A MONTE CARLO CALCULATION OF THE RESONANCE ESCAPE PROBABILITY OF THORIUM IN A HOMOGENEOUS REACTOR

by

David L. Bushnell

Dissertation submitted to the Graduate Faculty
of the Virginia Polytechnic Institute
in candidacy for the degree of

DOCTOR OF PHILOSOPHY
in
Physics

May 1961
Blacksburg, Virginia

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1.

INTRODUCTION

1.1 The Problem

It is the intent of this investigation to prepare a statistical model as an analog to a physical process by employing a random sampling technique which has come to be known as the Monte Carlo method. The physical process is the slowing down of neutrons by collisions with atomic nuclei where one type of nucleus can absorb. A parameter of absorptive moderating systems known as the resonance escape probability (REP) is of interest to reactor physicists and can be estimated from data produced by the statistical model.

The physical system to be considered consists of $Th(NO_3)_4$ dissolved in water to provide a finite homogeneous water moderated reactor in the form of a rectangular parallelipiped. A neutron source is produced at the center of one face by a beam of deuterons striking a deuteron target. The neutrons so produced have an energy of about 2.9 Mev. A tritium target can also be used producing neutrons of about 14 Mev. The (d,t) reaction provides larger neutron fluxes than the (d,d) reaction making possible better counting statistics for experiments.

The neutron cross section of a thorium nucleus manifests several resonances and varies rather rