor sys-
tem. This process can be described by the Boltzmann transport equation,
which is used to formulate the mathematical experiment. Alternatively,
the Boltzmann equation could be solved by standard numerical techniques,
but because of the resonance structure of the fuel and the geometry of
the reactor lattice, there is a danger that the systematic errors or pos-
sible instabilities inherent in numerical analysis would mask the small
but important effects that we are looking for in this problem. Monte Carlo
avoids this difficulty and can be made more determinably accurate by in-
creasing the number of histories processed.

B. SCOPE OF RESEARCH

The Monte Carlo method is used in this work to investigate the tem-

perature effects on the Doppler coefficient of reactivity and resonance capture probability due to a non-uniform temperature distribution in the fuel rods arrayed in a reactor lattice. Scattering is allowed in the fuel and moderator, and Doppler broadening of the resonances is taken into account. A new and direct method of evaluating the Doppler coefficient by Monte Carlo is obtained and discussed in succeeding chapters.

The investigation in Chapter II uses as a foundation the Boltzmann equation describing the transport of neutrons in a steady state condition. By use of the Green's function technique, the Boltzmann equation is transformed in this study to a transport integral equation, the solution of which is written in terms of the Neumann series. Although integral equivalents of the Boltzmann equation for specific conditions have been presented elsewhere,[25,26] the derivation presented in this investigation is kept general in order that the resulting integral transport equation be applicable for the same general conditions which apply to the Boltzmann equation. Furthermore this general form is required for our study of the problem of non-uniform fuel temperature. By using the mathematical properties of Banach abstract spaces, we can investigate the convergence of the Neumann series and establish a convergence criterion, which is required in the work of succeeding chapters.

In view of the fact that the purpose of this study is to include investigation of reactor parameters, such as the resonance capture probability and the Doppler coefficient, a general parameter is represented by the integral of the product of a function and the collision density. The de-

rivative of the parameter equals the derivative of the integral. It is
then shown in Chapter II that the Neumann series can be used to obtain
series equivalents for the integral and its derivative, and that these
series converge for conditions that are usually satisfied in physical sys-
tems. A perusal of these Neumann series representations, which are given
in Chapter II, indicates that closed form solutions are intractable be-
cause of the multiple integration involved in the terms of the series.
However, these series can be evaluated by Monte Carlo.

In 1953 Albert[27] introduced a stochastic model for describing a ran-
dom walk process, and in 1960 Spanier[28] studied and generalized this model
by using the rigorous mathematics of modern probability theory. Both au-
thors discussed the application of Albert's model to the study by Monte
Carlo of the solution of a Fredholm type integral equation by assuming
uniform convergence of the Neumann series associated with the integral
equation. Spanier recognized applicability to neutron transport problems
under the assumption of convergence. Since the convergence of the Neumann
series solution of the Boltzmann transport equation is established in Chap-
ter II, the basic stochastic model of Albert for a general random walk
process is used in Chapter III. Also in view of the convergence of the
Neumann series representations of reactor parameters and their derivatives,
the application of Albert's model to neutron transport is reformulated and
extended to the evaluation of reactor parameters and their derivatives.
The investigation presented in the second and third chapters results in
the complete and straightforward formulation of a rigorous stochastic model

for evaluating reactor parameters and their derivatives by Monte Carlo. The work in this chapter is kept general; in fact, the results can be applied to the behavior of gamma rays for shielding problems.

The stochastic model formulated in Chapter III is specialized in Chapter IV to the class of slowing down problems in a reactor. In this case the neutrons are emitted from a given high energy source and are processed by Monte Carlo according to random walk chains that are specialized in this chapter to specifically describe energy degradation and spatial propagation through the fuel and moderator regions. Since the type of collisions are restricted to those in which a neutron loses energy but cannot gain energy, this study is not applicable to the thermal energy region. However, this restriction is compatible with the study of temperature coefficient and capture probability due to Doppler broadening of the resonances in uranium fuel. The Monte Carlo treatment for this problem is formulated for a general temperature distribution in the fuel rod.

Previous to this work, the Doppler coefficient was obtained by an empirical fit to a curve of capture probability plotted versus temperature, or by a finite difference approximation to the differential, as described in Section I-A. This was done only in the case of a constant fuel temperature but could be applied to the case of a non-uniform temperature distribution. By applying the results of the investigation in Chapter III, a method of determining the Doppler coefficient directly by the Monte Carlo process is devised. In this way the Doppler coefficient is no longer dependent upon the inherent uncertainties of the two previous methods. Also

as discussed in Chapter VI, the direct method allows a very considerable saving of computer time in determining the Doppler coefficient to a given accuracy.

As an example of the method given in Chapter IV, a computer program was written for a circular cylindrical cell geometry. This cell geometry was used instead of a rectangular cell geometry in order to save computer time. This savings in time is possible because neutron paths incident on the cell boundary are reflected along a chord similar to the incident chord. The results are presented for a parabolic temperature distribution, water moderator and U-238 oxide resonance material.

This work results in a new method for determining the Doppler coefficient by Monte Carlo that is founded on a systematic deductive approach. Although the method could conceivably be formulated by intuition alone, evidently no one has done it. Furthermore the mathematical development avoids the introduction of assumptions that can be justified only by intuition. The method is shown to be applicable to physical systems of interest in reactor studies.

CHAPTER II

INTEGRAL TRANSPORT EQUATION AND NEUMANN SERIES

In this chapter an integral equation for the transport of neutrons is obtained from the steady-state Boltzmann equation. If one writes the integral equation in terms of neutron collision density rather than neutron flux, and represents a point in the 6-dimensional phase space (neutron energy, direction, and position) by the variable τ, then the integral equation may be written in standard form.

In Section II-B the Neumann series solution of the integral equation is determined by iteration. In investigating the convergence of the resulting Neumann series the more conventional techniques can not be relied upon since the kernel of the integral equation does not belong to Hilbert space. However the kernel does belong to the more general abstract space, namely Banach space. By using the appropriate definitions of norms and properties of transformations in Banach space the convergence for the Neumann series for neutron transport can be rigorously proven. The most important physical condition for the convergence is that the ratio of scattering to total cross section have a maximum value less than one. This is a reasonable condition for realistic reactor or shielding systems.

A. DERIVATION OF INTEGRAL TRANSPORT EQUATION FROM BOLTZMANN EQUATION

The Boltzmann equation describing the transport of neutrons serves as the foundation for this work. For the steady state case it is given by,[26]

$$\nabla \cdot \underline{\Omega} \; \Phi(\underline{r},E,\underline{\Omega}) + \Sigma_t(\underline{r},E) \; \Phi(\underline{r},E,\underline{\Omega}) = S(\underline{r},E,\underline{\Omega})$$

$$+ \int_{E'} \int_{\underline{\Omega}'} \Phi(\underline{r},E',\underline{\Omega}') \Sigma_s(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}) \; d\Omega' \; dE'$$

(2-1)

where the following definitions and identifications apply:

$n(\underline{r},E,\underline{\Omega}) \; d^3r \; dE \; d\Omega \equiv$ The expected number of neutrons in

d^3r about $\underline{r}$ with energies in dE about

E and going in the direction $d\Omega$ about $\underline{\Omega}$.

$\Phi(\underline{r},E,\underline{\Omega}) \equiv n(\underline{r},E,\underline{\Omega}) \; v(E)$

$= $ Neutron "flux"

$v(E) \quad = $ Speed of neutron of energy E

$S(\underline{r},E,\underline{\Omega}) \quad = $ Neutron source

$\Sigma_t(\underline{r},E) \quad = $ Total macroscopic cross section

$\Sigma_s(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}) \quad = $ Differential scattering cross section

In order to derive the integral equation equivalent to (2-1), consider the Green's function $G(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}')$ satisfying the differential equation

$$\nabla \cdot \underline{\Omega} G + \Sigma_t(\underline{r},E) \, G(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}')$$

(2-2)

$$= \delta(\underline{r} - \underline{r}') \, \delta(E - E') \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}')$$

and the boundary conditions

$$G = 0 \text{ at } |\underline{r} - \underline{r}'| = \infty$$

(2-3)

The notation δ is defined as the Dirac delta function and the notation δ_2 is defined as

$$\delta_2(\underline{\Omega} \cdot \underline{\Omega}') \equiv \frac{1}{2\pi} \delta(\underline{\Omega} \cdot \underline{\Omega}' - 1)$$

(2-4)

Let

$$\mu_L \equiv \underline{\Omega} \cdot \underline{\Omega}'$$

(2-5)

then it is noted that

$$\int_{\underline{\Omega}} \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \, d\Omega = \int_{\underline{\Omega}'} \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \, d\Omega'$$

(2-6)

$$= \frac{1}{2\pi} \int_{\mu_L=-1}^{1} \int_{\Phi=0}^{2\pi} \delta(\mu_L - 1) \, d\mu_L \, d\Phi = 1$$

Equation (2-2) is solved in Appendix A by Fourier Transform techniques. The solution for the Green's function is found to be

$$G(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}') \, d^3r' \, dE' \, d\Omega' = e^{-\int_0^{|\underline{r}-\underline{r}'|} \Sigma_t(E,\underline{r}' + \underline{\Omega}_R R')dR'}$$

(2-7)

$$\cdot \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}_R) \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \, \delta(E - E') \, \frac{d^3r' \, dE' \, d\Omega'}{|\underline{r} - \underline{r}'|^2}$$

where
$$\underline{\Omega}_R \equiv \frac{\underline{r} - \underline{r}'}{|\underline{r} - \underline{r}'|} = \frac{\underline{r} - \underline{r}'}{R} \tag{2-8}$$

Let $H(\underline{r}',E',\underline{\Omega}')$ represent the right hand side of equation (2-1), then by superposition,

$$\Phi(\underline{r},E,\underline{\Omega}) = \iiint\limits_{\underline{r}'E'\underline{\Omega}'} G(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}') \cdot$$
$$\tag{2-9}$$
$$\cdot H(\underline{r}',E',\underline{\Omega}') \, d^3r' \, dE' \, d\Omega'$$

is an integral equivalent of Eq. (2-1). The method of proving equivalence is given by Churchill[29]. Equation (2-1) can be obtained by multiplying Eq. (2-2) by $H(\underline{r}',E',\underline{\Omega}')$ and integrating over all $\underline{r}',E',\underline{\Omega}'$.

Substitute the right hand side of (2-1) for $H(\underline{r}',E',\underline{\Omega}')$ into (2-9). One can then integrate over E', and $\underline{\Omega}'$, employing the properties of the Dirac delta function, and obtain

$$\Phi(\underline{r},E,\underline{\Omega}) = \int\limits_{\underline{r}'} \frac{d^3r'}{|\underline{r} - \underline{r}'|^2} \, e^{-\int_0^{|\underline{r}-\underline{r}'|} \Sigma_t \, dR'} \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}_R) \left\{ S(\underline{r}',E,\underline{\Omega}) \right.$$
$$\tag{2-10}$$
$$\left. + \int\limits_{E''} \int\limits_{\underline{\Omega}''} \Phi(\underline{r}',E'',\underline{\Omega}'') \, \Sigma_s(E,\underline{\Omega}|E'',\underline{\Omega}'';\underline{r}') \, dE'' \, d\Omega'' \right\}$$

Equation (2-10) can be put in the form of a standard integral equation by introducing the following definitions:

$$\psi(\underline{r},E,\underline{\Omega}) \equiv \Sigma_t(\underline{r},E) \, \Phi(\underline{r},E,\underline{\Omega})$$
$$= \text{Collision density}$$

$$T(\underline{r}|\underline{r}';E,\underline{\Omega})\,d^3r \equiv e^{-\int_0^{|\underline{r}-\underline{r}'|} \Sigma_t(E,-\underline{\Omega}_R R')\,dR'}$$

$$\cdot\; \delta_2(\underline{\Omega}\cdot\underline{\Omega}_R)\,\frac{\Sigma_t(E,\underline{r})}{|\underline{r}-\underline{r}'|^2}\,d^3r$$

$$= \text{Transport kernel}$$

$$\widetilde{S}(\underline{r},E,\underline{\Omega}) \equiv \int_{\underline{r}'} S(\underline{r}',E,\underline{\Omega})\,T(\underline{r}|\underline{r}';E,\underline{\Omega})\,d^3r'$$

$$= \text{Collision density source}$$

$$C(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}')dEd\Omega \equiv \frac{1}{\Sigma_t(\underline{r}',E')}\,\Sigma_s(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}')dEd\Omega$$

$$= \text{Collision kernel}$$

$$K(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}') \equiv C(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}')\,T(\underline{r}|\underline{r}';E,\underline{\Omega})$$

$$= \text{Kernel of integral equation}$$

Finally the integral form of the Boltzmann transport equation can be written for the neutron collision density as

$$\psi(\underline{r},E,\underline{\Omega}) = \widetilde{S}(\underline{r},E,\underline{\Omega})$$

$$+ \int_{\underline{r}'}\int_{E'}\int_{\underline{\Omega}'} \psi(\underline{r}',E',\underline{\Omega}')\,K(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}')\,d^3r'\,dE'\,d\Omega'$$

$$\text{(2-11)}$$

It is further noted that the following relations exist:

$$\int_{\underline{r}} T(\underline{r}|\underline{r}';E,\underline{\Omega})\,d^3r = 1 \qquad \text{(2-12)}$$

$$\int_{E}\int_{\underline{\Omega}'} C(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}')\,dEd\Omega = \frac{\Sigma_s(E',\underline{r}')}{\Sigma_t(E',\underline{r}')} \qquad \text{(2-13)}$$

hence
$$\int\limits_{\underline{r}} \int\limits_{E} \int\limits_{\underline{\Omega}} K(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}') \; d^3r \; dE d\Omega \;=\; \frac{\Sigma_s(E',\underline{r}')}{\Sigma_t(E',\underline{r}')} \qquad (2\text{-}14)$$

The integral transport equation for neutrons can also be obtained directly by physical arguments if one notes that the kernels be expressed as the following conditional probabilities:

$K(\underline{r},E,\underline{\Omega}|\underline{r}',E',\underline{\Omega}') \; d^3r \; dE d\Omega \equiv$ The probability that a neutron with energy E' and going in direction $\underline{\Omega}'$ shall, upon suffering a collision at $\underline{r}'$, be scattered into dE about E and $d\Omega$ about $\underline{\Omega}$ after that collision and shall suffer its next collision in d^3r about $\underline{r}$.

$C(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}') \; dE \; d\Omega \equiv$ The probability that a neutron with energy E' and going in direction $\underline{\Omega}'$ shall, upon suffering a collision at $\underline{r}'$, be scattered into dE about E and $d\Omega$ about $\underline{\Omega}$ after that collision.

$T(\underline{r}|\underline{r}';E,\underline{\Omega}) \; d^3r \equiv$ The probability that a neutron at $\underline{r}'$ with energy E and going in direction $\underline{\Omega}$ shall suffer its next collision in d^3r about $\underline{r}$.

$\Sigma_s(\underline{r},E)/\Sigma_t(\underline{r},E) \equiv$ The probability that a collision suffered by a neutron with energy E at $\underline{r}$ was a scattering collision.

B. FORMULATION OF NEUMANN SERIES AND CONVERGENCE CRITERION

The integral equation for neutron transport can be put in a more compact form for use in this section by letting τ represent the 6-dimensional vector of phase space in Eq. (2-11),

$$\psi(\tau) \;=\; \tilde{S}(\tau) + \int\limits_{\tau'} K(\tau|\tau') \; \psi(\tau') \; d\tau' \qquad (2\text{-}15)$$

where
$$dτ = d^3r \, dEd\Omega \qquad (2\text{-}16)$$

The Neumann series solution of Eq. (2-15) can be obtained by successive iteration.[30] The first iteration is found by substituting the right hand side of (2-15) for $\psi(τ')$ appearing in the integral term of (2-15), obtaining

$$\psi(τ) = \tilde{S}(τ) + \int_{τ_0} K(τ|τ_0) \, \tilde{S}(τ_0) \, dτ_0$$

$$\qquad (2\text{-}17)$$

$$+ \int_{τ_1} \int_{τ_0} K(τ|τ_1) \, K(τ_1|τ_0) \, \psi(τ_0) \, dτ_0 \, dτ_1$$

The second iteration is formed by substituting the right hand side of (2-17) for $\psi(τ')$ into (2-15). Higher order iterations are formed by successively substituting the previous iterative value of $\psi(τ)$ into the integral term of (2-15). After m iterations there results,

$$\psi(τ) = \sum_{n=0}^{m} \psi_n(τ) + \text{Remainder} \qquad (2\text{-}18)$$

where
$$\psi_0(τ) = \tilde{S}(τ_0) \qquad (2\text{-}19)$$

and for $n \geq 1$

$$\psi_n(τ) \equiv \int_{τ_{n-1}} \cdots \int_{τ_0} K(τ|τ_{n-1}) \cdots K(τ_1|τ_0) \, \tilde{S}(τ_0) \, dτ_0 \cdots dτ_{n-1} \qquad (2\text{-}20)$$

and also

$$\text{Remainder} \equiv \int_{\tau_m} \cdots \int_{\tau_o} K(\tau|\tau_m) \cdots K(\tau_1|\tau_o) \, \psi(\tau_o) \, d\tau_o \cdots d\tau_m \quad (2\text{-}21)$$

The Neumann series is then formed by letting m approach infinity and neglecting the remainder term,

$$\psi(\tau) = \sum_{n=o}^{\infty} \psi_n(\tau) \qquad (2\text{-}22)$$

It is remarked that the nth term in (2-22) physically represents the contribution to the collision density at τ due to source neutrons which have undergone exactly n scattering collisions.

The question of convergence of the Neumann series has been thoroughly studied for the special case that Eq. (2-15) is a Fredholm integral equation of the 2nd kind and which has elements belonging to Hilbert L^2 space.[31,32] In that special case the Neumann series converges if the norm of the kernel is less than one, i.e., if

$$\|K\| \equiv \left[\int_{\tau} \int_{\tau'} |K(\tau|\tau')|^2 \, d\tau \, d\tau' \right]^{1/2} < 1 \qquad (2\text{-}23)$$

Unfortunately, the kernel for the neutron transport integral equation is not square integrable, which is a necessary condition for the solution of Eq. (2-15) to belong to L^2 space.

However, the criterion for the establishment of convergence of the Neumann series can be obtained by generalizing to Banach space (L^p space). Actually the functional space $L^p (1 \leq p \leq \infty)$ and the space of continuous

functions C are particular cases of the Banach abstract space. Briefly

a Banach space is a set of abstract elements, and is a linear space, a

complete space, and has a norm (positive) for every element of the ab-

stract set. The elements of the set may be points, measurable functions,*

transformed functions or functionals (operators). The mathematical des-

cription of a Banach space is given in Appendix B.

For a Banach space the norm of a measurable function, f, defined in

the region ϵ is[30]

$$\text{norm} \equiv \|f\| \equiv \left[\int_\epsilon |f(x)|^p \, dx \right]^{1/p} \tag{2-24}$$

in L^p space, $1 < p < \infty$, or

$$\text{norm} \equiv \|f\| \equiv \max |f(x)| \tag{2-25}$$

in C or L^∞ space.

The norm of a linear transformation, T, belonging to Banach space is

defined as

$$\text{norm} \equiv \|T\| \equiv M_a \tag{2-26}$$

where M_a is the smallest of the bounds M, and where

$$\|Tf\| \leq M\|f\| \tag{2-27}$$

---

*Functions which are continuous or have a finite number of finite discon-
tinuities are measurable. Functions that concern us here, namely those
which describe physical processes, are measurable. For a rigorous defini-
tion based on set theory the reader is referred to Halmos[33] or Doob.[34]

The convergence criterion for the Neumann series for neutron transport can now be established within the framework of Banach spaces and linear transformations. Writing Eq. (2-15) as a functional equation:

$$\psi(\tau) = \widetilde{S}(\tau) + \mathcal{K}\psi(\tau) \qquad (2\text{-}28)$$

or

$$(I - \mathcal{K})\,\psi = \widetilde{S} \qquad (2\text{-}29)$$

where I is the identity transformation and $\mathcal{K}$ is the linear transformation, associated with the kernel $K(\tau|\tau')$, which transforms the measurable function ψ into the measurable function $\mathcal{K}\psi$, i.e.,

$$\mathcal{K}\psi(\tau) \equiv \int_{\tau'} K(\tau|\tau')\,\psi(\tau')\,d\tau' \qquad (2\text{-}30)$$

the Neumann series in this notation becomes

$$\psi(\tau) = \sum_{n=o}^{\infty} \psi_n(\tau) = \widetilde{S} + \mathcal{K}\widetilde{S} + \mathcal{K}^2\widetilde{S} + \mathcal{K}^3\widetilde{S} + \cdots \qquad (2\text{-}31)$$

The elements of the integral Eq. (2-15) (or (2-29)) belong to Banach L^1 space under the conditions that the norm of $\widetilde{S}$ exists and is finite and the norm of K is bounded. In fact the source is a non-negative quantity; therefore, for L^1 space,

$$\|\widetilde{S}\| = \int_{\tau} |\widetilde{S}(\tau)|^1\,d\tau = \int_{\tau} \widetilde{S}(\tau)\,d\tau \qquad (2\text{-}32)$$

After referring to relation (2-12) and the definition of the collision

source, inverting the order of integration in $\underline{r}$ and $\underline{r}'$, and then integrating over all $\underline{r}$, one can write the norm of the collision source as

$$\|\tilde{S}\| = \int_\tau S(\tau)\, d\tau \qquad (2\text{-}33)$$

The norm equals one if the neutron source is normalized, and at least is finite for physical problems of interest, i.e., the class of slowing down problems in a reactor. Later it will also be required that the integral of the derivative of $\tilde{S}$ be bounded.

According to (2-26) and (2-27) the norm of the kernel is found from the norm of the function which was obtained by operating the kernel on the source term.

$$\|\mathcal{K}\tilde{S}\| = \int_\tau |\mathcal{K}\tilde{S}|^1\, d\tau = \int_\tau \left| \int_{\tau'} K(\tau|\tau')\, \tilde{S}(\tau')\, d\tau' \right| d\tau \qquad (2\text{-}34)$$

$$\leq \int_\tau \int_{\tau'} |K(\tau|\tau')\, \tilde{S}(\tau')|\, d\tau'\, d\tau \qquad (2\text{-}35)$$

By employing Fubini's Theorem (page 84, Riesz and Nagy,[30]) the limits of integration in (2-35) can be interchanged. After integrating over all τ and noting (2-14), there results

$$\|\mathcal{K}\tilde{S}\| \leq \int_{\tau'} \left| \frac{\Sigma_s}{\Sigma_t} \right| \cdot |\tilde{S}|\, d\tau' \leq \left| \frac{\Sigma_s}{\Sigma_t} \right|_{max} \cdot \|\tilde{S}\| \qquad (2\text{-}36)$$

Therefore the norm of the kernel is no larger than the largest ratio of scattering cross section to total cross section.

$$\|\mathcal{H}\| \;=\; M_a \;\le\; \left|\frac{\Sigma_s(\tau)}{\Sigma_t(\tau)}\right|_{max} \;<\; 1 \qquad\qquad (2\text{-}37)$$

Condition (2-37) would not be satisfied for a pure scattering system (e. g., pure Compton scattering for photons) but would be reasonable for true physical systems. In requiring conditions (2-37), the norm of the kernel is bounded. Also, as shown, the norm of the source exists, and therefore the solution of integral transport Eq. (2-15) belongs to Banach L^1 space. This condition will now be shown to satisfy the criterion for convergence of the Neumann series. Later we will require the norm of the derivative of the kernel to be bounded.

Consider the right hand side of Eq. (2-31) and denote the partial sum by S_n, then the norm of the partial sum is

$$\|S_n\| \;=\; \|\widetilde{S} + \mathcal{H}\widetilde{S} + \mathcal{H}^2\widetilde{S} + \mathcal{H}^3\widetilde{S} + \cdots + \mathcal{H}^n\widetilde{S}\| \qquad (2\text{-}38)$$

By using the properties of linear transformations (Eqs. (B-6) through (B-12) Appendix B), the norm of the partial sum becomes

$$\|S_n\| \;\le\; \|\widetilde{S}\| \cdot (1 + \|\mathcal{H}\| + \|\mathcal{H}\|^2 + \cdots + \|\mathcal{H}\|^n) \qquad (2\text{-}39)$$

which converges as n approaches ∞. This can be seen by employing condition (2-37) and comparing the resulting series to the geometric series. Hence the Neumann series (2-31) is "strongly" convergent ("strong convergence" in Banach space is a generalization of "convergence in the mean" in Hilbert space.[30]) Denote the limit of the partial sum S_n by ψ. By operating on the Neumann series with the transformation $\mathcal{H}$ and utilizing

the continuity property of linear transformations (Appendix B), one can

show that Eq. (2-31) is indeed a solution of the integral Eq. (2-15)

$$\mathcal{H}\psi = \mathcal{K}(\tilde{S} + \mathcal{H}\tilde{S} + \mathcal{H}^2\tilde{S} + \cdots)$$

$$= -\tilde{S} + \tilde{S} + \mathcal{H}\tilde{S} + \mathcal{H}^2\tilde{S} + \mathcal{H}^3\tilde{S} + \cdots \qquad (2\text{-}40)$$

$$= -\tilde{S} + \psi \qquad \text{Q.E.D.}$$

C. REPRESENTATION OF REACTOR PARAMETERS BY NEUMANN SERIES

In this work we are primarily concerned with evaluating reactor pa-

rameters such as resonance capture probability, resonance escape proba-

bility and Doppler coefficient. These parameters can be expressed in

terms of the Neumann series solution to the integral transport equation.

In this chapter let $w(\tau)$ represent a general function which is bounded

and has finite derivative, a.e., and which when "averaged" with respect

to the neutron collision density, gives the desired parameters of inter-

est. The quotation marks are used because, although the collision density

can be thought of as a probability density function, it does not necessar-

ily satisfy the requirement of normalization. Let I represent the integral

$$I = \int_T w(\tau)\,\psi(\tau)\,d\tau \qquad (2\text{-}41)$$

then the true average of $w(\tau)$ is

$$<w(\tau)> = \frac{I}{\int_T \psi(\tau)\,d\tau} \qquad (2\text{-}42)$$

Means of evaluating the integral I in terms of the Neumann series will now be considered. We will again rely on the mathematical theory of Banach space. Since it has been established that the elements of the integral Eq. (2-15) belong to L^1 space, and consequently so does its solution ψ, it is necessary that the measurable function $w(\tau)$ belong to L^∞ space in order that I represent the scalar product of w and ψ in Banach space.[30] The norm of w must exist in order for w to belong to L^∞ space. Then according to (2-25) the norm of w equals

$$\text{norm} \ = \ \|w\| \ = \ \max \ |w(\tau)| \tag{2-43}$$

and must be finite. Now substitute the Neumann series for $\psi(\tau)$ into the integral I (2-41), giving

$$I \ = \ \int_\tau w[\tilde{S} + \tilde{\mathcal{K}}\tilde{S} + \tilde{\mathcal{K}}^2\tilde{S} + \cdots] \, d\tau \tag{2-44}$$

According to Riesz and Nagy,[30] strong convergence of the Neumann series implies "weak" convergence of the Neumann series, which means that (2-44) can be integrated term by term and the resulting series converges strongly to I. Therefore,

$$I \ = \ \int_\tau w(\tau) \, \tilde{S}(\tau) \, d\tau$$
$$+ \ \sum_{n=1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_0} w(\tau_n) K(\tau_n | \tau_{n-1}) \cdots K(\tau_1 | \tau_0) \, \tilde{S}(\tau_0) \, d\tau_0 \cdots d\tau_n \tag{2-45}$$

Let α be a variable upon which w, $\tilde{S}$, and K depend parametrically. (The

temperature of the fuel would be an example of α since neutron cross sections in general depend on the temperature of the medium.) Rewriting (2-45) as an explicit function of α,

$$I(\alpha) = \int_T w(\tau,\alpha)\, S(\tau,\alpha)\, d\tau$$

$$+ \sum_{n=1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_0} w(\tau_n,\alpha)\, K(\tau_n|\tau_{n-1},\alpha)\cdots K(\tau_1|\tau_0,\alpha)\, \tilde{S}(\tau_0,\alpha)\, d\tau_0\cdots d\tau_n \qquad (2\text{-}46)$$

We will require that the conditions previously satisfied by the norms of w, $\tilde{S}$, and K hold for all values of interest for the variable α. Then by using the Weierstrass Test for uniform convergence[35,36] the Neumann series equivalent of the integral I (2-46) can be shown to be uniformly and absolutely convergent with respect to α over an interval in which the terms are continuous functions of α.

$$|I(\alpha)| \leq \left| \int_T w\tilde{S}\, d\tau \right| + \left| \int_T wK\tilde{S}\, d\tau \right| + \cdots \qquad (2\text{-}47)$$

$$\leq |w(\tau,\alpha)|_{max} \cdot \left(\int_T |\tilde{S}|\, d\tau + \int_T |K\,\tilde{S}|\, d\tau + \int_T |K^2\tilde{S}|\, d\tau + \cdots \right) \qquad (2\text{-}48)$$

But according to the definition of the norm of the source and the kernel for L^1 space, and by again using the properties of linear transformations reported in Appendix B, series (2-48) becomes

$$|I(\alpha)| \leq |w(\tau,\alpha)|_{max} \cdot \|\tilde{S}\| \cdot \left(1 + \|K\| + \|K\|^2 + \cdots \right) \qquad (2\text{-}49)$$

which converges since (2-39) converges as n approaches ∞. Therefore, Eq.

(2-46) converges uniformly since the function $w(\tau,\alpha)$ is bounded and the Neumann series exhibits strong convergence.

In later chapters the differential of I (2-41) with respect to the general variable will be needed.

$$\frac{\partial I(\alpha)}{\partial \alpha} = \int_\tau \frac{\partial}{\partial \alpha} \left(w(\tau,\alpha) \; \psi(\tau,\alpha) \right) \, d\tau \qquad (2\text{-}50)$$

assuming the limits of integration are independent of the variable α. In view of the uniform convergence of the Neumann series equivalent of I, Eq. (2-46) can be differentiated term by term if the resulting series converges uniformly. Performing term-wise differentiation,

$$\frac{\partial I(\alpha)}{\partial \alpha} = \int_{\tau_0} \left[\frac{1}{w_0} \frac{\partial w_0}{\partial \alpha} + \frac{1}{S_0} \frac{\partial \tilde{S}_0}{\partial \alpha} \right] w(\tau_0) \; \tilde{S}(\tau_0) \, d\tau_0$$

$$+ \sum_{n=1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_0} \left[\frac{1}{w_n} \frac{\partial w_n}{\partial \alpha} + \frac{1}{K_n} \frac{\partial K_n}{\partial \alpha} + \cdots \right. \qquad (2\text{-}51)$$

$$\left. + \frac{1}{K_1} \frac{\partial K_1}{\partial \alpha} + \frac{1}{\tilde{S}_0} \frac{\partial \tilde{S}_0}{\partial \alpha} \right] w_n \; K_n \cdots K_1 \; \tilde{S}_0 \; d\tau_0 \cdots d\tau_n$$

where the following notations are used

$$K_n \equiv K(\tau_n | \tau_{n-1}, \alpha) \qquad (2\text{-}52)$$

$$w_n \equiv w(\tau_n, \alpha) \qquad (2\text{-}53)$$

$$\tilde{S}_0 \equiv \tilde{S}(\tau_0, \alpha) \qquad (2\text{-}54)$$

By again using the Weierstrass Test and by imposing the requirements that

the derivative of w is bounded, that the integral over all τ of the derivative of $\tilde{S}$ is bounded, and that the integral over all $\underline{r}_n$ ($\tau_n = (\underline{r}_n, E_n, \underline{\Omega}_n)$) of the derivative of the kernel, K_n, is bounded for all n, then series (2-51) can be shown to be uniformly convergent with respect to α over an interval in which the terms are continuous functions of α. Under these conditions the absolute values of the terms of (2-51) can be shown to be less than the terms of the following geometric series:

$$\left| \frac{\partial I(\alpha)}{\partial \alpha} \right| \leq M \sum_{n=0}^{\infty} n \left| \frac{\Sigma_s}{\Sigma_t} \right|^{n-1}$$

which is convergent by the Ratio Test,[35,36] for condition (2-37). M is a finite constant.

D. MATHEMATICAL MODIFICATION OF KERNEL AND SOURCE

The remainder of this chapter will consider the modification of the kernel in a mathematical sense, and the resultant effect on the Neumann series. It is noted that if one thinks of ψ as just a mathematical density function, then a new density term ψ' can be introduced into the integral I (2-41) in the following manner:

$$I = \int_{\tau} w(\tau) \frac{\psi(\tau)}{\psi'(\tau)} \psi'(\tau) \, d\tau = \int_{\tau} w(\tau) \, W(\tau) \, \psi'(\tau) \, d\tau \qquad (2\text{-}55)$$

where the weight factor $W(\tau)$ is defined as

$$W(\tau) \equiv \psi(\tau)/\psi'(\tau) \qquad (2\text{-}56)$$

Hence the integral I represents in this second form the "average" of the product (w W) with respect to the "density" term ψ'. Likewise the source and kernel in the Neumann series representation of I can be modified without effecting the sum if the correct weighting factor is introduced. Let $\tilde{S}'$ and K' be the new non-physical source and kernel respectively, then

$$
I = \int_\tau w(\tau) \, W_o(\tau) \, \tilde{S}'(\tau) \, d\tau
$$

$$
+ \sum_{n=1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_0} w(\tau_n) W_n(\tau_0, \cdots \tau_n) K'(\tau_n|\tau_{n-1}) \cdots K'(\tau_1|\tau_0) \tilde{S}'(\tau_0) d\tau_0 \cdots d\tau_n \tag{2-57}
$$

where the weight factors are now defined as

$$
W_o(\tau) \equiv \tilde{S}(\tau)/\tilde{S}'(\tau) \tag{2-58}
$$

and for $n \geq 1$,

$$
W_n(\tau_0, \cdots \tau_n) \equiv \frac{K(\tau_n|\tau_{n-1}) \cdots K(\tau_1|\tau_0) \, \tilde{S}(\tau_0)}{K'(\tau_n|\tau_{n-1}) \cdots K'(\tau_1|\tau_0) \, \tilde{S}'(\tau_0)} \tag{2-59}
$$

Similarly the differential of I can be written in the form

$$
\frac{\partial I(\alpha)}{\partial \alpha} = \int_\tau \left(\frac{1}{w} \frac{\partial w}{\partial \alpha} + \frac{1}{\tilde{S}} \frac{\partial \tilde{S}}{\partial \alpha} \right) w(\tau) \, W_o(\tau) \, \tilde{S}'(\tau) \, d\tau
$$

$$
+ \sum_{n=1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_0} \left(\frac{1}{w_n} \frac{\partial w_n}{\partial \alpha} + \frac{1}{K_n} \frac{\partial K_n}{\partial \alpha} + \cdots + \frac{1}{K_1} \frac{\partial K_1}{\partial \alpha} \right. \tag{2-60}
$$

$$
\left. + \frac{1}{\tilde{S}_o} \frac{\partial \tilde{S}_o}{\partial \alpha} \right) w_n W_n(\tau_0, \cdots \tau_n) \, K'_n \cdots K'_1 \, \tilde{S}'_o \, d\tau_0 \cdots d\tau_n
$$

where the notation K'_n and $\tilde{S}'_o$ are similarly defined as in (2-52) and (2-54). The new kernel and source may be completely arbitrary without

effecting the value of I or $\partial I/\partial \alpha$ as long as the weight factors are defined as above. However in practice it would be reasonable to require the norm of new source to exist and the norm of the new kernel to be less than one, and both norms to belong to L^1 space, so that the corresponding Neumann series would be convergent. This discussion on the modification of the source and kernel in this chapter serves as insight to the non-analog random walk process that is examined in the next chapter.

CHAPTER III

RANDOM WALK PROCESS

In this chapter the mathematical description for a random walk proc-ess is formulated, and applied to the problem of neutron transport. The Neumann series and the random walk process are then related.

In 1953 Albert[27] presented a mathematical model based on stochastic process theory to describe a random walk process and discussed specialized applications to the problem of estimating the solutions of integral equa-tions. Spanier[28] reformulated and extended his work by using a clear and precise mathematical development based on modern probability theory. Both authors make the basic assumption that the Neumann series converges, which is needed to develop their mathematical theory rigorously. Since the cri-terion for convergence of the Neumann series solution to the integral equation for neutron transport was developed in Chapter II, the basic math-ematical model of Albert can be used in this chapter and related to the Neumann series.

Monte Carlo is a convenient method for processing random walk chains. This is accomplished by making decisions based on random variables selected from probabilities governing the random walk chains. These decisions de-termine the generation of the random walk process and in turn the evalua-tion of random variables that serve as estimators to desired parameters which depend upon neutron transport phenomena. As will be seen in this chapter, proofs of convergence that were given in Section II-C are needed

to determine the proper random variables, called estimators, which provide

an estimate of the quantities given by the integrals I(2-41) and $\partial I/\partial\alpha$(2-50)

in the preceding chapter. It will also be noted that Monte Carlo effec-

tively provides a method of evaluating the individual terms of the Neumann

series corresponding to the integral I(2-45) and $\partial I/\partial\alpha$(2-51).

Because this chapter draws upon probability theory as a background,

using definitions of probability density functions (or frequency functions),

distribution functions, conditional density functions, and expected values,

all in the multivariate sense, these definitions are presented in Appendix

C.

A. FORMULATION OF RANDOM WALK CHAINS FOR ANALOG PROCESSES

Random walk processes can be divided into two categories called ana-

log and non-analog. Analog processes can be described as processes in

which random walks are governed by probabilities simulating the physical

laws of the system under consideration. Non-analog processes are those in

which the probabilities are deliberately but carefully distorted. This

distortion will then permit the adoption of special Monte Carlo techniques.

A random walk chain can be described as follows: Consider a particle

propagating through a medium in a random manner and suffering collisions

at successive points in phase space, τ_0, τ_1, τ_2, $\cdots$. It may be absorbed

at any one of the points, say τ_n, with probability P thus terminating the

random walk chain, or it may continue on to the next point τ_{n+1} with proba-

bility Q. The selective process is continued until termination occurs.

The mathematical model can be developed by considering a random walk

chain consisting of a sequence of points $\{\tau_n\}$ at which are assigned definite probabilities of continuing or stopping the chain. Let

$$q_n(\tau_0, \cdots \tau_n) = \text{Probability of continuing the chain with sequence } \{\tau_n\}$$

$$\text{beyond point } \tau_n.$$

$$p_n(\tau_0, \cdots \tau_n) = \text{Probability of terminating the chain with sequence}$$

$$\{\tau_n\} \text{ at point } \tau_n.$$

where

$$p_n(\tau_0, \cdots \tau_n) + q_n(\tau_0, \cdots \tau_n) = 1, \text{ for all } n$$

and

$$0 < p_n(\tau_0, \cdots \tau_n) \leq 1, \text{ for all } n$$

$$(3\text{-}1)$$

Also let

$$f_0(\tau_0) = \text{the probability density function of } \tau_0, \; n=0$$

and

$$f_n(\tau_n \mid \tau_0, \cdots \tau_{n-1}) = \text{the conditional probability density function of}$$

$$\tau_n, \text{ providing the particle was not absorbed at}$$

$$\text{any preceding point of the chain, } n > 0.$$

It is noted that $f_n(\tau_n \mid \tau_0, \cdots \tau_{n-1})$ is written as a density function conditioned on the previous points of the chain and also that both p_n and q_n are allowed to depend on all previous collision points. This dependence is actually more general than we need in later work. In accordance with these definitions a random walk chain can be constructed by the following process:

1. Select τ_0 from the density function $f_0(\tau_0)$.

2. Decide termination (with probability $p_0(\tau_0)$) or continuation (with probability $q_0(\tau_0)$).

3. If continuation is selected then select τ_1 from the conditional

   density function $f_1(\tau_1|\tau_0)$.

4. Decide termination (with probability $p_1(\tau_0,\tau_1)$) or continuation

   (with probability $q_1(\tau_0,\tau_1)$).

5. If continuation is selected, continue the process by selecting

   decisions from appropriate probabilities of the next higher

   subscript until termination occurs.

In general, if previous n decisions are of continuation type and the se-

quence $(\tau_0,\tau_1,\cdots\tau_{n-1})$ has been generated, then select τ_n from the condi-

tional density function $f_n(\tau_n|\tau_0,\cdots\tau_{n-1})$.

Let us assume that termination occurs at τ_n with probability

$p_n(\tau_0,\cdots\tau_n)$, this random walk chain may then be represented by the nota-

tion

$$C_n = \left\{ (\tau_0,q_0(\tau_0)),\ (\tau_1,q_1(\tau_1)), \right.$$

$$\left. \cdots(\tau_{n-1},q_{n-1}(\tau_0,\cdots\tau_{n-1})),\ (\tau_n,p_n(\tau_0,\cdots\tau_n)) \right\}$$

The length of the random walk chain is defined as the subscript correspond-

ing to that phase point, among the sequence $(\tau_0,\tau_1,\tau_2,\cdots)$, at which a ter-

mination event was selected. Let L represent the chain length, which is

equal to n for the random walk chain, C_n. It is noted that the chain must

be of finite length in order to represent physical problems.

The probability density function, $f_n(\tau_0,\cdots\tau_n)$, for the chain of length

n and sequence $\{\tau_n\}$ can be determined by an iterative procedure from the

conditional density function governing the chain. It is in fact defined by

$$f_n(\tau_o, \cdots \tau_n) = f_n(\tau_n | \tau_o, \cdots \tau_{n-1}) \cdot f_{n-1}(\tau_o, \cdots \tau_{n-1}) \qquad (3\text{-}2)$$

By successive application of the definition, then

$$f_n(\tau_o, \cdots \tau_n) = f_n(\tau_n | \tau_o, \cdots \tau_{n-1}) \cdot f_{n-1}(\tau_{n-1} | \tau_o, \cdots \tau_{n-2})$$

$$\qquad (3\text{-}3)$$

$$\cdots f_2(\tau_2 | \tau_o, \tau_1) \cdot f_1(\tau_1 | \tau_o) \cdot f_o(\tau_o)$$

$$= \left(\prod_{m=1}^{n} f_m(\tau_m | \tau_o, \cdots \tau_{m-1}) \right) \cdot f_o(\tau_o) \qquad (3\text{-}4)$$

A random walk process consists of a sequence of random walk chains usually of variable length. Therefore, a random walk process is represented by a sequence of density functions $\{f_n(\tau_o, \cdots \tau_n)\}$ and a sequence of functions $\{q_n(\tau_o, \cdots \tau_n)\}$ and $\{p_n(\tau_o, \cdots \tau_n)\}$. For a random walk process certain valuable probabilities can be obtained. Let

$P\{L=n\} \equiv$ The probability that the chain length is exactly n.

Descriptively this would be the probability that among all possible chains the first n-1 collisions that occur are scattering collisions and that the nth collision is an absorption collision. Mathematically for the random walk process this probability is

$$P\{L=n\} \;=\; \int\limits_{\tau_0} f_0(\tau_0)\, q_0(\tau_0)\, d\tau_0 \int\limits_{\tau_1} f_1(\tau_1|\tau_0)\, q_1(\tau_0,\tau_1)\, d\tau_1$$

$$\cdots \int\limits_{\tau_{n-1}} f_{n-1}(\tau_{n-1}|\tau_0,\cdots\tau_{n-2})\, q_{n-1}(\tau_0,\cdots\tau_{n-1})\, d\tau_{n-1}$$

$$\quad (3\text{-}5)$$

$$\cdot\int\limits_{\tau_n} f_n(\tau_n|\tau_0,\cdots\tau_{n-1})\, p_n(\tau_0,\cdots\tau_n)\, d\tau_n$$

By using Eq. (3-3) this can also be written in shortened form as

$$P\{L=n\} \;=\; \int\limits_{\tau_n}\cdots\int\limits_{\tau_0} f_n(\tau_0,\cdots\tau_n)\, p_n(\tau_0,\cdots\tau_n)\, \prod_{i=0}^{n-1} q_i(\tau_0,\cdots\tau_i)\, d\tau_0\cdots d\tau_n$$

$$\quad (3\text{-}6)$$

In accordance with the restriction that random walk chains must be of finite length, we must have

$$P\{L=\infty\} \;=\; 0$$

This is a natural condition to impose in order to process random walk chains by Monte Carlo.

An analog random walk for the neutron transport problem can be generated by using the kernel and source term of the neutron integral transport Eq. (2-15). For convenience, assume normalization of the source and make the following identifications:

$$q_n(\tau_0,\cdots\tau_n) \;=\; \int\limits_{\tau} K(\tau|\tau_n)\, d\tau \;=\; \frac{\Sigma_s(\tau_n)}{\Sigma_t(\tau_n)} \qquad (3\text{-}7)$$

In this case, $q_n(\tau_0,\cdots\tau_n)$ is independent of chain points $\tau_0,\cdots\tau_{n-1}$ and

physically represents the probability of the neutron suffering a scattering collision at τ_n given that the collision occured there, and therefore the probability of continuing the chain. Furthermore from Eq. (3-1), $p_n(\tau_o, \cdots \tau_n)$ represents the probability of an absorption collision.

$$p_n(\tau_o, \cdots \tau_n) \;=\; 1 - q_n(\tau_o, \cdots \tau_n) \;=\; \frac{\Sigma_a(\tau_n)}{\Sigma_t(\tau_n)} \qquad (3\text{-}8)$$

The conditional density function is given by

$$f_n(\tau_n | \tau_o, \cdots \tau_{n-1}) \;=\; \frac{K(\tau_n | \tau_{n-1})}{q_n(\tau_o, \cdots \tau_{n-1})} \;=\; \frac{\Sigma_t(\tau_{n-1})}{\Sigma_s(\tau_{n-1})} K(\tau_n | \tau_{n-1}) \quad (3\text{-}9)$$

which is normalized as can be seen by integrating over all τ_n. The probability density function for n=0 is related to the neutron source as follows, assuming that the source is normalized,

$$f_o(\tau_o)\, d\tau_o \;=\; \tilde{S}(\tau_o)\, d\tau_o \qquad (3\text{-}10)$$

Upon substituting (3-7) through (3-10) into (3-3), the probability density function for n > 0 is given by

$$f_n(\tau_o, \cdots \tau_n) d\tau_o \cdots d\tau_n \;=\; \left[\prod_{i=o}^{n-1} \frac{\Sigma_t(\tau_i)}{\Sigma_s(\tau_i)} K(\tau_{i+1} | \tau_i) \right] \tilde{S}(\tau_o) d\tau_o \cdots d\tau_n \quad (3\text{-}11)$$

Eqs. (3-10) and (3-11) are also normalized as can be shown by integrating over all τ_o through τ_n and under assumption that the source is normalized.

The procedure previously mentioned for constructing the random walk chains can now be used for this analog problem. However in order to use

Monte Carlo for processing these random walks, it is necessary to show that

this analog problem produces chains of finite length with probability <u>one</u>.

Equivalently we can show that the probability of a chain of infinite length

is zero by using the convergence criterion of the Neumann series. From Eq.

(3-6) the probability that the chain is of infinite length is just

$$P\{L=\infty\} = \lim_{m\to\infty} \int_{\tau_m}\cdots\int_{\tau_0} f_m(\tau_0,\cdots\tau_m) \prod_{i=0}^{m} q_i(\tau_0,\cdots\tau_i)\ d\tau_0\cdots d\tau_m \qquad (3\text{-}12)$$

After substituting Eqs. (3-11) and (3-7) into Eq. (3-12) one obtains, after

simplification

$$P\{L=\infty\} = \lim_{m\to\infty} \int_{\tau_m}\cdots\int_{\tau_0} \frac{\Sigma_s(\tau_m)}{\Sigma_t(\tau_m)}\left[\prod_{i=0}^{m-1} K(\tau_{i+1}|\tau_i)\right]\tilde{S}(\tau_0)\ d\tau_0\cdots d\tau_m$$

$$\qquad (3\text{-}13)$$

$$= \lim_{m\to\infty} \int_{\tau_{m+1}}\cdots\int_{\tau} \left[\prod_{i=0}^{m} K(\tau_{i+1}|\tau_i)\right]\tilde{S}(\tau_0)\ d\tau_0\cdots d\tau_{m+1}$$

Since the source and kernel are non-negative quantities the inequality of

Eqs. (2-3) and (2-37), can be used in Eq. (3-13), obtaining

$$P\{L=\infty\} \le \lim_{m\to\infty} \left(\frac{\Sigma_s}{\Sigma_t}\right)^{m+1}_{max} \int_{\tau} \tilde{S}(\tau)\ d\tau$$

$$\qquad (3\text{-}14)$$

$$= 0$$

It is thus noted that the analog random walk chain is of finite length in

the applications where the Neumann series converges.

As mentioned in the previous chapter, we are concerned with evaluating

integrals of the form

$$I = \int_T w(\tau)\, \psi(\tau)\, d\tau \qquad (2\text{-}41)$$

where ψ is a solution of the integral Eq. (2-15).

It is desirable to obtain an estimator which when used in conjunction with the random walk process will give an unbiased estimate of I. Suppose $\hat{I}$ represents the random variable (or estimator) which is evaluated as the random walk chains are processed by Monte Carlo. After N histories of random walk chains are processed, the average of the estimator is given by

$$\bar{I} = \frac{1}{N} \sum_{j=1}^{N} \hat{I}(j) \qquad (3\text{-}15)$$

where N = total number of histories

  = total number of random chains

The requirement that $\bar{I}$ be an unbiased estimate of I is just that the expected value of $\bar{I}$ equals I,

$$E\{\bar{I}\} = I \qquad (3\text{-}16)$$

Let it be assumed that the estimator is evaluated only at the termination point of each chain. In order to identify the chain length with each history a special function, called a characteristic function (or indicator), is introduced. It is defined as

$$\chi_n(j) = \begin{cases} 1, & \text{if } j\underline{^{th}} \text{ history terminated at } \tau_n;\,(L=n) \\ 0, & \text{otherwise} \end{cases}$$

The estimator $\hat{I}$ can now be defined as

$$\hat{I}(j) = \lim_{k \to \infty} \sum_{n=0}^{k} \chi_n(j) \, \hat{I}_n(\tau_0, \cdots \tau_n) \qquad (3\text{-}17)$$

and the Eq. (3-15) can be written as

$$\bar{I} = \frac{1}{N} \lim_{k \to \infty} \sum_{j=1}^{N} \sum_{n=0}^{k} \chi_n(j) \, \hat{I}_n(\tau_0, \cdots \tau_n) \qquad (3\text{-}18)$$

where $\hat{I}_n$ can be called the partial estimator corresponding to histories terminating at τ_n. For unbiasedness, we must now determine $\hat{I}_n$ such that

$$E\{\hat{I}\} = E\{\bar{I}\} = I \qquad (3\text{-}19)$$

(The first equality in (3-19) is known from probability theory.[37]) It is convenient to employ conditional expectations to show unbiasedness. Using the property of the characteristic function, Eq. (3-19) becomes

$$E\{\hat{I}\} = E\left\{ \lim_{k \to \infty} \sum_{n=0}^{k} \chi_n(j) \, \hat{I}_n(\tau_0, \cdots \tau_n) \right\}$$

$$\qquad (3\text{-}20)$$

$$= \lim_{k \to \infty} \sum_{n=0}^{k} E\{\hat{I}_n | L=n\} \cdot P\{L=n\}$$

Because of (3-14) it is noted

$$P\{L < \infty\} = \lim_{k \to \infty} \sum_{n=0}^{k} P\{L=n\} = 1 \qquad (3\text{-}21)$$

The conditional expectations are of the form:

$$E\{\hat{I}|L=n\} = \int_{\tau_n}\cdots\int_{\tau_0} \hat{I}_n \, h_n(\tau_0,\cdots\tau_n|L=n) \, d\tau_0\cdots d\tau_n \qquad (3\text{-}22)$$

where h_n is the conditional probability density of chain C_n, conditioned on a chain of length exactly n,

$$h_0(\tau_0|L=0) = \frac{f_0(\tau_0)\,p_0(\tau_0)}{P\{L=0\}} \qquad (3\text{-}23)$$

and

$$h_n(\tau_0,\cdots\tau_n|L=n) = \frac{f_n(\tau_0,\cdots\tau_n)\left[\prod_{i=0}^{n-1} q_i(\tau_0,\cdots\tau_i)\right]p_n(\tau_0,\cdots\tau_n)}{P\{L=n\}} \quad (3\text{-}24)$$

Using Eqs. (3-22), (3-23), and (3-24) in Eq. (3-20),

$$E\{\hat{I}\} = \lim_{k\to\infty}\sum_{n=0}^{k}\int_{\tau_n}\cdots\int_{\tau_0}\hat{I}_n\,f_n(\tau_0,\cdots\tau_n)\prod_{i=0}^{n-1}q_i(\tau_0,\cdots\tau_i)$$

$$\cdot\, p_n(\tau_0,\cdots\tau_n)\,d\tau_0\cdots d\tau_n \qquad (3\text{-}25)$$

Upon substituting Eqs. (3-7) through (3-11) into (3-25) there results,

$$E\{\hat{I}\} = \int_{\tau_0}\hat{I}_0(\tau_0)\,\tilde{S}(\tau_0)\,p_0(\tau_0)\,d\tau_0$$

$$+ \lim_{k\to\infty}\sum_{n=1}^{k}\int_{\tau_n}\cdots\int_{\tau_0}\hat{I}_n(\tau_0,\cdots\tau_n)\,p_n(\tau_0,\cdots\tau_n)\,K(\tau_n|\tau_{n-1}) \qquad (3\text{-}26)$$

$$\cdots K(\tau_1|\tau_0)\,\tilde{S}(\tau_0)\,d\tau_0\cdots d\tau_n$$

Equation (3-26) is now in the form to determine the proper estimator $\hat{I}_n(\tau_0,\cdots\tau_n)$ so that $\bar{I}$ is an unbiased estimate of I. Comparison of Eq.

(3-26) to the Neumann series solution of I (2-45), leads to the following

choice of the partial estimator $\hat{I}_n$,

$$\hat{I}_n(\tau_0, \cdots \tau_n) = \frac{w(\tau_n)}{p_n(\tau_0, \cdots \circ \tau_n)} = \frac{\Sigma_t(\tau_n)}{\Sigma_a(\tau_n)} w(\tau_n) \qquad (3\text{-}27)$$

The division of w by p_n can be understood physically by recalling that the

estimator is averaged with respect to the termination of the random walk

chains which is analogous to capture density, however in order to obtain

I from the integral equation, w was averaged with respect to neutron coll-

sion density.

The proper derivative estimator for the integral $\partial I/\partial \alpha$ (2-50) can be

determined in a manner similar to the foregoing analysis for the estimator

of the integral I (2-41). Then after referring to the Neumann series solu-

tion of $\partial I/\partial \alpha$ (2-51), the proper choice for the partial differential esti-

mator is

$$\hat{DI}_0(\tau_0) = \left[\frac{1}{w(\tau_0)} \frac{\partial w_0}{\partial \alpha} + \frac{1}{\tilde{S}(\tau_0)} \frac{\partial \tilde{S}_0}{\partial \alpha} \right] \frac{w(\tau_0)}{p_0(\tau_0)}; \ n=0$$

and

$$\hat{DI}_n(\tau_0, \cdots \tau_n) = \left[\frac{1}{w(\tau_n)} \frac{\partial w_n}{\partial \alpha} + \frac{1}{K_n} \frac{\partial K_n}{\partial \alpha} + \cdots \qquad (3\text{-}28) \right.$$

$$\left. + \frac{1}{K_1} \frac{\partial K_1}{\partial \alpha} + \frac{1}{\tilde{S}(\tau_0)} \frac{\partial \tilde{S}_0}{\partial \alpha} \right] \frac{w(\tau_n)}{p_n(\tau_0, \cdots \tau_n)} ; \ n \geq 1$$

where the notations are the same as in Chapter II (2-52) through (2-54).

Because of the derivatives involved in estimator (3-28), the derivative

estimator is explicitly dependent on previous collision points of the random walk chain whereas the estimator (3-27) is dependent only on the terminal point of the chain for neutron transport phenomena. The estimate of the differentiated integral is given by the average of the partial derivative estimators.

$$\overline{DI} \;=\; \frac{1}{N} \sum_{j=1}^{N} \widehat{DI}(j) \tag{3-29}$$

$$= \frac{1}{N} \lim_{k \to \infty} \sum_{j=1}^{N} \sum_{n=0}^{k} \chi_n(j)\, \widehat{DI}_n(\tau_o, \cdots \tau_n) \tag{3-30}$$

where $\chi_n(j)$ is the same characteristic function defined previously.

By using the Monte Carlo method to generate the individual random walk chains of the analog process and thus averaging the partial estimators (3-27) and (3-29), estimates of the individual terms of the Neumann series solution of the integrals I(2-45) and $\partial I/\partial\alpha$(2-51) can be obtained.

B. FORMULATION OF RANDOM WALK CHAINS FOR NON-ANALOG PROCESSES

The techniques and mathematical descriptions of the random walk process developed in the previous section serve as basis for this section in which we consider the use of non-analog chains. These random walk chains may be completely arbitrary as long as the condition of finite length with probability one holds.

In Chapter II it was discussed that the kernel of the integral equation and of the Neumann series could be modified without mathematically

effecting the solution, if the correct weighting factor was introduced to compensate for the modification. Similarily, non-physical kernel and source terms will be used in this section. If this modified kernel is then used to govern the random walk chain, then a non-analog process would be produced. Let

$$C_n' = \left\{ (\tau_0, q_0'(\tau_0)), \cdots (\tau_{n-1}, q'_{n-1}(\tau_0, \cdots \tau_{n-1})), (\tau_n, p_n'(\tau_0, \cdots \tau_n)) \right\}$$

represent a random walk chain of length n that is determined by the arbitrary kernel $K'(\tau | \tau')$ and arbitrary source $\tilde{S}'(\tau)$. The source and kernel may be completely arbitrary except that they must have the properties required in Chapter II and in addition determine finite random walk chains. The continuation and termination probabilities and the conditional density function governing the chain C_n' are defined as follows:

$$q_n'(\tau_0, \cdots \tau_n) = \int_\tau K'(\tau | \tau_n) \, d\tau \qquad (3\text{-}31)$$

$$p_n'(\tau_0, \cdots \tau_n) = 1 - q_n'(\tau_0, \cdots \tau_n) \qquad (3\text{-}32)$$

$$f_n'(\tau_n | \tau_0, \cdots \tau_n) = \frac{K'(\tau_n | \tau_{n-1})}{q'_{n-1}(\tau_0, \cdots \tau_{n-1})} \qquad (3\text{-}33)$$

The probability density functions governing the chain C_n' are obtained as in Section III-A.

$$f_0'(\tau_0) \, d\tau_0 = \tilde{S}'(\tau_0) \, d\tau_0; \quad n=0 \qquad (3\text{-}34)$$

$$f_n{}'(\tau_o,\cdots\tau_n)d\tau_o\cdots d\tau_n = f_n{}'(\tau_n|\tau_o\cdots\tau_{n-1})\cdots f_1{}'(\tau_1|\tau_o)f_o{}'(\tau_o)d\tau_o\cdots d\tau_n$$

$$= \prod_{i=o}^{n-1} \frac{K'(\tau_{i+1}|\tau_i)}{q_i{}'(\tau_o,\cdots\tau_i)}\ \widetilde{S}'(\tau_o)d\tau_o\cdots d\tau_n;\ n \geq 1 \tag{3-35}$$

Equations (3-33), (3-34), and (3-35) are normalized as can be shown by integrating over all τ_n, τ_o, and τ_o through τ_n, respectively, and under the assumption that the source $\widetilde{S}'(\tau)$ is normalized.

The random walk process for this non-analog problem is now represented by a sequence of density functions $\{f_n{}'(\tau_o,\cdots\tau_n)\}$ and a sequence of functions $\{q_n{}'(\tau_o,\cdots\tau_n)\}$ and $\{p_n{}'(\tau_o,\cdots\tau_n)\}$. As in the previous section, the conditional probability density, $h_n{}'$, conditioned on a chain $C_n{}'$ of length exactly n will be needed for this non-analog process. It is given by

$$h_o{}'(\tau_o|L=0)\ =\ \frac{f_o{}'(\tau_o)\ p_o{}'(\tau_o)}{P\{L=n\}}\ ;\ n\ =\ 0 \tag{3-36}$$

and

$$h_n{}'(\tau_o,\cdots\tau_n|L=n)\ =\ \frac{f_n{}'(\tau_o,\cdots\tau_n)\ \prod\limits_{i=o}^{n-1} q_i{}'(\tau_o,\cdots\tau_i)\ p_n{}'(\tau_o,\cdots\tau_n)}{P\{L=n\}};\ n\geq 1$$

$$\tag{3-37}$$

In order to estimate the integral I(2-41) by the use of non-analog chains processed by Monte Carlo, the proper estimator must first be determined. As in Section III-A, an estimator is acceptable only if it gives an unbiased estimate of the integral I, i.e.,

$$E\{\hat{I}'\}\ =\ I \tag{3-38}$$

where

$$\hat{I}'(j) = \lim_{k \to \infty} \sum_{n=o}^{k} \chi_n(j) \, \hat{I}_n'(\tau_o, \cdots \tau_n) \qquad (3\text{-}39)$$

where the characteristic $\chi_n(j)$ assumes the same definition as in Section III-A and where $\hat{I}_n'$ is the partial estimator corresponding to histories terminating at τ_n for the non-analog random walk chain C_n'. After N histories have been generated by Monte Carlo the estimate of I is given by

$$\bar{I}' = \frac{1}{N} \sum_{j=1}^{N} \hat{I}'(j) \qquad (3\text{-}40)$$

The proper estimator is again determined by the use of conditional probabilities and the density functions governing the non-analog random walk chain,

$$E\{\hat{I}'\} = \lim_{k \to \infty} \sum_{n=o}^{k} E\{\hat{I}_n' | L'=n\} \cdot P\{L'=n\} \qquad (3\text{-}41)$$

where the conditional expectations are equal to

$$E\{\hat{I}_n' | L'=n\} = \int_{\tau_n} \cdots \int_{\tau_o} \hat{I}_n' \, h_n'(\tau_o, \cdots \tau_n | L'=n) \, d\tau_o \cdots d\tau_n \qquad (3\text{-}42)$$

After using Eqs. (3-31) through (3-37) in Eq. (3-42), and then substitute-ing the result into Eq. (2-41), the expected value of the estimator $\hat{I}'$ can be written as

$$E\left\{\hat{I}'\right\} = \int_{\tau_o} \hat{I}_o' \ \tilde{S}'(\tau_o) \ p_o'(\tau_o) d\tau_o$$

$$+ \lim_{k\to\infty} \sum_{n=1}^{k} \int_{\tau_n}\cdots\int_{\tau_o} \hat{I}_n'(\tau_o,\cdots\tau_n) p_n'(\tau_o,\cdots\tau_n) \prod_{i=o}^{n-1} K'(\tau_{i+1}|\tau_i)$$

$$\cdot \ \tilde{S}'(\tau_o) d\tau_o\cdots d\tau_n \tag{3-43}$$

The selection of partial estimator $\hat{I}'_n$ such that the expected value

of $\hat{I}'$ equals I, is obtained by comparing Eq. (3-43) with (2-57), this gives

$$\hat{I}'_n(\tau_o,\cdots\tau_n) = \frac{w(\tau_n)}{p'_n(\tau_o,\cdots\tau_n)} W_n(\tau_o,\cdots\tau_n) \tag{3-44}$$

where the weighting function is given by

$$W_o(\tau_o) = \frac{\tilde{S}(\tau_o)}{\tilde{S}'(\tau_o)} \ ; \ n = 0 \tag{3-45}$$

$$W_n(\tau_o,\cdots\tau_n) = \frac{K(\tau_n|\tau_{n-1})\cdots K(\tau_1|\tau_o) \ \tilde{S}(\tau_o)}{K'(\tau_n|\tau_{n-1}) \quad K'(\tau_1|\tau_o) \ \tilde{S}'(\tau_o)}; \ n \geq 1 \tag{3-46}$$

or expressed in terms of the probability density functions governing the

analog and non-analog random walk chains, by

$$W_n(\tau_o,\cdots\tau_n) = \frac{f_n(\tau_o,\cdots\tau_n) \prod_{i=o}^{n-1} q_i(\tau_o,\cdots\tau_n)}{f'_n(\tau_o,\cdots\tau_n) \prod_{i=o}^{n-1} q'_i(\tau_o,\cdots\tau_n)} \tag{3-47}$$

By using the same techniques as above, the proper choice for the par-

tial derivative estimator in the non-analog process can be obtained. Refer-

ring to Eq. (2-60), it is given by

$$\hat{DI}'_o(\tau_o) \;=\; \left[\frac{1}{w(\tau_o)} \frac{\partial w_o}{\partial \alpha} + \frac{1}{S(\tau_o)} \frac{\partial S_o}{\partial \alpha} \right] \frac{w(\tau_o)}{p'_o(\tau_o)} W_o(\tau_o); \quad n=0 \qquad (3\text{-}48)$$

$$\hat{DI}'_n(\tau_o,\cdots\tau_n) \;=\; \left[\frac{1}{w(\tau_n)} \frac{\partial w_n}{\partial \alpha} + \frac{1}{K_n} \frac{\partial K_n}{\partial \alpha} + \cdots \frac{1}{K_1} \frac{\partial K_1}{\partial \alpha} + \frac{1}{\tilde{S}(\tau_o)} \frac{\partial S_o}{\partial \alpha} \right] \qquad (3\text{-}49)$$

$$\cdot \; \frac{w(\tau_n)}{p'_n(\tau_o,\cdots\tau_n)} W_n(\tau_o,\cdots\tau_n) \; ; \; n \geq 1$$

where the notations are the same as in Chapter II, (2-52) through (2-54), and where the weighting factor is given by (3-45) and (3-46).

The estimate of the differentiated integral (2-50) is given by the average of the partial derivative estimators, averaged over N histories of the non-analog process.

$$\overline{DI}' \;=\; \frac{1}{N} \sum_{j=1}^{N} \hat{DI}'(j) \qquad (3\text{-}50)$$

where

$$\hat{DI}'(j) \;=\; \lim_{k\to\infty} \sum_{n=0}^{k} \chi_n(j) \, \hat{DI}'_n(\tau_o,\cdots\tau_n) \qquad (3\text{-}51)$$

Referring to Eqs. (3-44), (3-48) and (3-49), it is noted that both the partial estimator and partial derivative estimator for the non-analog process are explicitly dependent on all the phase points of the given random walk chain. Furthermore the probability of termination $p'_n(\tau_o,\cdots\tau_n)$ occurs in the denominators since the integrals I and $\partial I/\partial \alpha$ represent averages with respect to neutron collision density and not with respect to capture density.

CHAPTER IV

MONTE CARLO APPROACH

In this chapter the Monte Carlo chains are specialized to the neutron slowing down problems in a reactor. Implicit in this case is the fact that neutrons undergo only energy degrading collisions. Usually a neutron is introduced at some high initial energy and followed by random walk process until it is absorbed or its energy has decreased below some cutoff energy, which is above thermal energies. Certain properties can be obtained by averaging reactor parameters over the points of the random walk chain.

In the first section a non-analog process is formulated, which forces all collisions to be scattering collisions. It is then necessary to prove that the chain is finite with probability one and to determine the proper estimator that gives an unbiased estimate of the desired property. In order to obtain the proper estimator, the use of expected values is evolved from this non-analog process, i.e., the probability of terminating the chain by absorption is analytically calculated and also the quantity to be averaged is evaluated at each chain point not at just the terminal point. In practice, when the contribution of succeeding chain points to the averaged quantity becomes negligible, the chain is terminated even though the neutron energy may be greater than the cutoff energy.

In Section IV-B the non-analog slowing down problem is further specialized to obtaining information about resonance absorption probability and Doppler temperature coefficient. A heterogeneous reactor with infinite

lattice array is assumed; therefore, a single cell can be considered into which a neutron source is introduced and in which the neutrons undergo perfect reflection at the cell boundaries, i.e., angle of reflection equals angle of incidence.

In order to utilize experimentally obtained parameters describing the resonances, the fuel cross sections are expressed as a function of the Breit-Wigner formula. By neglecting any temperature expansion of fuel materials, all the temperature dependence for this problem is contained in the Doppler broadened cross sections, which are expressable in terms of the Doppler broadening functions. The estimators as well as the transport kernel used in generating the random walk chains are functions of the temperature dependent Doppler broadening functions. In addition the derivative estimators are related to the derivatives with respect to temperature of the Doppler broadening functions.

A. SPECIALIZATION TO SLOWING DOWN PROBLEMS IN A REACTOR LATTICE

For this type of problem it is convenient to use a high energy source and a non-analog process which forces all collisions to be scattering collisions, but being careful that an unbiased estimate of the desired reactor property is obtained. The chains are terminated only when the neutron energy is less than some arbitrary cutoff energy. Since all collisions are forced to be scattering collisions, the collision kernel in Chapter II is accordingly modified by replacing the ratio Σ_s/Σ_t by one. In this case H is normalized and is given by

$$H(\tau_n | \tau_{n-1}) = \frac{K(\tau_n | \tau_{n-1})}{\Sigma_s(\tau_{n-1})/\Sigma_t(\tau_{n-1})} \tag{4-1}$$

$$= T(\underline{r}_n | \underline{r}_{n-1}; E_n, \underline{\Omega}_n) \frac{\Sigma_s(E_n, \underline{\Omega}_n | E_{n-1}, \underline{\Omega}_{n-1}, \underline{r}_{n-1})}{\Sigma_s(E_{n-1}, \underline{r}_{n-1})} \tag{4-2}$$

The random walk chains are governed by the following probability density

function, termination, and continuation probabilities, respectively:

$$d_n(\tau_o, \cdots \tau_n), \ p^*(\tau_n), \ q^*(\tau_n)$$

where

$$d_n(\tau_n | \tau_o, \cdots \tau_n) = H(\tau_n | \tau_{n-1}) \tag{4-3}$$

$$q^*(\tau_n) = \begin{cases} 0, & \text{if } E_n < E_{cutoff} \\ 1, & \text{otherwise} \end{cases} \tag{4-4}$$

$$p^*(\tau_n) = 1 - q^*(\tau_n) \tag{4-5}$$

and therefore the probability density function for τ_n is given by

$$d_n(\tau_o, \cdots \tau_n) = d_n(\tau_n | \tau_o, \cdots \tau_{n-1}) \ d_{n-1}(\tau_{n-1} | \tau_o, \cdots \tau_{n-2}) \cdots d_o(\tau_o)$$

$$\tag{4-6}$$

$$= H(\tau_n | \tau_{n-1}) \cdots H(\tau_1 | \tau_o) \ \tilde{S}(\tau_o)$$

For convenience the source is assumed normalized in this section. It is

noted that the values of p* and q* do not depend on the sample sequence

but rather are determined by the given phase point in the chain.

As mentioned in Chapter III, the non-analog chains may be completely

arbitrary, provided the chain has probability one of being finite. There-
fore, as in Section III-A, it is necessary that the probability of generat-
ing a chain of infinite length is zero. This probability is given by

$$P\{L=\infty\} = \lim_{m\to\infty} \int_{\tau_m}\cdots\int_{\tau_0} d_m(\tau_0,\cdots\tau_m) \prod_{i=0}^{m} q^*(\tau_i)\, d\tau_0\cdots d\tau_m$$

$$(4\text{-}7)$$

$$= \lim_{m\to\infty} \int_{\tau_m}\cdots\int_{\tau_0} q^*(\tau_m)\, \tilde{S}(\tau_0) \prod_{i=0}^{m-1} H(\tau_{i+1}|\tau_i)\, q^*(\tau_i)\, d\tau_0\cdots d\tau_m$$

Because of the nature of q* in this non-analog problem for a hetero-
geneous lattice, it is difficult to simplify this expression and show that
the limit is zero directly. However it is shown in Appendix D by physical
arguments that the above process is finite with probability one. Since
elastic collisions in the epi-thermal region are energy degrading, it
seems reasonable that the neutron energy will decrease below the cutoff
energy in a finite number of collisions.

By combining the use of expected values with this non-analog chain,
it is possible to obtain more information from a given chain and hence a
more efficient determination of the desired reactor property. Briefly,
the use of expected values involves analytically calculating the expected
value of a random variable rather than using a sample value. For the prob-
lem of interest the use of expected values is applied by calculating at
each chain point the true probability of absorption, Σ_a/Σ_t, and multiply-
ing this by the quantity to be averaged, w, at each chain point. The esti-
mator for this problem will now be determined.

The random walk process governed by Eqs. (4-1) through (4-6) has the following conditional density function, conditioned on the chain length exactly n.

$$b_n(\tau_0, \cdots \tau_n | L=n) = \frac{d_n(\tau_0, \cdots \tau_n) \; p^*(\tau_n) \prod\limits_{i=0}^{n-1} q^*(\tau_i)}{P\{L=n\}} \qquad (4-8)$$

$$= \frac{p^*(\tau_n) \; \tilde{S}(\tau_0) \prod\limits_{i=0}^{n-1} H(\tau_{i+1} | \tau_i) \; q^*(\tau_i)}{P\{L=n\}} \qquad (4-9)$$

But the termination of the chain is determined only by the energy of the last point, i.e., the chain terminates only when a phase point has energy less than the cutoff energy.

In the previous chapter the estimator contributed to the knowledge of the integral I(2-41) only at the termination point of the chain, although it was allowed to depend on all previous points. However since each chain point can contribute to the estimate of I in this chapter, the estimator is written

$$\bar{I} = \frac{1}{N} \lim_{k \to \infty} \sum_{j=1}^{N} \sum_{n=0}^{k} \chi_n(j) \; \hat{I}_n(\tau_0, \cdots \tau_n) \qquad (4-10)$$

where *

$$\hat{I}_n(\tau_0, \cdots \tau_n) = \sum_{m=0}^{n} I^*_m(\tau_0, \cdots \tau_m) \qquad (4-11)$$

---

*Spanier[28] has shown that by using the integral equation adjoint to (2-15) and (2-41), a random variable determined by summing over all the phase points in the chain can be an unbiased random variable for an analog random walk process. In the investigation of slowing down problems, we obtain the proper estimator for I(2-41) for a non-analog process without relying on the adjoint equation.

As in Chapter III

$$\hat{I}(j) = \lim_{k \to \infty} \sum_{n=0}^{k} \chi_n(j) \; \hat{I}_n(\tau_0, \cdots \tau_n) \tag{4-12}$$

where $\chi_n(j)$ is the same as defined in Chapter III. According to the requirement of unbiasedness, $\hat{I}_n$ must be determined such that

$$E\{\hat{I}\} = I \tag{4-13}$$

Employing conditional expectations with the non-analog process,

$$E\{\hat{I}\} = E\left\{ \sum_{n=0}^{\infty} \sum_{m=0}^{n} \chi_n(j) \; I^*_m(\tau_0, \cdots \tau_m) \right\} \tag{4-14}$$

$$= \sum_{n=0}^{\infty} E\left\{ \sum_{m=0}^{n} I^*_m(\tau_0, \cdots \tau_m) \Big| L=n \right\} \; P\{L=n\} \tag{4-15}$$

But by Eq. (4-9),

$$E\left\{ \sum_{m=0}^{n} I^*_m(\tau_0, \cdots \tau_m) \Big| L=n \right\}$$

$$= \int_{\tau_n} \cdots \int_{\tau_0} \left(\sum_{m=0}^{n} I^*_m(\tau_0, \cdots \tau_m) \right) b_n(\tau_0, \cdots \tau_n | L=n) d\tau_0 \cdots d\tau_n \tag{4-16}$$

$$= \sum_{m=0}^{n} \int_{\tau_n} \cdots \int_{\tau_0} I^*_m(\tau_0, \cdots \tau_m) \frac{p^*(\tau_n) \; \tilde{S}(\tau_0) \prod_{i=0}^{n-1} H(\tau_{i+1}|\tau_i) \; q^*(\tau_i)}{P\{L=n\}} d\tau_0 \cdots d\tau_n$$

The next step is to substitute Eqs. (4-16) into (4-15) and employ the Cauchy product rule, which is given by

$$\sum_{n=0}^{\infty} \sum_{m=0}^{n} F(n,m) \;=\; \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} F(n+m,m) \;=\; \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} F(n,m)$$

Equation (4-15) becomes

$$E\{\hat{I}\} \tag{4-17}$$

$$= \sum_{n=0}^{\infty} \sum_{m=0}^{n} \int_{\tau_n} \cdots \int_{\tau_0} I^*_m(\tau_0, \cdots \tau_m) p^*(\tau_n) \tilde{S}(\tau_0) \prod_{i=0}^{n-1} H(\tau_{i+1}|\tau_i) q^*(\tau_i) d\tau_0 \cdots d\tau_n$$

$$= \sum_{m=0}^{\infty} \sum_{n=m}^{\infty} \int \cdots \int \text{ same integrand} \tag{4-18}$$

$$= \sum_{m=0}^{\infty} \int_{\tau_m} \cdots \int_{\tau_0} I^*_m(\tau_0, \cdots \tau_m) \prod_{i=0}^{m-1} H(\tau_{i+1}|\tau_i) \; q^*(\tau_i) \left\{ \begin{array}{c} \\ \\ \end{array} \right\} S(\tau_0) \; d\tau_0 \cdots d\tau_m$$

$$\tag{4-19}$$

where

$$\left\{ \begin{array}{c} \\ \\ \end{array} \right\} = p^*(\tau_m) + \sum_{n=m+1}^{\infty} \int_{\tau_n} \cdots \int_{\tau_{m+1}} p^*(\tau_n) \prod_{i=m}^{n-1} H(\tau_{i+1}|\tau_i) q^*(\tau_i) \; d\tau_{m+1} \cdots d\tau_n$$

$$\tag{4-20}$$

but since

$$p^*(\tau_n) \;=\; 1 - q^*(\tau_n) \text{ and} \int_{\tau_{i+1}} H(\tau_{i+1}|\tau_i) \; d\tau_{i+1} \;=\; 1$$

then

$$\int_{\tau_n}\cdots\int_{\tau_{m+1}} p^*(\tau_n) \prod_{i=m}^{n-1} H(\tau_{i+1}|\tau_i) \, q^*(\tau_i) \, d\tau_{m+1}\cdots d\tau_n$$

$$= q^*(\tau_m) \int_{\tau_{n-1}}\cdots\int_{\tau_{m+1}} \prod_{i=m+1}^{n-1} q^*(\tau_i) H(\tau_i|\tau_{i-1}) \, d\tau_{m+1}\cdots d\tau_{n-1} \qquad (4\text{-}21)$$

$$- q^*(\tau_m) \int_{\tau_n}\cdots\int_{\tau_{m+1}} \prod_{i=m+1}^{n} q^*(\tau_i) H(\tau_i|\tau_{i+1}) \, d\tau_{m+1}\cdots d\tau_n$$

Upon using Eq. (4-21), (4-20) becomes

$$\{\ \} = 1 - q^*(\tau_m) + q^*(\tau_m) \left[1 - \int_{\tau_{m+1}} q^*(\tau_{m+1}) H(\tau_{m+1}|\tau_m) \, d\tau_{m+1} \right]$$

$$+ q^*(\tau_m) \sum_{n=m+2}^{\infty} \int_{\tau_{n-1}}\cdots\int_{\tau_{m+1}} \left[1 - \int_{\tau_n} q^*(\tau_n) H(\tau_n|\tau_{n-1}) \, d\tau_n \right] \qquad (4\text{-}22)$$

$$\cdot \prod_{i=m+1}^{n-1} q^*(\tau_i) H(\tau_i|\tau_{i-1}) \, d\tau_{m+1}\cdots d\tau_{n-1}$$

After cancellation of like terms,

$$\{\ \} = 1 - \lim_{n\to\infty} q^*(\tau_m) \int_{\tau_n}\cdots\int_{\tau_{m+1}} \prod_{i=m+1}^{n} q^*(\tau_i) H(\tau_i|\tau_{i-1}) \, d\tau_{m+1}\cdots d\tau_n$$

$$\qquad (4\text{-}23)$$

$$= 1 \qquad (4\text{-}24)$$

Upon comparing the integral term in (4-23) to Eq. (4-7), the limit is zero

under the conditions of non-zero source and finiteness of the random walk

chains. Equation (4-15) now becomes

$$E\{\hat{I}\} =$$

$$= \sum_{m=0}^{\infty} \int_{\tau_m}\cdots\int_{\tau_0} I^*_m(\tau_0,\cdots\tau_m) \prod_{i=0}^{m-1} H(\tau_{i+1}|\tau_i)q^*(\tau_i)\tilde{S}(\tau_0)d\tau_0\cdots d\tau_m$$

$$(4\text{-}25)$$

$$= \int_{\tau_0} I^*_0(\tau_0)\ \tilde{S}(\tau_0)\ d\tau_0$$

$$(4\text{-}26)$$

$$+ \sum_{m=1}^{\infty} \int_{\tau_m}\cdots\int_{\tau_0} I^*_m(\tau_0,\cdots\tau_m) \prod_{i=0}^{m-1} H(\tau_{i+1}|\tau_i)\ \tilde{S}(\tau_0)\ d\tau_0\cdots d\tau_m$$

The $q^*(\tau_i)$ are all equal to one since the integral was conditioned on

a chain of length given by the index. Comparison of this series to the

Neumann series for I in Chapter II (2-57) leads to the following estimator

which satisfies the condition of unbiasedness:

$$I^*_m(\tau_0,\cdots\tau_m) = w(\tau_m)\ W_{m-1}(\tau_0,\cdots\tau_{m-1})$$

$$(4\text{-}27)$$

where

$$W_m(\tau_0,\cdots\tau_m) = \frac{\Sigma_s(\tau_m)}{\Sigma_t(\tau_m)}\cdots\frac{\Sigma_s(\tau_0)}{\Sigma_t(\tau_0)}$$

$$(4\text{-}28)$$

Therefore

$$\bar{I} = \frac{1}{N} \sum_{j=1}^{N} \sum_{n=0}^{\infty} \sum_{m=0}^{n} \chi_n(j)I^*_m(\tau_0,\cdots\tau_m)$$

$$(4\text{-}29)$$

is the estimate value of I(2-41) as determined by a Monte Carlo process generating non-analog random chains which terminate in a reactor only when the corresponding energy of the chain becomes less than some cutoff energy and in which each collision point of the chain contributes knowledge to the average value. In practice the chain may actually be terminated when the contributing knowledge becomes negligible (when the product of the ratios of Σ_s/Σ_t becomes $\ll 1$).

Because of the uniform convergence of the Neumann series representation of I(2-45) and $\partial I/\partial\alpha$(2-50), and the finiteness of the non-analog random walk chains in this chapter, the partial derivative estimator corresponding to $\partial I/\partial\alpha$ is determinable. By combining the methods of Chapter III and the preceding analysis of this chapter and referring to Eq. (2-60), the corresponding partial derivative estimator is found to be

$$DI^*_m(\tau_0, \cdots \tau_m) = w(\tau_m) \, W_{m-1}(\tau_0, \cdots \tau_{m-1}) \, DW_m(\tau_0, \cdots \tau_m) \quad (4\text{-}30)$$

where

$$DW_0(\tau_0) = \frac{1}{w(\tau_0)} \frac{\partial w_0}{\partial\alpha} + \frac{1}{\tilde{S}(\tau_0)} \frac{\partial \tilde{S}_0}{\partial\alpha} \quad (4\text{-}31)$$

and for $m \geq 1$

$$DW_m(\tau_0, \cdots \tau_m) = \frac{1}{w_m} \frac{\partial w_m}{\partial\alpha} + \frac{1}{K_m} \frac{\partial K_m}{\partial\alpha} + \cdots \frac{1}{K_1} \frac{\partial K_1}{\partial\alpha} + \frac{1}{\tilde{S}_0} \frac{\partial \tilde{S}_0}{\partial\alpha} \quad (4\text{-}32)$$

and where again the following notations are used:

$$w_m \equiv w(\tau_m) \quad (4\text{-}33)$$

$$K_m \equiv K(\tau_m | \tau_{m-1}) \quad (4\text{-}34)$$

$$\tilde{S}_o \equiv \tilde{S}(\tau_o) \tag{4-35}$$

The derivatives are evaluated at the chain points. Thence

$$\overline{DI} = \frac{1}{N} \sum_{j=1}^{N} \sum_{n=o}^{\infty} \sum_{m=o}^{n} \chi_n(j) \ DI^*_m(\tau_o, \cdots \tau_m) \tag{4-36}$$

is the Monte Carlo estimate of $\partial I/\partial\alpha$ (2-50).

B. SPECIALIZATION TO DOPPLER COEFFICIENT AND RESONANCE ESCAPE PROBABILITY

In this section the background provided by the previous sections are

applied to the specific problem of resonance absorption probability and

temperature coefficient in a heterogeneous reactor having a non-uniform

temperature in the fuel rod.

In order to determine the absorption probability, the random varia-

ble $w(\tau)$ is set equal to the ratio of neutron absorption cross section to

the total cross section. Recalling that ψ represents the collision density,

then

$$I = \int_R w(\tau) \ \psi(\tau) \ d\tau = \int_R \frac{\Sigma_a(\tau)}{\Sigma_t(\tau)} \ \psi(\tau) \ d\tau \tag{4-37}$$

represents the number of neutron absorptions per unit time in region R.

The resonance absorption probability can be thought of as the ratio of the

number of absorptions per unit time in the phase space with energy greater

than the thermal cutoff to the number of neutron births per unit time in

the same space. For numerical results this definition will be specialized

to the case of no absorptions in non-fuel regions. By using the nomenclature

p = Resonance escape probability

$1-p$ = Resonance absorption probability

then

$$1 - p = \frac{\int_R \frac{\Sigma_a(\tau)}{\Sigma_t(\tau)} \psi(\tau) \, d\tau}{\int_R \tilde{S}(\tau) \, d\tau} = \frac{I}{\bar{S}} \qquad (4\text{-}38)$$

where

R = region of the whole space τ with $E > E$ cutoff

$\bar{S}$ = number of source neutrons per unit time (or birth rate)

$$= \int_R \tilde{S}(\tau) \, d\tau = \int_R S(\tau) \, d\tau$$

The derivative with respect to temperature of the resonance absorption probability is given by

$$\frac{\partial(1-p)}{\partial T} = \frac{1}{\bar{S}} \frac{\partial I}{\partial T} = \int_R \frac{\partial}{\partial T} \left(\frac{\Sigma_a}{\Sigma_t} \psi \right) \frac{d\tau}{\bar{S}} \qquad (4\text{-}39)$$

That part of the temperature coefficient of reactivity due to absorptions of neutrons in the resonances of the fuel will be called the Doppler coefficient of reactivity, and is then given by

$$\frac{1}{p} \frac{\partial p}{\partial T} = \frac{-1}{\bar{S} - I} \frac{\partial I}{\partial T} \qquad (4\text{-}40)$$

$$= \frac{-\int_R \frac{\partial}{\partial T} \left(\frac{\Sigma_a}{\Sigma_t} \psi \right) d\tau}{\int_R S \, d\tau - \int_R \frac{\Sigma_a}{\Sigma_t} \psi \, d\tau} \qquad (4\text{-}41)$$

Since this work is concerned with the problem of temperature effects

due to the Doppler broadening of resonances in the fuel, any effects due

to changes in geometry or material density with temperature are purposely

neglected. Specifically, U-238 is considered in oxide form (UO_2) because

of its use in power reactors, although the methods proposed are valid for

the metal form. In order to exhibit the temperature dependence of the

fuel cross section explicitly, two assumptions are made, (1) the motion

of the fuel atoms which are bound in a crystal are described by the per-

fect gas model, i.e., their velocity distribution is approximated by the

Maxwell-Boltzmann distribution for free particles in a ideal gas, and (2)

the resonances of the fuel are spaced far enough apart that there is no

interaction among neighboring levels and therefore the single-level Breit-

Wigner formula[2,38] can be used to describe the microscopic cross section

in the center of mass coordinate system.

Lamb[24] studied the resonance capture of slow neutrons by atoms bound

in a crystal and developed a criterion for using the ideal gas model in

calculating the resonance cross section. The criterion depends on the

Debye temperature of the crystal, the natural width of the resonance, the

mass of the absorber nucleus, the neutron energy, and the environmental

temperature. According to Lamb's criterion the gas model is a good approx-

imation for the lowest resonance of U-238 (6.68ev) when the absorbing atoms

are bound in the metallic crystal at room temperature, and the approxima-

tion improves in accuracy with increase in temperature or with the higher

resonance levels. The uncertainty of the Debye temperature for uranium

dioxide does not allow reliable application of Lamb's criterion. The large

discrepancy among measurements and calculations of the Debye temperature

of uranium dioxide has been noted by Belle[21] who reported estimates vary-

ing from 160°K to 800°K. He does indicate that there is more evidence for

correctness of lower values, which would fulfill Lamb's criterion.

In 1960 Jackson, Bollinger, and Coté[39] performed an experiment for

determining the shape of the effective neutron cross section over the 6.68

ev. resonance peak of U-238. They observed no significant crystalline ef-

fect in uranium metal or U_3O_8 at room temperature. However at liquid ni-

trogen temperature a large discrepancy was noted between the observed shape

of the cross section in U_3O_8 and that predicted by the gas model correspond-

ing to the effective temperature given by Lamb. The authors used a Debye

temperature of about 450°K for U_3O_8 which corresponds to about the mean

in the Debye temperature range reported by Belle for UO_2. Since reactors

used for power purposes have fuel temperatures considerably above room

temperature, it appears that the gas model approximation is acceptable for

determination of the U-238 resonance cross section in both uranium metal

and UO_2.

The second assumption is substantiated by the experimental work of

Rosen, Dejardins, Rainwater, and Havens[40] in which they were able to re-

solve the individual resonances of U-238 in metal foils up to about 1000

ev. All but a few of the resonances were observed to be clearly separable.

Furthermore the resonances were sufficiently isolated that resonance pa-

rameters could be determined from the experimental data by a theoretical

analysis using the single level Breit-Wigner formula and the Maxwell-Boltz-mann distribution. In fact the authors use the same expressions for the Doppler broadened cross sections as those given by Eqs. (4-42) through (4-50).

The derivation of the Doppler broadened cross sections, using the single-level Breit-Wigner formula to describe the center of mass interaction probability and using the Maxwell-Boltzmann distribution to describe the motion of the struck nuclei, has been extensively investigated. Bethe and Placzek[3,41] and Dresner[42] make a basic approximation in their method, namely that the term involving the square of the ratio of atom speed divided by the neutron speed can be neglected in determining the kinetic energy of the neutron relative to the struck atom. This approximation is known as the Bethe approximation. Solbrig,[43] and Osborn (footnote in reference 44) both derive a more exact expression for the cross section, in which Solbrig later introduces approximations which he shows to be valid for incident neutron energies above .01ev and for heavy absorbers at temperatures not less than room temperature. Nordheim[9] has also investigated this latter method.

For the conditions present in this work, i.e., incident neutron and resonance energies above thermal energies, and fuel temperatures above room temperature, both methods produce the same expressions for the Doppler broadened neutron resonance cross sections. Since the experimentally determined resonance parameters are obtained from measurements in the laboratory coordinate system, the parameters in the usual expressions of Dop-

pler broadened cross sections should be appropriately modified by the ratio of neutron mass to reduced mass to take account of this fact. However for fuel nuclei this correction amounts to less than $\frac{1}{2}\%$ and will accordingly be neglected. Therefore all parameters in the following expressions for cross sections represent values in the laboratory coordinate system.

The Doppler broadened microscopic cross section for the capture of neutrons in the neighborhood of an isolated resonance is

$$\sigma_c(E,T) \;=\; \sigma_a\!\left(\frac{1}{v}\right) + \sigma_{co}\sqrt{\frac{E_o}{E}}\;\psi(x,\theta) \qquad (4\text{-}42)$$

The Doppler broadened microscopic cross section for the elastic scattering of neutrons in the neighborhood of an isolated resonance is

$$\sigma_s(E,T) \;=\; \sigma_p + \sigma_{so}\,\psi(x,\theta) + 2\sqrt{g\sigma_p\sigma_{so}}\;\chi(x,\theta) \qquad (4\text{-}43)$$

where $\sigma_a\!\left(\frac{1}{v}\right)$ and σ_p represent the background $"\frac{1}{v}"$ absorption cross section and potential scattering cross section respectively and where

$$\sigma_{co} \;=\; \sigma_o\frac{\Gamma_\gamma}{\Gamma} \qquad (4\text{-}44)$$

$$\sigma_{so} \;=\; \sigma_o\frac{\Gamma_{no}}{\Gamma} \qquad (4\text{-}45)$$

The unbroadened cross section for the formation of the compound nucleus, with neutron energy corresponding to the resonance peak, is

$$\sigma_o \;=\; 4\pi\lambda_o^2 g\,\frac{\Gamma_{no}}{\Gamma} \qquad (4\text{-}46)$$

where

E = energy of neutron in laboratory system.

E_o = energy of neutron corresponding to resonance peak.

λ_o = $\dfrac{\lambda_o}{2\pi}$, λ_o is the neutron wave length at resonance peak.

g = $\dfrac{2J+1}{2(2I+1)}$, I,J are the spins of target and compound nucleus respectively.

$\Gamma = \Gamma_{no} + \Gamma_\gamma$ = total resonance width, full width at half the maximum peak.

Γ_{no} = neutron width with $E = E_o$.

Γ_γ = capture width.

The Doppler broadening functions, also called spectroscopic integrals because of their original use in optics, are defined as

$$\psi'(x,\theta) \equiv \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\theta}} \frac{dy}{1+y^2} \qquad (4\text{-}47)$$

$$\chi(x,\theta) \equiv \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\theta}} \frac{ydy}{1+y^2} \qquad (4\text{-}48)$$

where

$$x = \frac{E - E_o}{\dfrac{\Gamma}{2}} \qquad (4\text{-}49)$$

$$\theta = \frac{4\,m\,k\,T\,E}{(m+M)\,\Gamma^2} \qquad (4\text{-}50)$$

m = mass of neutron

M = mass of target nucleus

T = Temperature of resonance medium

It is noted that the temperature dependence of the microscopic cross sections appear solely in the Doppler broadening functions. The potential scattering cross section is temperature independent for neutron energies above thermal.

In accordance with the restriction that there is no interaction between neighboring resonance levels and with the approximations discussed above, the total macroscopic cross section for a neutron of energy E is given by a simple sum of contributions from all the resonances, i.e.,

$$\Sigma_t(E,T) = N^A \left\{ \sigma_p + \sigma_a(1/v) \right.$$
$$\left. + \sum \left[(\sigma_{co}^i \sqrt{\frac{E_o^i}{E}} + \sigma_{so}^i) \, \psi(x^i,\theta^i) + 2\sqrt{g\sigma_p\sigma_{so}^{i-}} \, \chi(x^i,\theta^i) \right] \right\} \qquad (4\text{-}51)$$

where i represents the index of the resonance levels and N^A is the atom density of the resonance absorber.

For the sake of convenience in the mathematical description of the estimators and kernels in the random walk process, the cross sections will be written explicitly for only one resonance, the nearest dominating resonance, although the effect of the summation of resonances will be implied. In practice, for a given neutron energy the one resonance of U-238 or Th-232 with E_o nearest the neutron energy is dominant and all the rest of the resonances make a negligible contribution to the total cross section.

In the case where the fuel is a mixture of resonance atoms and non-resonance atoms, e.g., UO_2, let $\sigma_a(1/v)$ and σ_p be respectively the back-

ground absorption and potential scattering cross sections per atom of resonance absorber. Also let the total cross section in a reactor lattice composed of separate fuel and moderator regions be represented by the following notation:

$$\Sigma_t(\tau) = \left[N^A(\sigma_p^A + \sigma_a^A (1/v)) + \Sigma_{ra}^O \sqrt{\frac{E_o}{E}} \; \mathcal{Y}(x,\theta) \right.$$

$$\left. + \Sigma_{rs}^O \mathcal{Y}(x,\theta) + \Sigma_{ri}^O \mathcal{X}(x,\theta) \right] \eta(\tau) + \left[N^M(\sigma_p^M + \sigma_a^M (1/v)) \right] \nu(\tau)$$

(4-52)

where

$$\Sigma_{ra}^O = N^A \sigma_{co}^A \tag{4-53}$$

$$\Sigma_{rs}^O = N^A \sigma_{so}^A \tag{4-54}$$

$$\Sigma_{ri}^O = N^A 2\sqrt{g\sigma_p^A \sigma_{so}^A} \tag{4-55}$$

where the superscripts M and A denote the moderator and the resonance material respectively, and where η and ν are heterogeneity factors defined as

$$\eta(\tau) = \begin{cases} 1, & \text{if the neutron position } \underline{r} \text{ lies in the fuel.} \\ 0, & \text{otherwise.} \end{cases}$$

$$\nu(\tau) = \begin{cases} 1, & \text{if the neutron position } \underline{r} \text{ lies in the moderator.} \\ 0, & \text{otherwise.} \end{cases}$$

Recall that τ is the phase space vector of the neutron and thus denotes $(\underline{r}, E, \underline{\Omega})$. Also it is remarked that the temperature T is a function of $\underline{r}$, and hence of τ, since a general temperature distribution is allowed in the fuel. Thence the derivatives with respect to temperature of the cross sections are

$$\frac{\partial}{\partial T} \Sigma_t(\tau) \;=\; \frac{\partial}{\partial T} \Sigma_a(\tau) \;+\; \frac{\partial}{\partial T} \Sigma_s(\tau) \tag{4-56}$$

$$\frac{\partial}{\partial T} \Sigma_a(\tau) \;=\; \left[\Sigma_{ra}^{o} \sqrt{\frac{E_o}{E}} \; \frac{\partial \psi}{\partial T} \right] \eta(\tau) \tag{4-57}$$

$$\frac{\partial}{\partial T} \Sigma_s(\tau) \;=\; \left[\Sigma_{rs}^{o} \; \frac{\partial \psi}{\partial T} + \Sigma_{ri}^{o} \; \frac{\partial \chi}{\partial T} \right] \eta(\tau) \tag{4-58}$$

Methods of evaluating the derivative of the Doppler broadening functions are discussed in Appendix F.

One further approximation is necessary before writing explicitly the kernels governing the random walk chain. Once a scattering collision occurs, the scattering angle and new neutron energy must be selected from the collision kernel. When the neutron collides with a non-resonance nucleus there is no difficulty since the well known scattering frequency (4-60) for elastic collisions with struck particle at rest can be used for the neutron energies of interest, i.e., above thermal and below inelastic threshold energies. For collisions with resonance nuclei, this same frequency (4-60) is used for the scattering distribution. The assumption of struck particle at rest is harder to justify for collisions involving resonance nuclei and is investigated in Appendix E, where the resonance scattering frequency is formulated for the case of the target nucleus in motion, (E-8). Although the resonance cross section is effected by the motion of the struck particles, once a collision occurs and the decision is made that it is of a scattering type, then the dynamics of the scattering are similar to that in which the target is at rest since

the incident velocity of the neutron is much greater than that of the nucleus.

The collision kernels defined in Chapter II can now be written,

$$C(E,\underline{\Omega}|E',\underline{\Omega}';\underline{r}') \; dEd\Omega = \frac{\Sigma_s(\underline{r}',E')}{\Sigma_t(\underline{r}',E')} \; F(E'{\to}E;\underline{r}') \; dE \; \delta(\underline{\Omega} \cdot \underline{\Omega}' - g(E,E'))\frac{d\Omega}{4\pi}$$

$$(4\text{-}59)$$

Also $F(E'{\to}E,\underline{r}')$ becomes $F(E'{\to}E)$, once a decision is made as to the kind of nucleus involved in the scattering collision. The scattering frequency for an elastic collision with the struck nucleus of mass number A at rest is

$$F(E'{\to}E) \; dE \; = \; \frac{(A+1)^2}{4A} \frac{dE}{E'} \; ; \; \text{when} \; \left(\frac{A-1}{A+1}\right)^2 \; E' \leq E \leq E'$$

$$(4\text{-}60)$$

$$= \; 0 \qquad ; \; \text{otherwise}$$

Also

$$g(E,E') \; = \; \frac{A+1}{2} \sqrt{\frac{E}{E'}} - \frac{A-1}{2} \sqrt{\frac{E'}{E}} \qquad (4\text{-}61)$$

By utilizing the definition of the transport and collision kernels in Chapter II and Eqs. (4-59) and (4-60), the kernel H (4-5) for the non-analog process described in Section IV-B becomes

$$H(\tau|\tau')d\tau = e^{-\int_o^{|\underline{r}-\underline{r}'|} \Sigma_t(E,\underline{r}-\underline{\Omega}_R R')dR'} \; \delta_2(\underline{\Omega}\cdot\underline{\Omega}_R) \; \frac{\Sigma_t(E,\underline{r})}{|\underline{r}-\underline{r}'|^2} \; d^3r$$

$$(4\text{-}62)$$

$$\cdot \; F(E'{\to}E,\underline{r}') \; dE \; \delta(\underline{\Omega}\cdot\underline{\Omega}' - g(E,E')) \; \frac{d\Omega}{4\pi}$$

Thence the kernel K defined in Chapter II becomes

$$K(\tau|\tau')d\tau = e^{-\int_0^{|\underline{r}-\underline{r}'|} \Sigma_t(E,\underline{r}-\underline{\Omega}_R R')\, dR'} \quad \delta_2(\underline{\Omega}\cdot\underline{\Omega}_R)\, \frac{\Sigma_t(E,\underline{r})}{|\underline{r}-\underline{r}'|^2}$$

$$\cdot\, \frac{\Sigma_s(\underline{r}',E')}{\Sigma_t(\underline{r}',E')}\, F(E'\to E,\underline{r})\, dE\, \delta(\underline{\Omega}\cdot\underline{\Omega}' - g(E,E'))\, \frac{d\underline{\Omega}}{4\pi}$$

$$(4\text{-}63)$$

The derivative with respect to temperature of the kernel K is then

$$\frac{\partial}{\partial T} K(\tau|\tau') = \left[\frac{1}{\Sigma_t(\tau)} \frac{\partial}{\partial T} \Sigma_t(\tau) - \int_0^{|\underline{r}-\underline{r}'|} \frac{\partial}{\partial T} \Sigma_t(\tau)\, dR \right.$$

$$(4\text{-}64)$$

$$\left. + \frac{1}{\Sigma_s(\tau')} \frac{\partial}{\partial T} \Sigma_s(\tau') - \frac{1}{\Sigma_t(\tau')} \frac{\partial}{\partial T} \Sigma_t(\tau') \right] K(\tau|\tau')$$

In practice the initial phase point of the random walk chains are

selected from the conventional 'birth' source S, rather than the collision

source $\tilde{S}$, and the position of the first collision is selected from the

transport kernel. Since the energy of the source is established above

the resonance energy region, the cross sections are temperature independ-

ent at source energy. Therefore the derivative of the source $\tilde{S}$ with re-

spect to temperature appearing in (4-31) and (4-32) is set equal to zero.

With the random variable w defined as

$$w(\tau) \equiv \frac{\Sigma_a(\tau)}{\Sigma_t(\tau)} \qquad (4\text{-}65)$$

the problem of estimating the resonance capture probability and Doppler

coefficient in a heterogeneous lattice can now be solved by using the

Monte Carlo method to process the random walk chains described in Sec-

tion IV-B. Referring to Eqs. (4-59) through (4-64), the partial estimator (4-27) and partial derivative estimator (4-30) can be explicitly described as follows:

$$I^*_m(\tau_o, \cdots \tau_m) = \frac{\Sigma_a(\tau_m)}{\Sigma_t(\tau_m)} W_{m-1}(\tau_o, \cdots \tau_{m-1}) \tag{4-66}$$

and

$$DI^*_m(\tau_o, \cdots \tau_m) = \frac{\Sigma_a(\tau_m)}{\Sigma_t(\tau_m)} W_{m-1}(\tau_o, \cdots \tau_m) \, DW_m(\tau_o, \cdots \tau_m) \tag{4-67}$$

where

$$W_m(\tau_o, \cdots \tau_m) = \frac{\Sigma_s(\tau_m)}{\Sigma_t(\tau_m)} \cdots \frac{\Sigma_s(\tau_o)}{\Sigma_t(\tau_o)} \tag{4-68}$$

and

$$DW_o(\tau_o) = 0 \tag{4-69}$$

and for $m \gtrsim 1$

$$DW_m(\tau_o, \cdots \tau_m) = \frac{1}{\Sigma_a(\tau_m)} \frac{\partial}{\partial T} \Sigma_a(\tau_m) - \int_0^{\ell_m} \frac{\partial}{\partial T} \Sigma_t(\tau) \, dR$$

$$\tag{4-70}$$

$$+ \, \kappa_{m-1} + \cdots \kappa_1$$

where

$$\kappa_m \equiv \frac{1}{\Sigma_s(\tau_m)} \frac{\partial}{\partial T} \Sigma_s(\tau_m) - \int_0^{\ell_m} \frac{\partial}{\partial T} \Sigma_t(\tau) \, dR \tag{4-71}$$

and

$$\ell_m \equiv |\underline{r}_m - \underline{r}_{m-1}| \tag{4-72}$$

It is remarked that derivatives with respect to temperature of the total

cross sections do not appear outside the integrals in (4-70) even though

w is defined as (4-65). This is because all factors of $\Sigma_t(\tau)$ cancel from

the product of

$$w(\tau_m) \ K_m \cdots K_1 \ \tilde{S}_o$$

Estimates by the Monte Carlo method of capture probability and Doppler co-

efficient of reactivity are given by the following:

$$\bar{p} = 1 - \bar{I} \tag{4-73}$$

and

$$\frac{1}{\bar{p}} \left(\overline{\frac{\partial p}{\partial T}} \right) = \frac{-\overline{DI}}{1 - \bar{I}} \tag{4-74}$$

where

$$\bar{I} = \frac{1}{N} \sum_{j=1}^{N} \sum_{n=0}^{\infty} \sum_{m=0}^{n} \chi_n(j) \ I^*_m(\tau_o, \cdots \tau_m) \tag{4-75}$$

and

$$\overline{DI} = \frac{1}{N} \sum_{j=1}^{N} \sum_{n=0}^{\infty} \sum_{m=0}^{n} \chi_n(j) \ DI^*_m(\tau_o, \cdots \tau_m) \tag{4-76}$$

CHAPTER V

MONTE CARLO PROCEDURE AND COMPUTER PROGRAM

A. DESCRIPTION OF MONTE CARLO PROCEDURE

The procedure for processing Monte Carlo histories and for evaluating
the Doppler coefficient and the resonance capture probability on a digital
computer is described in this chapter. The procedure utilizes the mathe-
matical theory developed in the preceding chapters.

A semi-infinite lattice cell with a heterogeneous mixture of fuel and
moderator is considered for this problem. The fuel is contained in a cyl-
inder which has its axis colinear with that of the cell. Stated in brief,
Monte Carlo is used to generate a history by tracing neutron propagations
through the lattice cell as the neutron is degraded in energy by scatter-
ing collisions from source energy to cutoff energy. The value of the cut-
off energy is preset above thermal energies and below the energy of the
fuel resonances.

Decisions regarding the behavior of neutrons in a reactor lattice are
determined by random variables selected from the probability density func-
tions governing the random walk chains of Chapter IV. Data is collected
as the neutron histories are generated and is used to estimate values of
the desired reactor parameters, i.e., resonance capture probability and
Doppler coefficient of reactivity (Eqs. 4-73 and 4-74). The application
of sequences of pseudo-random numbers to select random variables from prob-

ability density functions which depict physical processes has been discussed by many authors.[45,...48] The assumption that the pseudo-random numbers are uniformly and independently distributed on the interval between zero and one is a very good one for numbers generated by the Method of Congruences,[49,...53] which is also used here. The mathematical details regarding the selection of random variables from the appropriate distribution functions are given in Appendix G. The verbal description of the Monte Carlo procedure for this problem follows.

1. Each history is started by selecting a pseudo-random number from the first random number generator (G-1), which is used to initiate the sequence of pseudo-random numbers generated by the second random number generator (G-2). This latter sequence of pseudo-random numbers is used to determine the behavior of the neutron for the given history. Since the number of random numbers used in each history depends upon its length and the paths taken in the cell, the use of two random number generators allows one to know beforehand the initial random number of each history.

2. The initial energy, position, and direction of the neutron is selected from the source distribution functions, Appendix G-3. The neutron source is taken to be isotropic in direction, uniformly distributed in the cell, and a line source in energy. The initial weight of the neutron is set equal to one (4-68).

3. Upon knowing the neutron energy, direction, and position at the source point (or last collision point), the distance, measured in terms of optical thickness, to the next collision point is selected from the

exponential distribution law of attenuation, Appendix G-4. The actual

position of the next collision is determined by knowledge of the total

macroscopic cross section, taking into account the crossing of boundaries

separating dissimilar media, the variation of the resonance cross section

due to the temperature distribution in the fuel, and the reflection of

the neutron path on the outer cell boundary. At the outer cell boundary,

the angle of reflection is set equal to the angle of incidence.

4. Upon knowing the position in the cell at which the collision

takes place, the species of the interacting nucleus is selected by random

variables according to the contribution to the total cross section at the

phase point of the collision. A scattering type collision is then forced

to occur by virtue of the modified kernel H (4-62) in Chapter IV and the

weight of the neutron is multiplied by the ratio of scattering to total

cross section (4-68). The derivatives with respect to temperature of the

Doppler broadening functions are integrated over the neutron path in the

fuel, and the partial estimators for p and $\partial p/\partial T$ are calculated by Eqs.

(4-66) and (4-67). If the neutron weight is less than a preset constant,

say .001,* the history is terminated and the procedure is continued as in

paragraph 6, otherwise the history is continued as in paragraph 5.

5. The scattering angle in the C.M.C.S. is selected from an isotropic

---

*The use of Russian roulette for deciding termination of a history was
provided for in the program and probably should be used if the input con-
stant is made considerably larger than .001. Russian roulette was tried
but did not produce an advantage in time or statistics over the straight-
forward use of the preset constant .001.

distribution, Appendix G-5. The new direction in the L.C.S. is determined by a transformation of coordinate systems, and the neutron energy after the scattering collision is calculated, according to the species of interacting nucleus, Appendix G-5. If the neutron energy is now greater than the preset thermal cutoff energy the history is continued by again following the procedure in paragraph 3, otherwise the history is terminated and the procedure in paragraph 6, is followed.

6. Once a decision has been made to terminate the history, either by conditions in paragraphs 4 or 5, the contributions of the history to p and $\partial p/\partial T$ are added to the sums in Eqs. (4-75) and (4-76). If the total number of histories processed is less than a preset maximum, another history is processed by again starting with the procedure in paragraph 1. Otherwise the Monte Carlo estimate is obtained for the resonance capture probability and Doppler coefficient of reactivity by evaluating Eqs. (4-73) through (4-76). In practice the histories are processed and the above estimates obtained for subgroups of histories so that trends can be observed and statistical variations noted. Also estimates of the variance of capture probability and its derivative are obtained by first calculating the average values of the square of the partial estimators (4-66) and (4-67).

B. BRIEF DESCRIPTION OF PROGRAM

Since part of the purpose of this work is to provide a computer program which utilizes the theory presented in the preceding chapters and

which is capable of handling the case of a non-uniform temperature distribution in the fuel, a brief description of the program is appropriate here. Most of this program was written in the MAD language (Michigan Algorithm Decoder[54]) for the IBM 709 digital computer. The Random subroutine discussed in paragraph 6 was written in symbolic machine language. The program requires a machine with 32,768 words in fast access memory. Because of the large size of the program, it was necessary to break it into component parts that could be separately translated by the MAD compiler. The division of the program according to separate functions has facilitated debugging and will make future modifications discussed in the succeeding chapters much easier. The program, called REPAD (Resonance Escape Probability and its Derivative with respect to temperature) includes the following routines:

1. The Main routine generates neutron histories and follows them in energy degradation and spatial propagation through the fuel and moderator regions of the reactor lattice. When the option of a non-uniform temperature distribution is selected, the following routine is used for the neutron propagation through the fuel.

2. The Non-uniform Temperature subroutine computes the optical thickness of the neutron path (and its derivative with respect to temperature) through the temperature zones of the fuel, using cross sections obtained from the Cross Section subroutine, and determines the next collision point. If the neutron energy is such that resonances need not be taken into account, this subroutine is bypassed.

3. The preparation subroutine prepares input data, cross sections of resolved resonances evaluated at the peak energy, and macroscopic cross-sections for the program. The radial temperature distribution can be completely arbitrary, however if the parabolic temperature distribution is selected, this subroutine calculates the value of the temperature in each of the desired temperature zones.

4. The Cross Section subroutine determines the appropriate macroscopic scattering, absorption, and total cross sections in the fuel for the current value of neutron energy. In the neutron energy region of unresolved resonances, the neutron width is selected from the Porter-Thomas distribution,[40] and the unbroadened resonance scattering, absorption, and interference scattering cross sections are calculated. In the region of resolved resonances the decision is made whether the neutron energy is in a limited range between resonances where the resonance cross sections are negligible with respect to the potential scattering cross section or not. If not, the unbroadened cross sections are determined for the appropriate resonance or resonances. The Doppler broadening of resonances is accounted for in the next subroutine. The "1/v" absorption cross section is calculated if it is important with respect to potential scattering cross section for the given neutron energy.

5. The Psi-Chi subroutine evaluates the Doppler broadening functions for the appropriate resonance parameters and fuel temperature to a prescribed accuracy, and calculates their derivatives with respect to temperature. Mathematical details of calculating these functions are given in Appendix F.

6. The Random subroutine generates pseudo-random numbers and variables used in the problem. Selection of random variables from uniform, exponential, polar cosine, azimuthal sine and cosine, and parabolic distributions are required.

7. The Random Input/Output subroutine accepts the initial random numbers for input and prepares initial, final, and intermediate random numbers for output. This routine is necessary for running a series of many histories on the digital computer with the same physical conditions but different random numbers.

8. The Edit subroutine computes averages, and estimated variances and standard errors of the reactor lattice parameters for subgroups of histories and for the completed problem. The parameters include resonance capture probability and its derivative with respect to temperature, resonance escape probability and Doppler coefficient of reactivity. The first two parameters are also given for three separate energy groups. This subroutine also punches output cards to be used as input for succeeding problems.

The program REPAD is written for a cylindrical fuel rod and lattice cell, both of arbitrary dimensions. Both cell and fuel rod are circular and have colinear axes.

CHAPTER VI

RESULTS

A. PROGRAM CONSTANTS AND INPUT PARAMETERS

For the total time available on The University of Michigan IBM 709

computer for this problem, it was decided that for purposes of comparison

it would be better to run only a few cases with 12,000 Monte Carlo histo-

ries rather than more cases with fewer histories and larger statistical

error. The production runs were for a .25 in. diameter rod of $U^{238}O_2$ fuel

and a 1/1 fuel to moderator volume ratio. These and other input parameters,

such as fuel surface temperatures and non-resonance cross sections, were

selected to be compatible with those appearing in practice and consistent

with those in WCAP-1572 in order to make a comparison with the results of

Arnold and Dannels[15] for the case of uniform fuel temperature. Values of

input parameters that are common for all the runs are given in Table I.

The recent resonance parameters determined at Columbia University by

Rosen, Dejardins, Rainwater and Havens[40] are used for U-238. Since the

resonance parameters used in REP[16] were older measurements which included

only 28 resolved resonances, this number of resonances was also used in

the production runs with REPAD.

Unresolved resonances were not included because a considerable savings

of computer time could be realized by omitting the unresolved resonances,

and because it seemed incongruous to select unresolved resonances parameters

from a probability distribution when actually another 27 resonances are

TABLE I

VALUES OF INPUT PARAMETERS FOR REPAD PROGRAM

Parameters	Value	Description
V^f/V^m	1.000	Fuel-Moderator volume ratio
R^f	.3175 cm	Radius of fuel rod (.25 in.)
R^m	.4490 cm	Radius of moderator cell
Σ_p^f	.416 cm^{-1}	Potential scattering cross section of fuel-UO$_2$
Σ_p^m	1.468 cm^{-1}	Potential scattering cross section of moderator-H$_2$O
Σ_p^m	1.468 cm^{-1}	Total cross section of moderator-H$_2$O
Σ_a^f	.0522 cm^{-1}	"1/v" absorption cross section of fuel at 1 ev
ERN(1)	100,000 ev	Reference value - source energy
ERN(2)	5530 ev	Reference value - not used
ERN(3)	545.75 ev	Reference value - max energy of resolved resonance region
ERN(4)	250.00 ev	Reference value - cutoff energy for "1/v" cross section
ERN(5)	.625 ev	Reference value - thermal cutoff energy

now resolved. According to the results presented in WCAP-1572 for a uniform fuel temperature, the 28 resonances of U-238 below 545 ev, which also include the strong resonances, contribute more than 80% to both the resonance capture probability and the Doppler coefficient; it is, therefore especially important to investigate the effects of a non-uniform temperature distribution due to these resonances. Furthermore, for fuel temperatures above 800°K, unresolved resonances corresponding to the average reduced neutron width $(< \Gamma_n^o > = < \Gamma_{no}/\sqrt{E_o}>)$ are broadened sufficiently so that at peak energies the average neutron path through the fuel rod is of the order of 1 mean free path, and consequently neutrons incident on the fuel rod have a good chance of passing through most of the temperature regions in the fuel. It is expected therefore that the concept of an average fuel temperature would have more meaning for the unresolved resonances than the resolved resonances.

B. NUMERICAL RESULTS AND DISCUSSION

The running time of REPAD is about .01 min/history for uniform fuel temperature and .02 min/history for non-uniform fuel temperature on the IBM 709. The latter time is for 24 temperature regions in the fuel. Runs of 12,000 histories each were made for the following conditions:

Uniform fuel temperature

Run	T_s, °K
1	840
2	1700
3	2800

Parabolic fuel temperature
        (radially)

Run	T_s, °K	T_p, °K	T_s/T_p
4	840	2800	3.34
5	1820	3780	2.08

where T_s = surface temperature

    T_p = peak temperature at centerline

Also let

$$T_{av} = \frac{T_s + T_p}{2}$$

$$T_{rm} = \left(\frac{\sqrt{T_s} + \sqrt{T_p}}{2}\right)^2$$

As mentioned previously one of the features of REPAD is that the derivative with respect to temperature of the capture probability is directly evaluated by Monte Carlo. This then allows calculation of that part of the temperature coefficient of reactivity due to the resonance capture probability and also of the Doppler coefficient. Given these results one may determine β in the empirical $T^{1/2}$ law for resonance integrals,[10,17]

$$RI(T) = RI(T_o) \cdot (1 + \beta \ (\sqrt{T} = \sqrt{T_o})) \tag{6-1}$$

From Eq. (1-2), and Eq. (6-1), β can be expressed as

$$\beta = \frac{\partial p/\partial T}{p \cdot \ln (p)} \cdot 2\sqrt{T} \tag{6-2}$$

The results of the Monte Carlo runs are given in Table II and are summarized in Figs. 1 through 3. (The error indications shown in the figures are for probable error.) Results from WCAP-1572 are also included

TABLE II

RESULTS FROM 12,000 MONTE CARLO HISTORIES

	Flat Temperature Distribution, °K			Parabolic Temperature Distribution, °K	
	T_s 840	T_s 1700	T_s 2800	T_s T_p 840 2800	T_s T_p 1820 3780
$(1-p)$	.21329	.22777	.24180	.22533	.24094
$\pm .6745\ \sigma$	$\pm .00207$	$\pm .00213$	$\pm .00218$	$\pm .00211$	$\pm .00224$
$-\partial p/\partial T$ (10^{-4})	.2134	.1666	.1355	.1796	.1348
$\pm .6745\ \sigma$ (10^{-4})	$\pm .0185$	$\pm .0106$	$\pm .0073$	$\pm .0135$	$\pm .0085$
p	.78671	.77223	.75820	.77467	.75906
$-\ell n\ p$	.23990	.25848	.27681	.25532	.27587
$-\ell n(-\ell n\ p)$	1.428	1.352	1.283	1.365	1.289
$\dfrac{1}{p}\dfrac{\partial p}{\partial T}$ (10^{-4})	.271	.216	.179	.232	.178
$\dfrac{1}{p\ell n\ p}\dfrac{\partial p}{\partial T}$ (10^{-4})	1.131	.834	.646	.909	.644
β (10^{-2})	.655	.687	.683	.744	.671

$$\bar{\beta} = .675 \times 10^{-2} \pm .030 \times 10^{-2}$$

Fig. 1. The variation of resonance capture probability with fuel temperature; uniform temperature case, runs 1, 2, 3. Values for parabolic temperature distribution indicated on lower curve, runs 4, 5. .25 in. dia. UO_2 fuel, 28 resolved resonances.

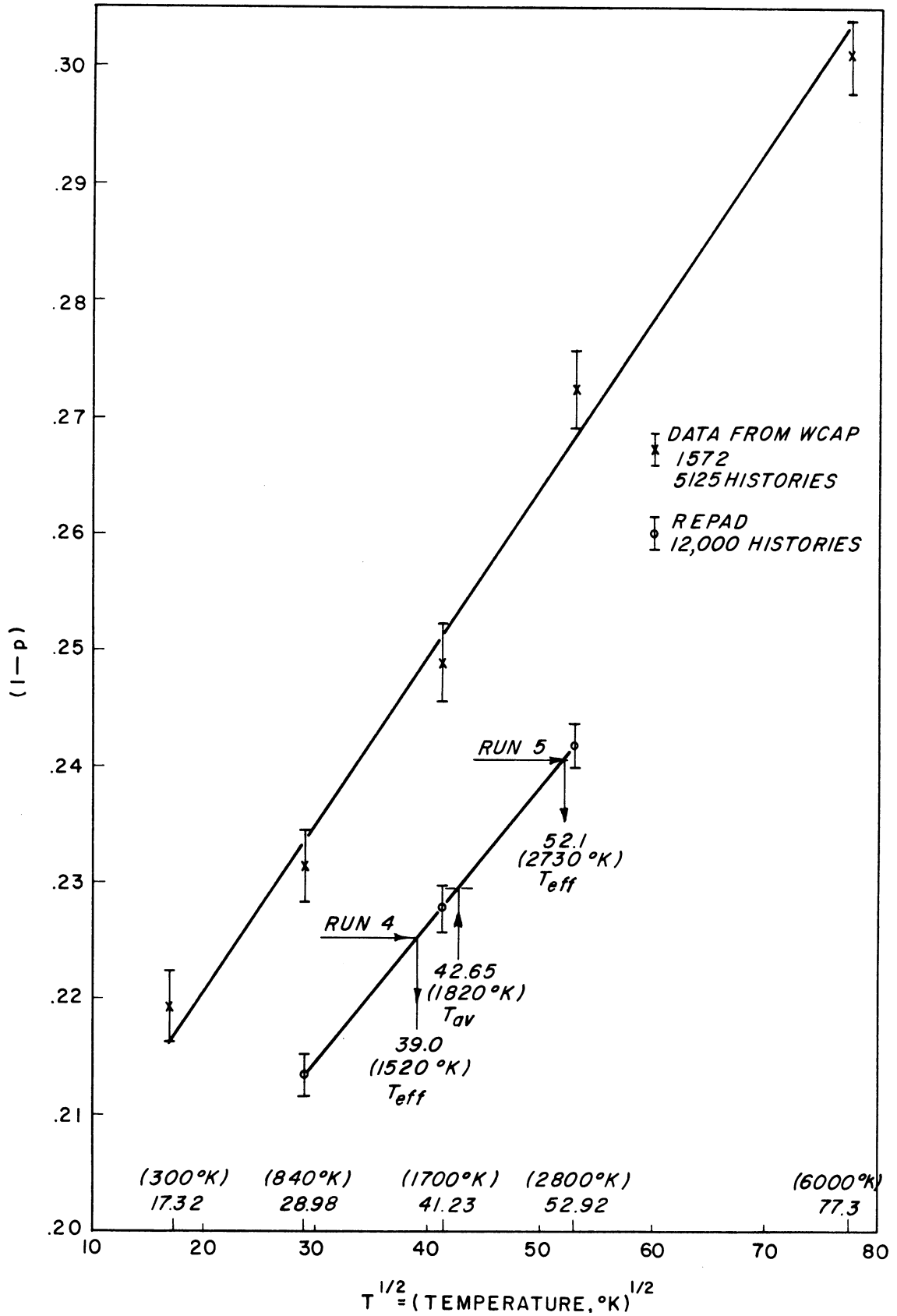Fig. 2. The variation of the Doppler coefficient of reactivity and the derivative of resonance escape probability with fuel temperature; uniform temperature case, runs 1, 2, 3. Values for parabolic temperature distribution indicated on curves, runs 4, 5. .25 in. dia. UO_2 fuel, 28 resolved resonances.
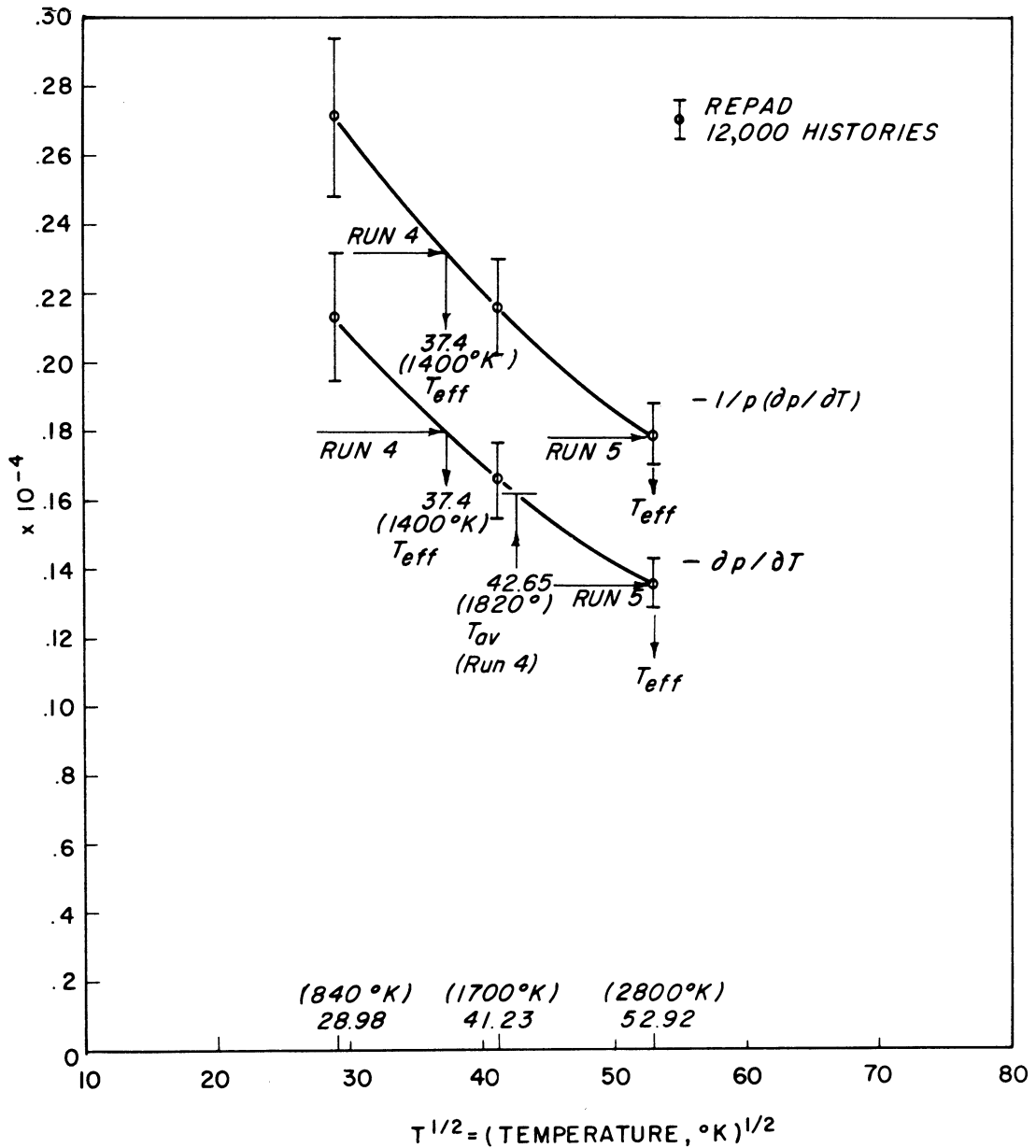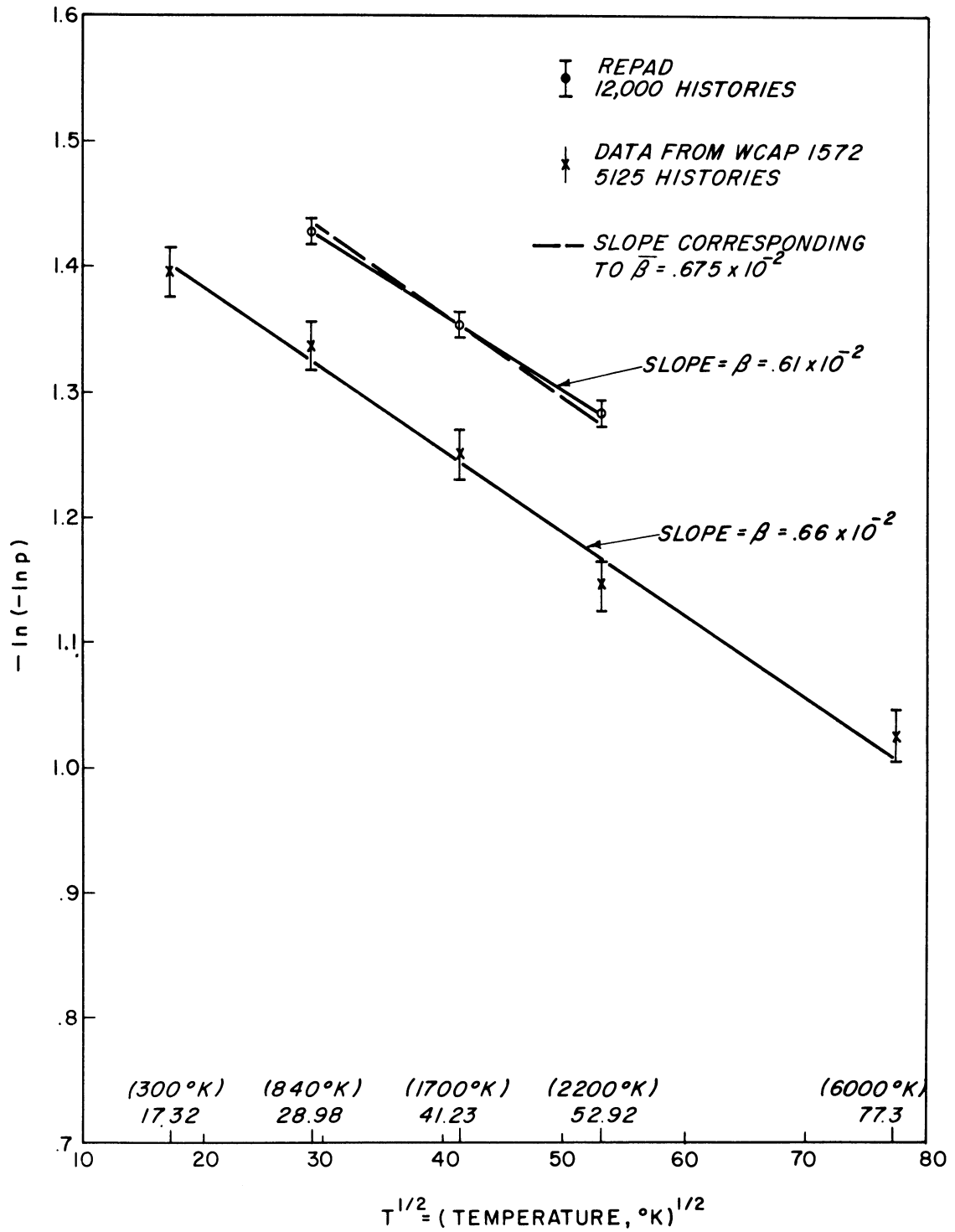
Fig. 3. The variation of ln(-lnp) with fuel temperature; uniform temperature case, runs 1, 2, 3. .25 in. dia. UO_2 fuel, 28 resolved resonances.

for comparison. Values of capture probability were obtained by using data in WCAP-1572 from the resolved resonance energy region only. The differences between the results of WCAP-1572 and REPAD for flat fuel temperature are attributed to the difference in outside cell boundaries, i.e., rectangular and circular, respectively. The average value of β obtained by Eq. (6-2) from the three flat fuel temperature runs of REPAD was found to be $.675 \times 10^{-2}$, which is close to the value obtained from WCAP-1572 data (see Fig. 3). By representing the slope corresponding to $\beta = .675 \times 10^{-2}$ by the dashed line superimposed on the upper curve in Fig. 3, one notices that the dashed line lies within the error limits, and thus helps to substantiate relations (6-1) and (6-2). Figure 2 illustrates the dependence upon temperature of $\partial p/\partial T$, the derivative of capture probability, and $(1/p) \cdot \partial p/\partial T$, the temperature coefficient due to Doppler effect. The curves are for a flat temperature in the fuel. It is noted that both values decrease about 35% as the temperature increases from 840 to 2800°K.

The curves of $(1-p)$, $\partial p/\partial T$, and $(1/p) \cdot \partial p/\partial T$, and the average value of β for the flat temperature are useful for illustrating the effect of a non-uniform temperature distribution and the determination of an effective temperature. Let the effective temperature, T_{eff}, be defined as that temperature at which the case of a flat temperature gives the same value of the parameter of interest as the case of a parabolic temperature distribution in the fuel. A characteristic effective temperature applies to only one parameter under a given set of conditions. Since the functional dependence on temperature of the capture probability and its derivative are dif-

ferent, it is not expected that their effective temperature would be the
same.

By superimposing the values of capture probability for the parabolic
temperature distribution cases on the lower curve in Fig. 1, the effective
temperatures are obtained. Similarly the effective temperatures for $\partial p/\partial T$
and $(1/p) \cdot (\partial p/\partial T)$ are obtained in Fig. 2. Values for T_{eff}, T_{av} and T_{rm}
are given below:

Run	T_s,°K	T_p, °K	T_{av},°K	T_{rm},°K	T_{eff},°K
4	840	2800	1820	1670	$\left\{ \begin{array}{l} 1520 \text{ for } (1-p) \\ 1400 \text{ for } \partial p/\partial T \\ 1400 \text{ for } (1/p) \ \partial p/\partial T \end{array} \right.$
5	1820	3780	2800	2720	$\left\{ \begin{array}{l} 2730 \text{ for } (1-p) \\ 2800 \text{ for } \partial p/\partial T \\ 2800 \text{ for } (1/p) \ \partial p/\partial T \end{array} \right.$

For the higher temperature run, the parabolic temperature distribu-
tion can be characterized by the average temperature since T_{av}, T_{rm}, and
T_{eff} appear to give the same values of $(1-p)$, $\partial p/\partial T$, and $(1/p) \cdot \partial p/\partial T$ with-
in limits of the statistical error. However for the lower temperature run,
which corresponds more nearly to practical operating fuel temperatures in
a power reactor, the average temperature is a poorer approximation to the
effective temperature. Use of the average temperature to characterize the
parabolic distribution in this case would cause the following errors:

T_s,°K	T_p,°K	Parameter	% Error caused by replacing T_{eff} by	
			T_{av}	T_{rm}
		$1 - p$	1.7	1.
840	2800	$\partial p/\partial T$	-10.	-7.
		$(1/p)\ \partial p/\partial T$	- 9.	-6.5

For the case of (1-p) the discrepancy in using T_{av} is outside the limits of probable error, however for the other two parameters there is a slight overlap in the error limits.

The concept of a constant β (Eq. 6-1) for a large temperature range also provides determination of the effective temperature. For the first run of parabolic temperature, the effective temperature is found from Eq. (6-2) to be 1380°K, which is within the statistical error of that given for the Doppler coefficient of reactivity.

The reasons that the average temperature appears to be a much better approximation to the effective temperature for the second run at the high temperatures than the first may be attributed to two factors. 1) The peak to surface temperature ratio is smaller in the second run. 2) At higher temperatures the resonances become lowered and broadened by the Doppler effect and therefore the self-shielding factor is decreased. At the lower temperature, neutrons incident on the fuel surface near the resonance peak do not travel far before being absorbed, and hence experience cross sections corresponding more nearly to the surface temperature. However in the limit of extremely high temperature the resonances are com-

pletely broadened and the self-shielding factor vanishes, hence incident

neutrons could penetrate further into the fuel and thus experience cross-

sections over a larger range of the temperature distribution. At this

limit the volume average of the cross section would equal the effective

cross section. For a parabolic temperature distribution this averaged

cross section corresponds to the cross section at the average temperature.

The error in using the average temperature concept is due to an attempt

of replacing the average of a function by the function of an average, how-

ever as the rod temperature becomes higher and the temperature distribu-

tion becomes less extreme, the results indicate that this error decreases.

CHAPTER VII

CONCLUDING REMARKS

A. CONCLUSIONS

Pearce[10] has indicated that there is a definite need for investigating the effect of a non-uniform temperature distribution in the fuel on capture probability and Doppler coefficient. He states that "there are two distributions of temperature within fuel elements that are of particular interest: (1) the distribution present in an operating reactor, where the temperature is highest away from the coolant channels, and (2) the distribution present in a reactor runaway, where the temperature is highest in the region of highest thermal flux. Both these distributions are difficult to realize in either activation or reactivity experiments and there have been no experiments reported on the Doppler effect in these distributions. The theory of Doppler effect in non-uniform distributions is also in an unsatisfactory state." The current theory reviewed in his article "shows that one cannot simply take a surface Doppler coefficient with a surface temperature and a volume coefficient with a volume temperature."

It is hoped that the program written in this work partially fulfills this need, since REPAD provides the first means of evaluating the effects of an arbitrary, radially dependent temperature distribution without introducing approximations that are difficult to justify. The numerical

results are for a parabolic temperature distribution since it closely approximates the distribution existing in a UO_2 fueled reactor.[21]

The results of this work indicate that the substitution of a parabolic temperature distribution in the fuel by a uniform distribution at the average temperature as suggested by Keane[22] and Dresner[23] can be done for the conditions considered in Section VI-B only if one is satisfied with an error of about 2% in resonance capture probability. However the results further indicate a trend toward a larger error as the peak to surface temperature ratio becomes larger than 3.3 and/or as the average fuel temperature becomes lower than 1820°K. Both of these tendencies are quite probable in operating power reactors using UO_2 fuel.

The error caused by using a uniform average temperature as a substitute for the parabolic temperature distribution is much greater for the Doppler coefficient of reactivity, being of the order of 10% for a parabolic temperature distribution in a .25 in. UO_2 fuel rod with surface and peak temperatures of 840°K and 2800°K respectively. The results indicate that the Doppler coefficient has the same trend toward a larger error as indicated above for capture probability. This 10% error is significant when one considers that the Doppler coefficient is of prime importance in reactor safety because it reacts promptly with changes in fuel temperature. Furthermore, as pointed out by Pearce[10] the temperature coefficient of reactivity is more sensitive to the Doppler coefficient than to changes in thermal utilization and resonance capture due to thermal expansion of the fuel in power reactors.

The root mean square temperature (Section VI-B) represents a better approximation than the average value as a substitute to a parabolic temperature distribution for purposes of evaluating the capture probability and Doppler coefficient, but it is still not satisfactory for the usual operating conditions of a power reactor.

The Monte Carlo program REPAD includes a new and direct method of evaluating the derivative with respect to temperature of the capture probability that was rigorously derived from the Neumann series solution of the Boltzmann equation by utilizing the mathematical model of Albert[27] for random walk chains. This formulation for determining the Doppler coefficient circumvents the approximations inherent in the other two methods discussed in Chapter I, and the results indicate that this new method compares favorably with these other methods. For the special case of a flat fuel temperature, a direct comparison was made with the method of describing the temperature dependence of the resonance integral by an empirical $T^{1/2}$ law. Both methods agree within experimental error. The use of a finite difference approximation to the derivative would give a large error for our results since the temperatures were widely spaced, and therefore this approximation was not used. However Morton[14] used this technique in his Monte Carlo program for a uniform temperature distribution and obtained a probable error of about 25% for 4096 histories. For 12,000 histories one would then expect the finite difference method to give a probable error of about 14%. This compares with an average of about 7% for the runs reported in the results using the direct method, and about 12% using the empirical

method. Furthermore both the empirical fitting and finite difference tech-
niques require at least two runs at different temperatures in order to ob-
tain an estimate for the Doppler coefficient. Therefore for a given prob-
able error, the new method allows a savings in computer time by a factor
between 6 and 8 in comparison to the two other methods.

In summary, it is felt that this work fulfills two purposes. 1) It
illustrates the application of the method of constructing random walk
chains from the Boltzmann equation to develop a mathematical formulation
for determining the Doppler coefficient directly in a Monte Carlo process.
The method developed produces a considerable savings in computer time.
2) On the basis of this work the quantative influence of a fuel tempera-
ture distribution on the resonance capture probability and Doppler coeffi-
cient of reactivity is evaluated by means of the present digital computer
program.

B. FUTURE WORK

There are many interesting problems that can be investigated with the
Monte Carlo program REPAD as presently written; these include the follow-
ing:

1. One could evaluate the temperature dependence of the resonance
capture probability and Doppler coefficient for the 54 resolved resonances
and the unresolved resonances of U-238 and Th-232,[8] in order to compare
with the experimental results of Hellstrand, Blumberg, and Hörner[17] for a
uniform temperature.

2. One could investigate further the apparent divergence of the effective temperature for a parabolic distribution from the average temperature as the average fuel temperature decreases and the peak to surface temperature ratio increases. Also one could investigate the effect of fuel rod diameter and fuel-moderator volume ratio on this trend.

3. One could use temperature distributions more appropriate to a reactor in a runaway condition where the temperature is highest in the fuel region of highest flux.

With some modification of REPAD, the following features could be included:

1. Doppler broadened U-235 resonances in fuel of low enrichment using the Breit-Wigner single-level formula and Doppler broadening functions;

2. variation of fuel composition in the separate radial fuel zones; (This is important for fuel burnup studies.)

3. provision for the determination of spatial dependence of Doppler effect;[55]

4. provision for p wave and higher angular momentum neutron interaction for the unresolved resonances;

5. provision for a more generalized geometry to include a rectangular lattice cell;

6. use of the Breit-Wigner multi-level resonance formula for U-235 at high enrichments;

7. provision for a spatial and energy dependent source to investigate source effects on Doppler coefficient and capture probability.

APPENDIX A

DERIVATION OF GREEN'S FUNCTION

The solution of Eq. (2-2) can be determined by Fourier Transform

techniques, however in order to gain insight to the method, the special

case of spatially uniform cross section will be considered first.

Case I: $\Sigma_t \rightarrow \Sigma_t(E)$; function of E only.

Equation (2-2) then becomes

$$\nabla \cdot \underline{\Omega}\, G \;+\; \Sigma_t(E)\, G(\underline{r}, E, \underline{\Omega} \mid r', E', \underline{\Omega}') \;=$$

$$= \delta(\underline{r}-\underline{r}')\, \delta(E-E')\, \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \tag{A-1}$$

The definition of the symbols and the boundary condition remains the

same as in Chapter II.

Let the Fourier Transform of the Green's function be

$$\overline{G} \;=\; \int_{\underline{r}} e^{\,i\,\underline{k}\cdot\underline{r}}\; G(\underline{r}, E, \underline{\Omega} \mid \underline{r}', E', \underline{\Omega}') \tag{A-2}$$

then by definition of the inverse transform

$$G \;=\; \int_{\underline{k}} e^{\,-i\,\underline{k}\cdot\underline{r}}\; \overline{G}\; \frac{d^3 k}{(2\pi)^3} \tag{A-3}$$

also let

$$\overline{\delta} \;=\; \int_{\underline{r}} e^{\,i\,\underline{k}\cdot\underline{r}}\; \delta(\underline{r}-\underline{r}')\, d^3 r \;=\; e^{\,i\,\underline{k}\cdot\underline{r}'} \tag{A-4}$$

In this case the transform of Eq. (A-1) with respect to the variable $\underline{r}$ becomes

$$-\underline{\Omega} \cdot \underline{k} \, i\, \overline{G} + \Sigma_t(E)\overline{G} = e^{i \underline{k} \cdot \underline{r}'} \delta(E - E') \delta_z(\underline{\Omega} \cdot \underline{\Omega}') \qquad (A-5)$$

hence

$$\overline{G}(\underline{k}, E, \underline{\Omega} \mid \underline{r}', E', \underline{\Omega}') =$$

$$= \frac{1}{\Sigma_t(E) - i\,\underline{\Omega} \cdot \underline{k}} \, e^{i \underline{k} \cdot \underline{r}'} \delta(E - E') \delta_z(\underline{\Omega} \cdot \underline{\Omega}') \qquad (A-6)$$

define:

$$\Delta' \equiv \delta(E - E') \delta_z(\underline{\Omega} \cdot \underline{\Omega}')$$

In integral form, the solution is then obtained by the property of the inverse transform and is

$$G(\underline{r}, E, \underline{\Omega} \mid \underline{r}', E', \underline{\Omega}') = \frac{\Delta'}{(2\pi)^3} \int_{\underline{k}} \frac{e^{-i\,\underline{k} \cdot (\underline{r} - r')}}{\Sigma_t(E) - i\,\underline{\Omega} \cdot \underline{k}} \, d^3 k \qquad (A-7)$$

define

$$\underline{R} \equiv \underline{r} - \underline{r}' = R\, \underline{\Omega}_R \qquad ; \quad R \equiv |\underline{R}| \qquad (A-8)$$

$$\underline{\Omega}_R \equiv \frac{\underline{R}}{R} \qquad (A-9)$$

Let $\underline{\Omega}$ be along x axis for convenience, then

$$\underline{\Omega} \cdot \underline{k} = k_x$$

$$\underline{R} = \underline{i} R_x + \underline{j} R_y + \underline{h} R_z$$

where $\underline{i}$, $\underline{j}$, $\underline{h}$ are unit vectors along x, y, z axis respectively, then (A-7) becomes

$$G = \frac{\Delta'}{(2\pi)^3} \underset{k_x \, k_y \, k_z}{\iiint} e^{-i\left(k_x R_x + k_y R_y + k_z R_z\right)} \frac{dk_x \, dk_y \, dk_z}{\xi_t - i k_x} \qquad (\text{A-10})$$

but one definition of the Dirac delta function is

$$\delta(\alpha) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\alpha \xi} d\xi = \delta(-\alpha) \qquad (\text{A-11})$$

Hence

$$G = \frac{\Delta'}{2\pi} \delta(R_y) \delta(R_z) \int_{k_x} e^{-i k_x R_x} \frac{dk_x}{\xi_t - i k_x} \qquad (\text{A-12})$$

but according to Volume 1 of the Bateman Manuscript Project,[56]

$$\frac{1}{2\pi} \int_{k_x} e^{-i k_x R_x} \frac{dk_x}{\xi_t - i k_x} = \begin{cases} 0 & , \text{ if } R_x < 0; \ (\underline{\Omega} \cdot (\underline{r} - \underline{r}') < 0) \\ e^{-\xi_t R_x} & , \text{ if } R_x \geq 0; (\underline{\Omega} \cdot (\underline{r} - \underline{r}') \geq 0) \end{cases} \qquad (\text{A-13})$$

let

$$\eta(x) \equiv \begin{cases} 0 & , \text{ if } x < 0 \\ 1 & , \text{ if } x \geq 0 \end{cases} \qquad (\text{A-14})$$

now

$$G = \Delta' \, \delta(R_y) \, \delta(R_z) \, \eta(R_x) \, e^{-\Sigma_t R_x}$$

but note

$$\delta_z(\underline{\Omega}\cdot\underline{\Omega}_R) = \delta(R_y)\,\delta(R_z)\,\eta(R_x) \tag{A-15}$$

therefore

$$G(\underline{r},E,\underline{\Omega}\mid \underline{r}',E',\underline{\Omega}')\,dR =$$

$$= e^{-\Sigma_t(E)\underline{\Omega}\cdot\underline{R}} \, \delta_z(\underline{\Omega}\cdot\underline{\Omega}_R)\delta_z(\underline{\Omega}\cdot\underline{\Omega}')\,\delta(E-E')\,dR \tag{A-16}$$

Since $d^3R = |\underline{R}|^2\,dR\,d\Omega_R$, then

$$G(\underline{r},E,\underline{\Omega}\mid \underline{r}',E',\underline{\Omega}')\,d^3r = G\,d^3R$$

$$\tag{A-17}$$

$$= e^{-\Sigma_t(E)\underline{\Omega}\cdot\underline{R}} \, \delta_z(\underline{\Omega}\cdot\underline{\Omega}_R)\,\delta_z(\underline{\Omega}\cdot\underline{\Omega}')\,\delta(E-E')\,\frac{d^3R}{|\underline{R}|^2}$$

is a solution to (A-1) and is the Green's function for the case of

spatially constant cross section. Substituting (A-17) in (2-9) and in-

tegrating over all E', $\underline{\Omega}'$, the integral equivalent of Eq. (2-1) can be

written in this case as

$$\Phi(\underline{r},E,\underline{\Omega}) = \int_{\underline{r}'} \frac{d^3r'}{|\underline{r}-\underline{r}'|^2}\, e^{-\Sigma_t(E)\left[\underline{\Omega}\cdot(\underline{r}-\underline{r}')\right]} \, \delta_z(\underline{\Omega}\cdot\underline{\Omega}_R) \left\{ S(\underline{r}',E,\underline{\Omega}) \right.$$

$$\tag{A-18}$$

$$+ \int_{E''}\int_{\underline{\Omega}''} \left. \Phi(\underline{r}',E'',\underline{\Omega}'')\,\Sigma_s(E,\underline{\Omega}\mid E'',\underline{\Omega}'';\underline{r}')\,dE''\,d\underline{\Omega}'' \right\}$$

Since

$$\frac{d^3r'}{|\underline{r}-\underline{r}'|^2} = \frac{d^3R}{|\underline{r}-\underline{r}'|^2} = dR\, d\Omega_R \tag{A-19}$$

and

$$\underline{r}' = \underline{r}-\underline{R} = \underline{r} - \underline{\Omega}_R\, R$$

then an alternate form is

$$\phi(\underline{r},E,\underline{\Omega}) = \int_{R=0}^{\infty} dR\, e^{-\Sigma_t(E)R} \left\{ S(\underline{r}-\underline{\Omega}R, E, \underline{\Omega}) \right.$$

$$\left. + \int_{E'}\int_{\underline{\Omega}'} \phi(\underline{r}-\underline{\Omega}R, E',\underline{\Omega}')\, \Sigma_s(E,\underline{\Omega}\,|\,E',\underline{\Omega}'; \underline{r}-\underline{\Omega}R)\, dE'\, d\underline{\Omega}' \right\} \tag{A-20}$$

is the integral equivalent of the Boltzmann transport equation with

cross section spatially constant.

Case II: $\Sigma_t \to \Sigma_t(E,\underline{r})$; function of both E and $\underline{r}$.

With insight afforded by Case I, Eq. (2-2) can be solved with the

cross section a function of E and $\underline{r}$. Physically the solution represents

the transport of particles with energy E in direction $\underline{\Omega}$ from $\underline{r}'$ to $\underline{r}$

only if $\underline{\Omega} = \underline{\Omega}_R$ (A-9).

We can impose this condition immediately on Eq. (2-2) by utilizing

the delta function; $\delta_2(\underline{\Omega}\cdot\underline{\Omega}_R)$. Let s be in direction $\underline{\Omega}$ then

$$\underline{\Omega}\cdot\nabla = \frac{d}{ds} \tag{A-21}$$

Equation (2-2) then becomes

$$\frac{d}{ds} G + \Sigma_t (E, \underline{r}) G (\underline{r}, E, \underline{\Omega} | \underline{r}', E', \underline{\Omega}') =$$

$$= \delta(R) \delta_2 (\underline{\Omega} \cdot \underline{\Omega}_R) \delta_2 (\underline{\Omega} \cdot \underline{\Omega}') \delta (E \cdot E')$$

(A-22)

Define:

$$\Delta \equiv \delta_2 (\underline{\Omega} \cdot \underline{\Omega}_R) \delta_2 (\underline{\Omega} \cdot \underline{\Omega}') \delta (E - E')$$

Multiply Eq. (A-22) by

$$e^{\int_0^R \Sigma_t (E, \underline{r}' + \underline{\Omega}_R R') dR'}$$

and note

$$\frac{d}{ds} \left(e^{\int_0^R \Sigma_t (E, \underline{r}' + R' \underline{\Omega}_R) dR'} \right) = e^{\int_0^R \Sigma_t' dR'} \frac{d}{ds} \int_0^R \Sigma_t' dR'$$

$$= e^{\int_0^R \Sigma_t' dR'} \Sigma_t (E, \underline{r})$$

Since

$$\frac{d}{ds} R = \frac{d}{dR} R = 1$$

$$\underline{\Omega} = \underline{\Omega}_R$$

for non-trivial solution, then (A-22) becomes

$$\frac{d}{ds} \left(G e^{\int_0^R \Sigma_t' dR'} \right) = e^{\int_0^R \Sigma_t' dR'} \delta(R) \Delta$$

(A-23)

Let

$$E \equiv e^{\int_0^R \Sigma_t' dR'}$$

(A-24)

then (A-23) becomes

$$\frac{d}{ds} \left(G E' \right) = E' \delta(R) \Delta \tag{A-25}$$

Taking the Fourier Transform with respect to R of (A-25)

$$-ik \, \overline{GE'} = \int_0^\infty e^{ikR + \int_0^R \Sigma_t' dR'} \delta(R) \, dR \, \Delta \tag{A-26}$$

$$= \Delta$$

hence

$$\overline{GE'} = \frac{-\Delta}{ik}$$

and by definition of the inverse transform

$$GE' = \frac{-1}{2\pi} \int_{-\infty}^\infty e^{-ikR} \frac{dk}{ik} \Delta = \eta(R) \, \Delta \tag{A-27}$$

where again

$$\eta(R) = \left\{ \begin{array}{ll} 0, & \text{if } R < 0 \\ 1, & \text{if } R \geq 0 \end{array} \right\} \qquad \left(\begin{array}{l} \text{this effect included} \\ \text{in } \delta_2(\underline{\Omega} \cdot \underline{\Omega}_R) \end{array} \right)$$

Therefore

$$G\left(\underline{r}, E, \underline{\Omega} \mid \underline{r}', E', \underline{\Omega}' \right)$$

$$= e^{-\int_0^R \Sigma_t(E, \underline{r}' + \underline{\Omega}_R R') dR'} \delta_2(\underline{\Omega} \cdot \underline{\Omega}_R) \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \delta(E - E') \tag{A-28}$$

Hence

$$G\left(\underline{r}, E, \underline{\Omega} \mid \underline{r}', E', \underline{\Omega}' \right) d^3 r' = G \, d^3 R$$

$$= e^{-\int_0^R \Sigma_t' dR'} \delta_2(\underline{\Omega} \cdot \underline{\Omega}_R) \, \delta_2(\underline{\Omega} \cdot \underline{\Omega}') \delta(E - E') \frac{d^3 R}{R^2} \tag{A-29}$$

is the Green's function for Eq. (2-2).

APPENDIX B

MATHEMATICAL DESCRIPTION OF BANACH SPACE

This section presents the mathematical description and some useful

properties of the Banach abstract space, and is summarized from the book

by Riesz and Nagy.[30]

BACKGROUND

The fundamental spaces L^p (where $1 \leqslant p \leqslant \infty$) and the space of contin-

uous functions C are particular cases of the Banach abstract space

(generalization of Hilbert space).

A <u>Banach space</u> is a set B of abstract elements f, g,...which satis-

fies the following conditions:

(a) B is a <u>linear</u> space, i.e., the operations of addition and

multiplication by real or complex numbers are defined for its elements,

and these operations follow the rules of vector algebra.

(b) To every element f of B there is a <u>norm</u> with properties:

norm $\cong \| f \| > 0$

$$\| f \| = 0 , \quad \text{if and only if } f = 0, \text{ a.e.}$$

$$\| f + g \| \leq \| f \| + \| g \| ; \qquad \| \alpha f \| = |\alpha| \, \| f \|$$

a = constant

(c) B is a <u>complete</u> space in the following sense, if $\{f_n\}$ is a

sequence of elements in B that satisfies

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$$\left\| f_n - f_m \right\| \longrightarrow 0 \qquad \text{for} \quad m, n \longrightarrow \infty$$

then there exists an element f of B $\ni$

$$\left\| f_n - f \right\| \longrightarrow 0 \qquad \text{for} \quad n \longrightarrow \infty$$

(Riesz-Fischer Theorem)

Remark: the elements of the set may be points, measurable functions, transformed functions, or functionals (or operators).

Measurable functions can be simply defined as a function which is the limit a.e. (almost everywhere) of a sequence of step functions (see Reference 30, p. 44).

The norm of the measurable function defined in a measurable region e, for which $|f|^p$ is summable, is defined in Banach space as

$$\text{norm} \equiv \left\| f \right\| \equiv \left[\int_e \left| f(x) \right|^p dx \right]^{1/p} ; \qquad \text{in } L^p \text{ space} \qquad \text{(B-1)}$$
$$1 \leq p \leq \infty$$

$$\equiv \left\| f \right\| \equiv \max \left| f(x) \right| \qquad \text{in C or } L^\infty \text{ space}$$
$$\text{(B-2)}$$

A linear operation or linear functional belonging to Banach space is an operation which assigns to every element f of B a numerical value Af and which is

1: additive: $\quad A(f_1 + f_2) = Af_1 + Af_2$

2: homogeneous: $\quad A(cf) = cAf$, where c is arbitrary constant

3: bounded: there exists a constant M such that for all f

$$\left| A f \right| \leq M \left\| f \right\|$$ (B-3)

Denote the smallest of the possible bounds M by M_A or $\left\| A \right\|$ called

norm of the linear functional A. Hence

$$\left| A f \right| \leq \left\| A \right\| \left\| f \right\|$$ (B-4)

hence

$$\left\| A \right\| \equiv M_A$$ (B-5)

A linear transformation belonging to Banach space is a tranforma-

tion of the space B into itself which transforms the element h into the

element Th and which is

1: additive: $\quad T(h_1 + h_2) = T h_1 + T h_2$

2: homogeneous: $\quad T(c h) = c T h$

3: bounded: there exists a constant M such that for all h

$$\left\| T h \right\| \leq M \quad \left\| h \right\|; \quad \text{if } M_A \text{ is the smallest of}$$ (B-6)

these bounds then

$$\text{norm} \equiv \left\| T \right\| \equiv M_A$$ (B-7)

Multiplication of linear transformations is defined as

$$(T_1 T_2) h = T_1 (T_2 h)$$ (B-8)

and

$$T^2 = TT \quad ; \quad T^3 = T(T^2) \; ; \; \ldots \tag{B-9}$$

for iterated transforms. Their norms have the properties:

$$\| cT \| = |c| \cdot \| T \| \; ; \quad \| T_1 + T_2 \| \leq \| T_1 \| + \| T_2 \| \tag{B-10}$$

$$\| T_1 T_2 \| \leq \| T_1 \| \; \| T_2 \| \tag{B-11}$$

hence for iterated transformations:

$$\| T^2 \| \leq \| T \|^2 \; ; \quad \| T^n \| \leq \| T \|^n \tag{B-12}$$

Continuity of linear transforms:

Every linear transformation is <u>continuous</u> in the sense that if the sequence $\{h_n\}$ converges strongly to h in B, then the sequence $\{Th_n\}$ also converges strongly to Th.

Proof:

$$\| Th_n - Th \| = \| T(h_n - h) \| \leq \| T \| \; \| h_n - h \| \to 0 \tag{B-13}$$

APPENDIX C

PROPERTIES OF DENSITY FUNCTIONS AND OTHER PROBABILITY FUNCTIONS

Consider a probability density function, or in shortened nomenclature, density function or frequency function, $f(x)$, which satisfies the condition:

$$\int_{-\infty}^{\infty} f(x)\,dx = 1 \tag{C-1}$$

then for the random variable,

$$P\left\{x \leq \xi \leq x + dx\right\} = f(x)\,dx \tag{C-2}$$

The cumulative distribution function (or distribution function), $F(x)$ for the random variable, ξ is

$$P\left\{\xi \leq x\right\} = F(x) = \int_{-\infty}^{x} f(x')\,dx = \int_{-\infty}^{x} dF(x') \tag{C-3}$$

hence

$$P\left\{\xi \leq -\infty\right\} = F(-\infty) = 0$$

$$P\left\{\xi \leq \infty\right\} = F(\infty) = 1$$

if

$$f(x) = 0 \qquad \text{for } x \leq 0,$$

then

$$P\left\{\xi \leq 0\right\} = F(0) = 0$$

The expected value of a function $g(x)$ w/r to the density function

f(x) is

$$\langle g(x) \rangle \equiv E\left\{ g(x) \right\} \equiv \int_{-\infty}^{\infty} g(x') \, f(x') \, dx' \qquad \text{(C-4)}$$

This one-dimensional concept can be generalized to many dimensions. Let $\xi_1,\ \xi_2,\ldots\ \xi_k$ be k random variables on sample space, Ω, with density function

$$P\left\{ x_i \le \xi_i \le x_i + dx_i \ ; \quad i = 1, \cdots k \ \right\}$$

$$= f_k \, (x_1, x_2, \ldots x_k) \, dx_1 \, dx_2 \cdots dx_k \qquad \text{(C-5)}$$

The multivariate distribution function is then

$$P\left\{ \xi_i \le x_i \ ; \ i = 1, \cdots k \ \right\} = F_k \, (x_1, \ldots x_k)$$

$$= \int_{-\infty}^{x_1} \cdots \int_{-\infty}^{x_k} f_k \, (x_1, \cdots x_k) \, dx_1 \cdots dx_k \qquad \text{(C-6)}$$

The normalization condition is then

$$\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_k \, (x_1, \cdots x_k) \, dx_1 \cdots dx_k \ = \ 1 \qquad \text{(C-7)}$$

If k = 2, with density function, $f_2(x,y)$, then

$$f_1 (x) = \int_{-\infty}^{\infty} f_2(x,y) \, dy \quad \text{and} \quad f_1'(y) = \int_{-\infty}^{\infty} f_2(x,y) \, dx \qquad \text{(C-8)}$$

are called marginal density functions for x and y respectively. This concept can be generalized by considering the above frequency functions and normalization conditions:

$$f_n (x_1, \cdots x_n) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_k \, (x_1, \cdots x_n, \cdots x_k) \, dx_{n+1} \cdots dx_k \qquad \text{(C-9)}$$

where

$$n \leqslant k$$

The corresponding distribution function is then

$$F_k \left(x_1, \cdots x_n, \infty \cdots \infty \right)$$

$$= \int_{-\infty}^{x_1} \cdots \int_{-\infty}^{x_n} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f_k \left(x_1, \cdots x_n, \cdots x_k \right) dx_1 \cdots dx_n \cdots dx_k$$

$$= \int_{-\infty}^{x_1} \cdots \int_{-\infty}^{x_n} f_n \left(x_1, \cdots x_n \right) dx_1 \cdots dx_n \qquad \text{(C-10)}$$

$$= F_n \left(x_1, \cdots x_n \right)$$

$$= P \left\{ \xi_i \leq x_i , \; i = 1, \cdots n ; \; \xi_i \leq \infty , \; i = n+1, \cdots k \right\}$$

Conditional density functions are defined as

$$f_k \left(x_{n+1}, \cdots x_k \mid x_1, \cdots x_n \right) dx_{n+1} \cdots dx_k$$

$$= \frac{f_k \left(x_1, \cdots x_n \cdots x_k \right)}{f_n \left(x_1, \cdots x_n \right)} dx_{n+1} \cdots dx_k \qquad \text{(C-11)}$$

= probability of random variables $x_{n+1}, \ldots x_k$ lying in intervals $dx_{n+1}, \ldots dx_k$, respectively, upon given $x_1, \ldots x_n$.

Conditional probability is defined as

$$P \left\{ E_2 \mid E_1 \right\} = \frac{P \left\{ E_1, E_2 \right\}}{P \left\{ E_1 \right\}} \qquad \text{(C-12)}$$

where E_1 and E_2 are events in the sample space Ω, and $P\{E_1, E_2\}$ is the probability for both events to occur.

For mutual independence we have for probabilities

$$P\{E_2|E_1\} = P\{E_2\} \, ,$$

since

$$P\{E_1 \cap E_2\} = 0$$

and

$$P\{E_1, E_2\} = P\{E_1\} \, P\{E_2\}$$

and for random variables, ξ_i,

$$P\left\{x_i \leq \xi_i \leq x_i + dx_i \; ; \; i = 1, \cdots k\right\} = \prod_{i=1}^{k} P\left\{x_i \leq \xi_i \leq x_i + dx_i\right\} \qquad \text{(C-13)}$$

$$= \prod_{i=1}^{k} f^i(x_i) \, dx_i \qquad \text{(C-14)}$$

APPENDIX D

PROOF OF FINITENESS OF NON-ANALOG RANDOM WALK
CHAINS DESCRIBED IN CHAPTER IV

In a heterogeneous reactor containing an infinite array of lattice

cells, the neutrons slow down by striking moderator or fuel atoms. Under

the assumption of elastic collisions and struck nuclei at rest, the long-

est chain from birth to death results if the neutron were to slow down

to the cutoff energy entirely within the fuel regions.

The expected number of collisions with one kind of nucleus sustained

by a neutron in slowing down from source energy E_0 to cutoff energy E_C

is approximated by

$$\frac{1}{\xi} \ln \left(\frac{E_0}{E_c} \right) \qquad \text{(D-1)}$$

where ξ is the average logarithmic energy decrement for the given kind

of nucleus.

Therefore the expected length of the chain for the non-analog ramdom

walk process described in Section IV-A, in which all collisions are

scattering collisions, is

$$\langle n \rangle \leq \frac{\ln \left(E_0 / E_c \right)}{\xi_{fuel}} \qquad \text{(D-2)}$$

In measure theory language using Lebesque integration

$$\langle n \rangle = \int_{\Omega} n(\omega) \, d\mu(\omega) \qquad \text{(D-3)}$$

where

$\mu(\omega)$ is the probability measure of the set ω

Ω is the complete sample space

$\mu(\Omega) = 1.$

Consider the set A and its complement defined by

$$A = \left\{ \omega \mid n(\omega) < b \right\}$$
$$A' = \left\{ \omega \mid n(\omega) = b \right\} \qquad b = \infty \tag{D-4}$$

Thus

$$<n> = \int_A n(\omega)d\mu(\omega) + \int_{A'} n(\omega)d\mu(\omega) \tag{D-5}$$

But by the definition of the set A'

$$<n> = \int_A n(\omega)d\mu(\omega) + b\mu(A') \tag{D-6}$$

Since $<n>$ is finite and b is unbounded then $\mu(A')$ must be zero in view of Eq. (D-2). But $\mu(A')$ is just the probability measure of the set containing random walk chains of infinite length, therefore the probability of a chain of infinite length is zero and therefore Eq. (4-7) becomes

$$P\left\{ L = \infty \right\} = 0 \tag{D-7}$$

Osborn has proposed using the hydrogen model to prove (D-7) for the case of non-analog random walk chains in which all collisions are forced to be scattering collisions.

In lethargy units the scattering frequency for elastic neutron collisions with the struck hydrogen nucleus at rest is given by

$$F(u', u'') \, du' = e^{u'-u''} \, du'' \quad , \quad u' \le u'' \le \infty$$

(D-8)

$$= 0 \quad , \quad \text{otherwise}$$

Let P_n be the probability of crossing lethargy u in exactly n collisons, then

$$P\{L = n\} = P_n$$

With the source at lethargy zero, then

$$P_1 = \int_{u'=u}^{\infty} F(0,u') \, du' = \int_{u}^{\infty} e^{-u'} \, du' = e^{-u}$$

(D-9)

$$P_2 = \int_{u'=0}^{u} \int_{u''=u}^{\infty} F(0,u') \, F(u',u'') \, du' du'' = u \, e^{-u}$$

(D-10)

$$P_3 = \int_{u'=0}^{u} \int_{u''=u'}^{u} \int_{u'''=u}^{\infty} F(0,u') F(u',u'') \, F(u'',u''') \, du' du'' du''' = \frac{u^2}{2} e^{-u}$$

(D-11)

$$P_4 = \int_{u'=0}^{u} \int_{u''=u'}^{u} \int_{u'''=u''}^{u} \int_{u^{IV}=u}^{\infty} F(0,u') F(u',u'') \cdots F(u''',u^{IV}) \, du' \cdots du^{IV} = \frac{u^3}{3 \cdot 2} e^{-u}$$

(D-12)

The nth term is determined by induction to be

$$P_n = \frac{u^{n-1}}{(n-1)!} e^{-u}$$

(D-13)

The limit:

$$\lim_{n \to \infty} P_n = 0 \qquad\qquad\text{(D-14)}$$

can be shown by taking the logarithm of (D-13) and using Sterling's formula for the factorial with large n. And therefore

$$P\{ L = \infty \} = P_\infty = 0 \qquad\qquad\text{(D-15)}$$

It is also noted that

$$\sum_{n=1}^{\infty} P_n = 1 \qquad\qquad\text{(D-16)}$$

by substituting (D-14) into the summation and recognizing the resulting sum to be an expansion formula for e^u.

APPENDIX E

SCATTERING PROBABILITY FOR STRUCK NUCLEUS IN MOTION

In the previous sections, the Monte-Carlo process was developed under the assumption that the collision kernel

$$C\left(E, \underline{\Omega} \mid E', \underline{\Omega}'; \underline{r}'\right)$$

could be defined for elastic collisions of neutrons with the struck nuclei at rest. The motion of the nuclei, which produces the Doppler broadening of the resonances, was considered in determining the total cross section in the transport kernel and the ratio of scattering to total cross section. However once it was determined that a scattering collision occurred, the new energy and direction of the neutron were selected as if the struck nucleus were at rest, i.e., it was assumed that at the energies of interest (above 10 kT) the motion of the nucleus had negligible effect on the collision dynamics.

For resonance scattering, this last assumption is somewhat questionable, and it is the purpose of this section to investigate this assumption in some detail. The method employed for this discussion is to derive the correct scattering frequency for the case of elastic collisions and the struck nuclei in motion. The correct scattering frequency and the assumed scattering frequency can then be compared and perhaps some evaluation made of the assumption. The work is an extension of the method of Osborn[57] in which the scattering frequency is

given in integral form for an arbitrary differential scattering cross

section and in closed form for a constant scattering cross section in

the CMCS. Since details are given in Reference 57, the steps are only

outlined here.

The desired probability is $P(\underline{v}|\underline{v}'; A,T)$ = the probability that a

neutron of initial velocity $\underline{v}'$, shall,upon suffering a scattering col-

lision with a nucleus of mass number A and whose velocity distribution

is Maxwellian and characterized by a temperature T, have a final veloc-

ity in d^3v about $\underline{v}$.

This scattering probability can be derived by formulating the scat-

tering rate density of neutrons from all possible initial velocities

into d^3v about $\underline{v}$. After a coordinate transformation this can be written

as

$$d^3_v \int_{\underline{v}'} n(\underline{r},v') \, v' \, d^3_v' \, \Sigma_s (v') \, P(\underline{v}|\underline{v}'; T, A)$$

(E-1)

where $n(\underline{r},\underline{v}')$ is the initial neutron density in phase space.

$$P(\underline{v}|\underline{v}',T,A) =$$

$$= \frac{1}{\Sigma_s(v')} \int_{\underline{\Omega}_R'} \frac{R'}{v'} \, \sigma_s (R',\underline{\Omega}_R') \, m(\underline{V}') \, J\left(\frac{\underline{V}', \underline{\Omega}_R'}{\underline{V}, \underline{\Omega}_R'}\right) d\underline{\Omega}_R'$$

(E-2)

Primes indicate precollision variables

$\underline{v}'$ =   initial neutron velocity

$\underline{V}'$ =   initial atom velocity

$m(\underline{V}')$ =   Maxwellian distribution of atom velocities.

$$R' = \underline{v}' - \underline{V}' \qquad\qquad \underline{\Omega}'_R = \underline{R}'/R'$$

$$\underline{k} = \underline{v} - \underline{v}' \qquad\qquad \underline{\Omega}'_k = \underline{k}/k$$

Upon evaluating the Jacobian, assuming that the differential scattering cross section is isotropic in the CMCS, and performing the azimuthal integration, the scattering probability can be written as

$$P(\underline{v}|\underline{v}';T,A) =$$

$$= \frac{2N}{(2\beta)^4 \xi_s(v')} \frac{k}{v'} \left(\frac{h}{\pi}\right)^{3/2} \int_0^{\pi/2} \sigma_s \, e^{-hD} J_0(ihB) \frac{\sin\gamma \, d\gamma}{\cos^3\gamma} \qquad (E-3)$$

where

N = number scattering atoms per cm^3

J_0 = zero order Bessel function of first kind

$h \equiv \dfrac{M}{2kT}$

$D \equiv v'^2 + \dfrac{k^2}{(2\beta\cos\gamma)^2} - \dfrac{kv'}{\beta}\cos\zeta$

$B \equiv \dfrac{kv'}{\beta} \tan\gamma \, \sin\zeta$

$\sin\zeta = \dfrac{v}{k}\sin\Theta \qquad\qquad \Theta$ = LCS scattering angle

$\alpha \equiv \dfrac{m}{m+M}$

$\beta \equiv \dfrac{M}{m+M}$

It has been assumed that Θ_c is the center-of-mass scattering angle, then the angle γ, and the relative speed R', are related by

$$\gamma = \frac{\pi - \Theta_c}{2}$$

$$R' = \frac{k}{2\beta\cos\gamma}$$

The usual form for the scattering cross section is related to the form appearing in Eq. (E-3) under the assumption of isotropy in the center-of-mass coordinate system.

$$
\begin{aligned}
\sigma_s(R', \Omega_c)d\Omega_c &= \sigma_s(R', \Omega_c)\sin\theta_c \, d\theta_c \, d\phi \\
&= \sigma_s(R')\frac{\sin\theta_c \, d\theta_c \, d\phi}{4\pi} \qquad \left(\text{isotropy in} \atop \text{CMCS}\right) \\
&= \sigma_s\left(\frac{k}{2\beta\cos\gamma}\right)\frac{4\cos\gamma\sin\gamma \, d\gamma \, d\phi}{4\pi}
\end{aligned}
$$

(E-4)

For the case of potential scattering, for which the microscopic cross-section is constant in the center-of-mass system, the scattering probability can be written

$$
P(\underline{v}|\underline{v}';T,A) = \frac{1}{4\pi}\left(\frac{h}{\pi}\right)^{\frac{1}{2}}\frac{1}{\beta^2 k \, v'}e^{-h\overline{X}}
$$

(E-5)

where

$$
\begin{aligned}
X &= \frac{\alpha}{\beta}v^2 + \left(\frac{\beta-\alpha}{2\beta}\right)^2(v^2+v'^2) + 2\frac{\beta-\alpha}{(2\beta)^2}\underline{v}\cdot\underline{v}' \\
&\quad - \frac{v^2v'^2 - (\underline{v}\cdot\underline{v}')^2}{v^2+v'^2 - 2\underline{v}\cdot\underline{v}'}
\end{aligned}
$$

(E-6)

In the limit as $\sqrt{h}v'$ becomes large $\left(hv'^2 = \frac{AE'}{kT}\right)$, and upon integrating over angles, the scattering probability for potential scattering reduces to the common probability for struck nuclei at rest,

$$
\begin{aligned}
\lim_{\sqrt{h}v'\to\infty}\int_\Omega P(\underline{v},\underline{\Omega}|\underline{v}',\underline{\Omega}';A,T)d\Omega \, v^2 dv &= \\
&= \frac{(A+1)^2}{4A}\frac{2v\,dv}{v'^2} \quad ; \quad \frac{A-1}{A+1}v' \leq v \leq v' \\
&= \frac{(A+1)^2}{4A}\frac{dE}{E'} \quad ; \quad \left(\frac{A-1}{A+1}\right)^2 E' \leq E \leq E' \\
&= F(E'\to E)dE
\end{aligned}
$$

(E-7)

For the case of resonance scattering, the Breit-Wigner single-level formula is introduced into Eq. (E-3) before integration. Straight forward integration does not seem possible in this case but by expanding the cross section in Tchebicheff polynomials of the second kind, integrating the individual terms of the series as Hankel transforms and thereby producing Laguerre polynomials, and then performing a sum of some of the terms, the resonance scattering probability can be written as

$$P_R(v | v'; T, A)$$

$$= \frac{1}{4\pi} \left(\frac{h}{\pi}\right)^{1/2} \frac{1}{\beta^2 k v'} \, e^{-hX} \frac{N \sigma_{Rs}^0}{\xi_s(v')} \frac{1 + \beta S}{1 + \frac{4}{\Gamma^2}\left(E_0 - C_1(1 + \xi_0^2)\right)^2} \qquad \text{(E-8)}$$

where

$$\kappa_1 \equiv h \left(\frac{k}{2\beta}\right)^2$$

$$C_1 \equiv \frac{m\beta}{2h} \kappa_1 = \frac{m}{8\beta} k^2$$

$$C_1 \xi_0^2 \equiv \frac{m\beta}{2} v'^2 \sin^2 \xi = \beta E' \sin^2 \xi$$

$$\beta = \frac{1 + \frac{4}{\Gamma^2}\left[E_0 - C_1(1 + \xi_0^2)\right]^2}{1 + \frac{4}{\Gamma^2}\left[E_0 - C_1\right]^2}$$

$$S = \sum_{n=0}^{\infty}{}' U_n \left(\frac{E_0 - C_1}{\sqrt{\frac{\Gamma^2}{4} + (E_0 - C_1)^2}}\right) \frac{C_1^n}{\left[\frac{\Gamma^2}{4} + (E_0 - C_1)^2\right]^{n/2}} \cdot \left\{ \; \right\}$$

$$\left\{ \; \right\} = \left\{ \frac{n!}{\kappa_1^n} L_n\left(-\kappa_1 \xi_0^2\right) - \xi_0^{2n} \right\}$$

U_n is the Tchebicheff polynomial of the second kind

L_n is the Laguerre polynomial.

In the resonance energy range of U-238, Eq. (E-8) can be simplified by replacing (1+BS) by 1. This causes a negligible effect for all scattering angles except backward scattering, in which case the maximum error is about .8% at room temperature and 8% at 3000°C. The term in the exponential equals zero when the scattering angle and the final speed are determined for the case of struck nucleus at rest and becomes large rapidly for other scattering angles and final speeds. Hence the motion of the struck nuclei cause the probability function for the final speeds to be distributed in Gaussian form about the speed corresponding to struck nuclei at rest, and therefore, the exponential term causes Eq. (E-8) to approximate the Dirac delta function, and qualitatively the effect of the motion of the struck nuclei is small. However it is difficult to evaluate quantitative effects due to the complexity of the resonance scattering probability. Further insight can be obtained by considering special cases of scattering. Since for heavy nuclei, scattering is almost isotropic in the laboratory system for the energy range of interest, the average scattering angle is $\pi/2(\overline{\cos \theta} = 0)$. Change the scattering probability from velocity to energy and direction coordinates.

$$P_R \left(\underline{v} \mid \underline{v}'; T, A \right) d^3v = P_R \left(E, \underline{\Omega} \mid E', \underline{\Omega}'; T, A \right) dE \, d\Omega$$

$$= P_R \left(E, \mu \mid E'; T, A \right) dE \, d\Omega \qquad (E-9)$$

$\mu \equiv \cos \Theta$

Θ = scattering angle in LCS.

Let E* be the final energy of the neutron for a given scattering angle for the case of struck nuclei at rest, i.e., for a given scattering angle in CMCS,

$$\frac{E^*}{E'} = \frac{1}{2}\left[1 + \alpha' + (1-\alpha')\cos\Theta_c \right] = \alpha^2 + \beta^2 + 2\alpha\beta\cos\Theta_c \qquad (E-10)$$

where

$$\alpha' \equiv \left(\frac{A-1}{A+1}\right)^2$$

or for a given scattering angle in LCS,

$$\frac{E^*}{E} = \beta^2 + \alpha^2(2\mu^2 - 1) + 2\alpha\mu\sqrt{\beta^2 - \alpha^2(1-\mu^2)} \qquad (E-11)$$

Let the final energy of the neutron due to motion of the nuclei be written as

$$E = E^*(1 + \Delta) \qquad (E-12)$$

where

$$\Delta \equiv \frac{\Delta E}{E^*} = \frac{E - E^*}{E^*}$$

The approximation that $\Delta \ll 1$ can be satisfactorily made since the mass number of the struck nucleus is large. The scattering probability for large scattering mass and $\mu = 0(\Theta = \pi/2)$ becomes

$$P_R\left(E, 0 \mid E'; T, A\right)$$

$$\simeq \frac{1}{8\pi}\left(\frac{\alpha}{2\pi kT}\right)^{1/2}\frac{1}{\sqrt{E'}} \; e^{-\frac{AE'}{8kT}\Delta^2} \frac{N\sigma_{RS}^0/\xi_s(E')}{1 + x^2\left(1 + \frac{E'}{\Gamma x}\Delta\right)^2} \qquad (E-13)$$

where

$$x \equiv \frac{2}{\Gamma} \left(\beta E' - E_0 \right)$$

The coefficient of Δ^2 in the exponential is about 7000 at room temperature for $E' = 6$ ev, hence Δ must be very small, and the final energy very close to E^*. But since the ratio of the neutron half-width to the "peak" energy of the resonance can also be quite small, Δ can be comparable to Γ/E. Therefore near a resonance let Δ be proportional to some multiple, y, of the half-width,

$$\Delta = \frac{\Delta E}{E^*} = y \frac{\Gamma}{E_0} \frac{E^*}{E_0} \approx y \frac{\Gamma}{E_0}$$

Also let Γ^0 be the reduced total width, i.e.,

$$\Gamma^0 \equiv \frac{\Gamma}{\sqrt{E_0}}$$

Therefore

$$\frac{A E'}{8kT} \Delta^2 \approx \frac{A}{8kT} \left(\Gamma^0 \right)^2 y^2$$

$$1 + \frac{E'}{x\Gamma} \Delta \approx 1 + \frac{y}{x}$$

Equation (E-13) in approximated form becomes

$$P_R \left(E, 0 \mid E'; T, A \right)$$

$$\approx \frac{1}{8\pi} \left(\frac{\alpha}{2\pi kT} \right)^{1/2} \frac{1}{\sqrt{E'}} \; e^{-\frac{A}{8kT} \Gamma^{0^2} y^2} \; \frac{N \sigma_{RS}^0 / \Sigma_s (E')}{1 + x^2 \left(1 + \frac{y}{x} \right)^2} \qquad \text{(E-14)}$$

Intuitively, one would expect that if the motion of nuclei in the collision dynamics is an important consideration for the resonance escape probability and Doppler coefficient, then the motion must manifest importance for the strong resonances which contribute a large portion to the resonance absorption probability. However it would seem that a definite trend in modification of the collision dynamics would have to be established in order to realize an important effect, e.g., if the motion of the nuclei could with reasonable probability cause the neutron to lose enough energy in a single collision to completely jump over the Doppler broadened resonance, then surely the effect would be important. For the strong resonances the practical width (resonance width at which the resonance cross section equals the non-resonance cross section) is about 50 half-widths (x = 50) and the reduced total width is about 10 mv/ $\sqrt{ev}$. For the strong resonances the exponential term is then approximately,

$$e^{-\frac{A}{8kT}\Gamma^{o^2}y^2} \simeq \begin{cases} e^{-.12y^2} & , \quad kT = .0253 \, ev. \, (Room \, Temp.) \\ e^{-.012y^2} & , \quad kT = .253 \, ev. \, (\sim 3000°K) \end{cases}$$

For a unique case in which the expected energy loss for the struck nucleus at rest is 25 half-widths and if E' corresponds to x = 50, then E* = E_O. Furthermore if y = -50, then the neutron could lose enough energy to jump over this hypothetical resonance. However the exponential term would be

$$e^{-\frac{A}{8kT}\Gamma'^{o^2}y^2} \approx \begin{cases} e^{-300}, & kT = .0253 \; ev. \\ e^{-30} & kT = .253 \; ev. \end{cases}$$

and therefore the scattering probability, Eq. (E-14), would be so small that the event would be extremely rare. In reality it takes on the order of 10 collisions with U-238 nuclei for the neutron to skip over the strong Doppler broadened resonances of U-238. Therefore the motion of the nuclei probably cannot cause an effect as important as jumping over the resonances. By studying the combination of exponential and denominator terms, it seems that on the average the nuclei motion can cause the neutron to lose more energy when $E' > E_o$ and less energy when $E' < E_o$, than it would lose under the assumption of struck nuclei at rest. Intuitively these small changes would not necessarily change the number of collisions required to skip over the resonance. And since the ratios Γ_n/Γ_γ and Σ_s/Σ_t remain constant throughout a given resonance, under the assumption of negligible potential and interference scattering, then the probability that a neutron suffers a sufficient number of scattering collisions to skip across the resonance does not change.

APPENDIX F

EVALUATION OF THE DOPPLER BROADENING FUNCTIONS AND THEIR DERIVATIVES

Various methods of evaluating the Doppler broadening functions, which were introduced in Chapter IV, will be discussed in this appendix. Among these methods, a new one is presented which utilizes the Moebius Inversion Technique for evaluating the inverse of a Fourier transform. In Chapter IV, the Doppler broadening functions were defined as

$$\psi(x,\theta) \equiv \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\theta}} \frac{dy}{1+y^2} \tag{F-1}$$

$$\chi(x,\theta) \equiv \frac{1}{2\sqrt{\pi\theta}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4\theta}} \frac{y\,dy}{1+y^2} \tag{F-2}$$

which satisfy the following partial differential equations and boundary conditions:

$$\frac{\partial\psi}{\partial\theta} = \frac{\partial^2\psi}{\partial x^2}$$

$$\psi(x,0) = \frac{1}{1+x^2}$$

$$\psi(0,\theta) = \frac{1}{2}\sqrt{\frac{\pi}{\theta}}\, e^{\frac{1}{4\theta}} erfc\left(\frac{1}{2\sqrt{\theta}}\right)$$

and

$$\frac{\partial\chi}{\partial\theta} = \frac{\partial^2\chi}{\partial x^2}$$

$$\chi(x,0) = \frac{x}{1+x^2}$$

$$\chi(0,\theta) = 0$$

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where

$$\operatorname{erfc}(y) = \frac{2}{\sqrt{\pi}} \int_y^\infty e^{-x^2} dx = 1 - \operatorname{erf}(y)$$

It can also be shown that the Doppler broadening functions also satisfy the following differential equations:

$$\frac{\partial \psi}{\partial \theta} = \frac{1}{\theta} \left\{ \left(\frac{x^2-1}{4\theta} - \frac{1}{2} \right) \psi - \frac{x}{2\theta} \chi + \frac{1}{4\theta} \right\} \qquad (F-3)$$

$$\frac{\partial \chi}{\partial \theta} = \frac{1}{\theta} \left\{ \left(\frac{x^2-1}{4\theta} - \frac{1}{2} \right) \chi + \frac{x}{2\theta} \psi - \frac{x}{4\theta} \right\} \qquad (F-4)$$

Equations (F-3) and (F-4) offer a convenient way of evaluating the derivatives with respect to temperature of the Doppler broadening functions. Recall that values of these derivatives are needed to determine the Doppler broadening function in the Monte Carlo program. Equations (F-3) and (F-4) are useful for finding higher order derivatives of Psi and Chi.

By recognizing the exponential and non-exponential parts of the integrands of the Doppler broadening functions, (G-1) and (G-2), as inverse Fourier transforms and recognizing a resultant form of the Dirac delta function the Psi and Chi can be written as

$$\psi(x,\theta) = \int_0^\infty e^{-v-\theta v^2} \cos x v \, dv \qquad (F-5)$$

$$\chi(x,\theta) = \int_0^\infty e^{-v-\theta v^2} \sin xv \; dv \qquad\qquad \text{(F-6)}$$

which are the inverse transforms of

$$\Omega_c(v,\theta) \equiv e^{-v-\theta v^2} = \frac{2}{\pi} \int_0^\infty \psi(x,\theta) \cos xv \; dx \qquad\qquad \text{(F-7)}$$

$$\Omega_s(v,\theta) \equiv e^{-v-\theta v^2} = \frac{2}{\pi} \int_0^\infty \chi(x,\theta) \sin xv \; dx \qquad\qquad \text{(F-8)}$$

Therefore Psi and Chi can be thought of as the inverse Fourier cosine and sine transform of Omega.

1. MOEBIUS INVERSION METHOD

Goldberg and Varga[58] and, independently, Duffin[59] have developed a method of numerically evaluating the inverse Fourier transform by employing the Moebius inversion formula from number theory and the Poisson formula from Fourier analysis. In the notation of Goldberg and Varga,

$$\phi(t) = \frac{2}{\pi} \int_0^\infty F(u) \cos tu \; du \qquad\qquad \text{(F-9)}$$

is the inversion of

$$F(t) = \int_0^\infty \phi(u) \cos tu \; du \qquad\qquad \text{(F-10)}$$

Upon being given an arbitrary sequence of numbers $\left\{ a_k \right\}_{k=1}^{\infty}$, let

the sequence $\left\{ b_n \right\}_{n=1}^{\infty}$ be defined by

$$\sum_{k} a_k \, b_{m/k} = \begin{cases} 1 & , \ m = 1 \\ 0 & , \ m = 2, 3, 4 \cdots \end{cases} \tag{F-11}$$

(all divisors of m)

Then the Moebius inversion formulae are given by

$$G(t) = \sum_{k=1}^{\infty} a_k \, \phi(kt) \tag{F-12}$$

$$\phi(t) = \sum_{n=1}^{\infty} b_n \, G(nt) \tag{F-13}$$

Suppose the a_k are given by

$$a_k : \begin{cases} a_{2k-1} = 1 & , \ k = 1, 2, 3, \cdots \\ a_{2k} = 0 & , \ k = 1, 2, 3, \cdots \end{cases} \tag{F-14}$$

then b_n are defined by

$$b_n : \begin{cases} b_{2n-1} = \mu_{2n-1} & , \ n = 1, 2, 3, \cdots \\ b_{2n} = 0 & , \ n = 1, 2, 3, \cdots \end{cases} \tag{F-15}$$

Where the μ are Moebius numbers,

$$\mu_m = \begin{cases} 1 & , \quad m = 1 \\ (-1)^s & , \quad \text{if m is the product of s distant primes} \\ 0 & , \quad \text{if m is divisible by a square.} \end{cases}$$

If we let

$$G(t) = \frac{1}{t} \left[\frac{F(0)}{2} + \sum_{k=1}^{\infty} (-1)^k F\left(\frac{k\pi}{t}\right) \right] \tag{F-16}$$

and use the sequences (F-14) and (F-15) and Eq. (F-10), then

$$G(t) = \sum_{k=1}^{\infty} \phi\left(t[2k-1]\right) \tag{F-17}$$

and hence

$$\phi(t) = \sum_{n=1}^{\infty} \mu_{2n-1} \, G\left(t[2n-1]\right)$$

$$= \frac{1}{t} \sum_{n=1}^{\infty} \frac{\mu_{2n-1}}{2n-1} \left\{ \frac{F(0)}{2} + \sum_{k=1}^{\infty} (-1)^k F\left(\frac{k\pi}{t(2n-1)}\right) \right\} \tag{F-18}$$

is a solution of Eq. (F-9).

The fact that the result (F-18) is a double infinite series is some-what disconcerting, however in applying the method of Moebius inversion to the functions Psi and Chi certain techniques can be employed to obtain more rapid convergence. This will be illustrated for the Psi function.

By defining

$$F(\theta, v) \equiv \frac{\pi}{2} e^{-v-\theta v^2} \tag{F-19}$$

then Eq. (F-5) can be written in the form

$$\Psi(x, \theta) = \frac{2}{\pi} \int_0^{\infty} F(\theta, v) \cos xv \, dv \tag{F-20}$$

hence

$$F(\theta,\nu) = \int_{0}^{\infty} \Psi(x,\theta) \cos x\nu \, d\nu \qquad \text{(F-21)}$$

Let $m = 2n-1$

$$G(mx) = \frac{1}{mx}\left[\frac{F(0)}{2} + \sum_{k=1}^{\infty} (-1)^k F\left(\frac{k\pi}{mx}\right) \right]$$

$$= \frac{\pi}{2mx}\left[\frac{1}{2} + \sum_{k=1}^{\infty} (-1)^k e^{-\frac{k\pi}{mx} - \theta\left(\frac{k\pi}{mx}\right)^2} \right] \qquad \text{(F-22)}$$

Defining $\phi \equiv \dfrac{x}{2\sqrt{\theta}}$, $\Psi(x,\theta)$ becomes

$$\Psi(x,\phi)$$

$$= \frac{\pi}{2x} \sum_{n=1}^{\infty} \frac{\mu_{2n-1}}{2n-1}\left[\frac{1}{2} + \sum_{k=1}^{\infty} (-1)^k e^{-\frac{k\pi}{mx} - \left(\frac{k\pi}{2m\phi}\right)^2} \right] \qquad \text{(F-23)}$$

Since it is desired to evaluate Psi for a set of values of x and ϕ, it is convenient to evaluate the exponentials on the computer only once and store the values—this of course requires that the two series be truncated.

The non-linear transformation method of Shanks[60] was employed to speed up the convergence of the k-series.

In order to obtain rapid convergence of the n-series the terms were compared to the terms of a series that can be written in closed form. Insight into this method was obtained using the Euler-Maclaurin

sum formula on the k-series, expanding the resulting functions in Taylor series, and recognizing the n-sum of the first few terms of the k-sum.

Employing the Euler-Maclaurin sum formula, Eq. (F-22) can be written after some manipulation as

$$
\begin{aligned}
G(mx) &= \frac{\pi}{2mx}\left\{ \frac{-1}{2} + \frac{m\phi}{2\sqrt{\pi}}\, e^{\frac{1}{4\Theta}}\left[erf\left(\frac{1}{2\sqrt{\Theta}} + \frac{\pi}{2m\phi}\right) - erf\left(\frac{1}{2\sqrt{\Theta}}\right)\right]\right. \\
&+ \left[\frac{1}{2}(1-E) + \frac{\pi}{m\phi}\,\frac{B_1}{2!}\left(H_1\left(\frac{1}{2\sqrt{\Theta}}\right) - E\cdot H_1\left(\frac{1}{2\sqrt{\Theta}} + \frac{\pi}{2m\phi}\right)\right)\right. \\
&\left.\left. - \left(\frac{\pi}{m\phi}\right)^3 \frac{B_3}{4!}\left(H_3\left(\frac{1}{2\sqrt{\Theta}}\right) - E\cdot H_3\left(\frac{1}{2\sqrt{\Theta}} + \frac{\pi}{2m\phi}\right)\right) + \cdots \right]\right\}
\end{aligned} \tag{F-24}
$$

where

$$
E \equiv e^{-\frac{\pi}{mx} - \left(\frac{\pi}{2m\phi}\right)^2}
$$

B_i = Bernouli numbers

H_i = Hermite polynomials.

After expansion for $m\phi$ and mx greater than 1,

$$
\begin{aligned}
G(mx) &\approx \frac{1}{2}\left(\frac{\pi}{2mx}\right)^2\left\{ 1 + \frac{1}{2}\left(\frac{\pi}{2m\phi}\right)^2 - \frac{1}{12}\left(\frac{\pi}{mx}\right)^2 \right. \\
&\left. + \frac{17}{10}\left(\frac{\pi}{2m\phi}\right)^4 + \cdots \right\}
\end{aligned} \tag{F-25}
$$

Now consider the sum

$$
\begin{aligned}
\Psi_1 &= \sum_{n=1}^{\infty} \mu_{2n-1}\,\frac{1}{4}\left(\frac{\pi}{2mx}\right)^2\left(\frac{\pi}{2m\phi}\right)^2 = \sum_{n=1}^{\infty} \mu_{2n-1}\left(\frac{\pi}{2}\right)^4\frac{1}{4x^2\phi^2}\,\frac{1}{(2n-1)^4} \\
&= \sum_{n=1}^{\infty} \mu_{2n-1}\, G_1(m\sqrt{x\phi}) \tag{F-26} \\
&= \frac{6}{(2x\phi)^2}
\end{aligned}
$$

where we define

$$G_1 \left(m \sqrt{x\phi} \right) \equiv \left(\frac{\pi}{2\sqrt{2x\phi}\, m} \right)^4 \tag{F-27}$$

The sum is performed by using the Moebius inversion formula and the Fourier cosine series for

$$f(y) = y^3 \,, \qquad 0 \le y \le \pi$$

and letting

$$y \to 0$$

Another useful sum can also be obtained, namely

$$\psi_2 = \frac{1}{1+x^2} = \psi(x, \infty) \,, \qquad \left(\phi = \infty \,, \ i.e\ \theta = 0 \right)$$

$$= \sum_{n=1}^{\infty} \mu_{2n-1}\, G_2 (mx) \tag{F-28}$$

$$\doteq \sum_{n=1}^{\infty} \mu_{2n-1}\, \frac{\pi}{2mx} \left\{ \frac{1}{1 + e^{-\pi/mx}} - \frac{1}{2} \right\}$$

where

$$G_2 (mx) \equiv \frac{\pi}{2mx} \left\{ \frac{1}{1 + e^{-\pi/mx}} - \frac{1}{2} \right\}$$

$$\simeq \frac{1}{2} \left(\frac{\pi}{mx} \right)^2 \left[1 - \frac{1}{12} \left(\frac{\pi}{mx} \right)^2 + \frac{1}{120} \left(\frac{\pi}{mx} \right)^4 + \cdots \right] \tag{F-29}$$

In this case the k-sum involving x alone can be written in the closed form: G_2.

Therefore, for large x and ϕ and by comparing Eqs. (F-27) and (F-29) with (F-25),

$$G(mx) \simeq G_1 + G_2$$

hence

$$\Psi(x,\phi) \simeq \Psi_1 + \Psi_2 \quad = \frac{6}{2x\phi^2} + \frac{1}{1+x^2}$$

$$\simeq \frac{1}{x^2}\left(1 + \frac{3}{2\phi^2}\right)$$

This same result can be obtained in the limit of large x and ϕ by

considering (F-1) as a Weierstrass transform and formally evaluating

by the method of Hirschman and Widder.[61]

For small x and ϕ but large m, we still have

$$G(mx) \approx G_1 + G_2$$

Hence the sum (F-23) can be written

$$\Psi(x,\phi) =$$

$$= \Psi_1 + \Psi_2 + \sum_{n=1}^{\infty}{}' \mathcal{A}_{2n-1}\left[G(mx) - G_1\left(m\sqrt{x\phi}\right) - G_2(mx)\right]$$

$$= \frac{1}{1+x^2} + \frac{6}{(2x\phi)^2} + \qquad\qquad\qquad\qquad\qquad \text{(F-30)}$$

$$+ \sum_{n=1}^{\infty}{}' \mathcal{A}_{2n-1}\frac{\pi}{2mx}\left[1 - \frac{1}{4}\left(\frac{\pi}{2mx}\right)\left(\frac{\pi}{2m\phi}\right)^2 - \frac{1}{1+e^{-\pi/mx}} + \right.$$

$$\left. + \sum_{k=1}^{\infty}{}' (-1)^k\, e^{-\frac{\pi k}{mx} - \left(\frac{\pi k}{2m\phi}\right)^2}\right]$$

In the program written for the computer and using this method, it
was desired to evaluate Psi for x and ϕ quite small, therefore the sub-
tracting of G_1 and G_2 was delayed until the 6th term of the n-series so
that mx and $m\phi$ were less than one. The Ψ_1 and Ψ_2 terms were cor-
respondingly modified.

For this case the series for Psi becomes

$$\Psi(x,\phi) = \frac{1}{1+x^2} - \frac{.000\,157\,576\,88}{(x\phi)^2} +$$

$$+ \frac{\pi}{2x}\left[\frac{17}{105} - \frac{1}{1+e^{-\pi/x}} + \frac{1/3}{1+e^{-\pi/3x}} + \frac{1/5}{1+e^{-\pi/5x}} + \frac{1/7}{1+e^{-\pi/7x}}\right] +$$

$$+ \sum_{n=1}^{\infty} \mu_{2n-1}\frac{\pi}{2mx}\left\{\frac{1}{2} + \sum_{k=1}^{\infty}(-1)^k e^{-\frac{\pi k}{mx} - \left(\frac{\pi k}{2m\phi}\right)^2}\right.$$

$$\left. - I_n(6)\left[\frac{1}{4}\left(\frac{\pi}{2mx}\right)\left(\frac{\pi}{2m\phi}\right)^2 - \frac{1}{1+e^{-\pi/mx}} + \frac{1}{2}\right]\right\}$$

<div align="right">(F-31)</div>

where the indicator I_n is defined as

$$I_n(6) = \begin{cases} 0 & , \; n < 6 \\ 1 & , \; n \geq 6 \end{cases}$$

By this method values of Psi were calculated to at least 5-figure
accuracy and were compared to those obtained by methods described in
the next section.

2. OTHER METHODS

Other methods of evaluating the Doppler broadening functions have
been tried. The Runge-Kutta technique of numerically evaluating dif-

ferential equations on a digital computer was applied to (F-3) and (F-4).
The numerical evaluation of the partial differential equations satisfied
by Psi and Chi is used to build up a table in the REP Code.[16] Further-
more the derivation of asymptotic and convergent series for Psi and Chi
has been done by others.[20,42] None of these methods (including Moebius
Inversion) of evaluating Psi and Chi over their full range of arguments
are entirely satisfactory for use in the program REPAD, either because
of inaccuracies for certain values of x and theta, or because they re-
quire too much time to evaluate on the computer for this Monte Carlo pro-
gram, or both. In consideration of these various possibilities of eval-
uating the Doppler broadening functions and the necessity of evaluating
their derivatives, it was decided to use a combination of convergent
and asymptotic series.

Define:

$$\phi = \frac{x}{2\sqrt{\theta}}$$

Convergent series:

$$\Psi(x,\theta) = e^{-\phi^2} \sum_{n=0}^{\infty} \frac{\phi^{2n}}{n!} \frac{1}{(4\theta)^n} \Gamma_n \tag{F-32}$$

$$\chi(x,\theta) = x e^{-\phi^2} \sum_{n=0}^{\infty} \frac{\phi^{2n}}{n!} \frac{1}{(4\theta)^{n+1}} \Gamma_{n+1} \tag{F-33}$$

where

$$\Gamma_o = \Psi(0,\theta) = \frac{\sqrt{\pi}}{2\sqrt{\theta}}\ e^{\frac{1}{4\theta}}\ erfc\left(\frac{1}{2\sqrt{\theta}}\right)$$

$$\frac{1}{(4\theta)^{n+1}}\ \Gamma_{n+1} = \frac{2}{2n+1}\ \frac{1}{4\theta}\left[1 - \frac{1}{(4\theta)^n}\ \Gamma_n\right] \quad, \quad n \geq 0$$

Asymptotic series:

$$\Psi(x,\theta) =$$

$$= \frac{1}{1+x^2}\sum_{m=0}^{M}\frac{\left(\frac{1}{2}\right)_m}{\left[\phi\left(1+\frac{1}{x^2}\right)\right]^{2m}}\sum_{n=0}^{m}\frac{(2m+1)!\ (-1)^n}{(2n+1)!\ (2m-2n)!}\ \frac{1}{x^{2n}} \qquad (\text{F-34})$$

$$\chi(x,\theta) =$$

$$= \frac{x}{1+x^2}\sum_{m=0}^{M}\frac{\left(\frac{1}{2}\right)_m}{\left[\phi\left(1+\frac{1}{x^2}\right)\right]^{2m}}\sum_{n=0}^{m}\frac{(2m+1)!\ (-1)^{m+n}}{(2n+1)!\ (2m-2n)!}\ \frac{1}{x^{2m-2n}} \qquad (\text{F-35})$$

$$\frac{\partial \Psi}{\partial \theta} =$$

$$= \frac{1}{1+x^2}\sum_{m=0}^{M}\frac{\left(\frac{1}{2}\right)_m\ \frac{2m}{\theta}}{\left[\phi\left(1+\frac{1}{x^2}\right)\right]^{2m}}\sum_{n=0}^{m}\frac{(2m+1)!\ (-1)^n}{(2n+1)!\ (2m-2n)!}\ \frac{1}{x^{2n}} \qquad (\text{F-36})$$

$$\frac{\partial \chi}{\partial \theta} =$$

$$= \frac{x}{1+x^2}\sum_{m=0}^{M}\frac{\left(\frac{1}{2}\right)_m\ \frac{2m}{\theta}}{\left[\phi\left(1+\frac{1}{x^2}\right)\right]^{2m}}\sum_{n=0}^{m}\frac{(2m+1)!\ (-1)^{m+n}}{(2n+1)!\ (2m-2n)!}\ \frac{1}{x^{2m-2n}} \qquad (\text{F-37})$$

where

$$\left(\tfrac{1}{2}\right)_m \;=\; \left(\tfrac{1}{2}\right)\left(\tfrac{1}{2}+1\right)\cdots\left(\tfrac{1}{2}+m-1\right)$$

The convergent series were used in REPAD to evaluate Psi and Chi for values of x and θ such that $\phi < 3$. The derivatives of Psi and Chi with respect to theta was determined by (F-3) and (F-4), when the convergent series was used. In order to obtain a 1% accuracy in the derivatives it was found that the convergent series should be truncated only when the contribution of the last term in Chi to the sum was less than .01%. The asymptotic series were used for values of x and θ such that $\phi > 4$. The asymptotic series for the derivatives, (F-36) and (F-37), were obtained by differentiating (F-34) and (F-35). The resulting series were checked for accuracy before using in REPAD. For x and θ such that $3 \leqslant \phi \leqslant 4$, it was found that by adding the first term of each convergent series to the asymptotic series for Psi and Chi, satisfactory accuracy resulted. Likewise the derivatives with respect to θ of these first terms were added to (F-36) and (F-37) for this same range of ϕ. The number of terms to be used in the asymptotic series was determined by a careful comparison of evaluating techniques; the decision for specifying the proper number of terms is built into REPAD.

APPENDIX G

COMPUTATIONAL DETAILS USED IN THE MONTE CARLO PROGRAM,
REPAD, FOR SELECTING RANDOM VARIABLES

1. RANDOM NUMBER GENERATORS

The two pseudo-random number sequences used in the Monte Carlo program, REPAD, are obtained from generators using the Method of Congruences. On binary computers with 35 numeric bits and one sign bit, this method involves multiplying two numbers together and taking the 35 least significant bits of the product as the random number. The pseudo-random numbers for the first generator are given by

$$a_n \equiv 3^{21} \, a_{n-1} \, \bmod \, 2^{35} \qquad (G-1)$$

for $n = 1,2,\ldots$. The initial integer, a_0, can be read in as an arbitrary number, however provision is made in REPAD to use $a_0 = 2^{35}-1$ if desired. The pseudo-random numbers for the second generator are given by

$$b_i \equiv 5^{13} \, b_{i-1} \, \bmod \, 2^{35} \qquad (G-2)$$

for $i = 1,2,\ldots$. (G-1) is used to generate the initial random number of each history and (G-2) is used for successive elements in the chain; therefore, $b_0 = a_n$ for the nth history. In practice, the random numbers, b_i, are divided by 2^{35} to obtain fractions on the interval $(0,1)$.

2. GENERAL METHOD

Given the probability density function, f(x),

$$P\left\{ y \leq x \leq y + dy \right\} = f(y)\, dy \qquad \text{(G-3)}$$

its cumulative distribution function, F(x), defined as

$$P\left\{ y \leq x \right\} = F(x) \equiv \int_{-\infty}^{x} f(y)\, dy \qquad \text{(G-4)}$$

The random variable x is selected from its probability function by first

selecting the random number, RN,

$$RN \subset (0,1)$$

then determine x such that

$$RN = F(x) = \int_{-\infty}^{x} f(y)\, dy \qquad \text{(G-5)}$$

If the inverse of F(x) is known, then

$$x = F^{-1}\, RN \, . \qquad \text{(G-6)}$$

3. NEUTRON SOURCE POSITION AND DIRECTION

For a source uniformly distributed in the circular, semi-infinite,

lattice cell with circular fuel rod, only the distance, r, from the axis

is required because of symmetry. Let

$$R = \text{radius of cell}$$

then the density function is

$$P\{y \le r \le y + dy\} = \frac{2\pi y \, dy}{\pi R^2} \quad , \quad \text{for } 0 \leqslant r \leqslant R$$

$$= 0 \quad , \quad \text{otherwise}$$

and

$$P\{y \le r\} = F(r) = \int_0^r \frac{2y \, dy}{R^2} = \frac{r^2}{R^2}$$

Now select $RN \subset (0,1)$, find r such that

$$RN = F(r) = r^2/R^2$$

i.e.,

$$r = R\sqrt{RN} . \tag{G-7a}$$

Alternatively,[48] select RN_1 and $RN_2 \subset (0,1)$; let $RN = \max(RN_1, RN_2,)$; find r such that

$$RN = r/R$$

i.e.,

$$r = R \cdot RN = R \cdot \max(RN_1, RN_2) . \tag{G-7b}$$

The neutron direction is selected from an isotropic distribution. The density function for the polar angle, γ, measured with respect to the radial line extending from the source point r to the axis, is

$$P\{y \le \gamma \le y + dy\} = \frac{\sin y \, dy}{2} \quad , \quad \text{for } 0 \leqslant \gamma \leqslant \pi$$

$$= 0 \quad , \quad \text{otherwise}$$

The distribution function is then

$$P\{y \le \gamma\} = F(\gamma) = \int_0^\gamma \frac{\sin y \, dy}{2} = \frac{1}{2}(1 - \cos \gamma)$$

Now select RN $\subset$ (0,1), find cos γ such that

$$RN = \frac{1}{2}(1 - \cos \gamma)$$

i.e.,

$$\cos \gamma = 2 RN - 1 \tag{G-8}$$

Then

$$\sin \gamma = \sqrt{1 - \cos^2 \gamma} \tag{G-9}$$

The density function for the azimuthal angle, ν , measured with respect to the same reference line as above, is

$$P\{y \le \nu \le y + dy\} = \frac{1}{2\pi} \, dy \qquad , \quad \text{for } 0 \le \nu \le 2\pi$$

$$= 0 \qquad , \quad \text{otherwise}$$

Then

$$P\{y \le \nu\} = G(\nu) = \int_0^\nu \frac{dy}{2\pi} = \frac{\nu}{2\pi}$$

Now select RN $\subset$ (0,1), find ν such that

$$RN = \frac{\nu}{2\pi}$$

i.e.,

$$\nu = 2\pi \ RN \qquad\qquad (G\text{-}10)$$

Then evaluate $\sin\nu$ and $\cos\nu$.

Alternatively[16,45] select RN_1 and $RN_2 \subset (0,1)$. Test: is $(2RN_2-1)^2 + RN_1^2 \leqslant 1$? If no, select two new random numbers and test again. If yes, then

$$\cos\nu = \frac{(2RN_2-1)^2 - RN_1^2}{(2RN_2-1)^2 + RN_1^2} \qquad\qquad (G\text{-}11)$$

$$\sin\nu = \frac{2(2RN_2-1)RN_1}{(2RN_2-1)^2 + RN_1^2} \qquad\qquad (G\text{-}12)$$

4. OPTICAL THICKNESS

The density function for the optical thickness, κ, traveled by a neutron, between successive collision points, is given by the exponential law of attenuation;

$$P\{y \leq \kappa \leq y+dy\} = e^{-\kappa} d\kappa \qquad , \ \text{for } 0 \leqslant \kappa$$
$$= 0 \qquad , \ \text{otherwise}$$

Therefore,

$$P\{y \leq \kappa\} = F(\kappa) = \int_0^\kappa e^{-y} dy = 1 - e^{-\kappa}$$

Now select $RN \subset (0,1)$, find κ such that

$$RN = 1 - e^{-\kappa}$$

i.e.,

$$\kappa = -\ln(1-RN). \qquad\qquad (G\text{-}13)$$

Alternatively, the evaluation of the logarithm may be avoided by using

a rejection technique devised by von Neumann.[45]

Upon selecting the optical thickness the actual distance traveled

by the neutron, t, is determined from

$$\kappa = \int_{0}^{t} \Sigma_t (E, \underline{r}' + \underline{\Omega}_R R') \, dR' \qquad\qquad (G\text{-}14)$$

where Σ_t is given by Eq. (4-52). When the cross section is tempera-

ture independent (G-14) can be integrated, otherwise t is found by trial

and error.

5. NEUTRON SCATTERING

The conditions of scattering are the same as established in Chapter

IV, namely, elastic collision, struck nucleus at rest, scattering iso-

tropic in the CMCS. Let

θ_c = polar angle, CMCS

θ = polar angle, LCS

ϕ_c = azimuthal angle, CMCS

ϕ = azimuthal angle, LCS

E' = neutron energy, precollision

E = neutron energy, postcollision.

The azimuthal angle is uniformly distributed on the interval $(0, 2\pi)$ for

both CMCS and LCS. Select the random variables, $\cos \Theta_c$, $\sin \Theta_c$, $\cos \phi$, and $\sin \phi$ as in Section G-3 for the polar and azimuthal angles.

For the conditions given above, the scattering angle, Θ, and neutron energy E can be determined from Θ_c by the following relations:

$$\frac{E}{E'} = \frac{1}{2} \left(1 + \alpha + (1-\alpha) \cos \Theta_c \right) \equiv D \tag{G-15}$$

$$\cos \Theta = \frac{A+1}{2} \sqrt{\frac{E}{E'}} - \frac{A-1}{2} \sqrt{\frac{E'}{E}}$$

$$= \frac{\sqrt{D}}{2} \left(A+1 - \frac{A-1}{D} \right) \tag{G-16}$$

$$\sin \Theta = \sqrt{1 - \cos^2 \Theta} \tag{G-17}$$

where

$$\alpha \equiv \left(\frac{A-1}{A+1} \right)^2$$

Hydrogen scattering is treated as a special case since $\alpha = 0$,

$$\frac{E}{E'} = \frac{1}{2} \left(1 + \cos \Theta_c \right) \equiv D' \tag{G-18}$$

$$\cos \Theta = \sqrt{D'} \tag{G-19}$$

But by Eq. (G-8), for the polar angle of scattering, Θ_c, we have

$$RN = \frac{1}{2} \left(1 + \cos \Theta_c \right) \tag{G-20}$$

Therefore,

$$D' = RN \tag{G-21}$$

and

$$\cos\theta = \sqrt{RN} \tag{G-22}$$

The evaluation of the square root of RN can be avoided by using the same trick as in Section G-3 (Eq. G-7b), giving

$$\cos\theta = \max\left(RN_1, RN_2\right) \tag{G-23}$$

And then

$$E = E'\cos^2\theta \tag{G-24}$$

$$\sin\theta = \sqrt{1-\cos^2\theta} \tag{G-25}$$

The direction of the neutron after the collision, measured with respect to the radial line extending from the collision point $\underline{r}$ to the axis, can now be determined since the precollision angles, γ' and ν' (Section G-3), are known and the scattering angles, θ and ϕ are known,

$$\cos\gamma = \sin\theta\cos\phi\sin\gamma' + \cos\theta\cos\gamma' \tag{G-26}$$

$$\sin\gamma = \sqrt{1-\cos^2\gamma} \tag{G-27}$$

$$\cos\nu = \frac{1}{\sin\gamma}\left[-(\sin\theta\cos\phi\cos\gamma')\cos\nu' -(\sin\theta\sin\phi)\sin\nu' + (\cos\theta\sin\gamma')\cos\nu'\right] \tag{G-28}$$

$$\sin\nu = \frac{1}{\sin\gamma}\left[-(\sin\theta\cos\phi\cos\gamma')\sin\nu' + (\sin\theta\sin\phi)\cos\nu' + (\cos\theta\sin\gamma')\sin\nu'\right] \tag{G-29}$$

APPENDIX H

A LIST OF SUPPLEMENTARY COMPUTER PROGRAMS WRITTEN

FOR THIS INVESTIGATION

In addition to the main digital computer program discussed in Chapter

V, several programs were developed for preliminary information and for

checking subroutines of the main program.

The following programs were written to investigate methods of evalua-

ting the Doppler broadening functions, Psi and Chi, and derivatives, and

to study the behavior of these functions with respect to their arguments:

1. evaluation of Psi by the method of Moebius Inversion,

2. evaluation of Chi by the method of Moebius Inversion,

3. evaluation of Psi and Chi by the method of Runge-Kutta,

4. evaluation of Psi and Chi by the use of convergent series,

5. evaluation of Psi and Chi by the use of asymptotic series,

6. evaluation of Psi for argument x=0, using the approximation

   of Hastings[62] for the error function,

7. approximation to Psi by extension of Hastings' approximation

   to the error function with complex argument,

8. check on other approximations to Psi and Chi,

9. evaluation of first and higher order derivatives of Psi and

   Chi by application of differential equations, Eqs. (F-3) and

   (F-4),

10. evaluation of first derivatives of Psi and Chi by asymptotic

series plus empirical functions, and comparison to results of item 9.

The following programs were written in order to study the behavior of the Doppler broadened resonance cross sections of U-238 with varying neutron energy and fuel temperature:

1. calculation of peak cross sections from resonance parameters,

2. evaluation of practical widths of resonances of U-238 metal and oxide for various fuel temperatures for two cases: 1) neglect of interference scattering, 2) inclusion of interference scattering,

3. comparison of the Doppler broadened cross sections of U-238 with the UO_2 potential scattering cross section for various energy increments and fuel temperatures. Provision for overlapping of resonances included.

The following programs were written to check the subroutines of the main Monte Carlo program:

1. checking of random number generators and of random variables obtained from the various distributions discussed in Appendix G,

2. generation and listing of random numbers used to initiate each history,

3. other auxiliary programs for checking the various subroutines discussed in Chapter V.

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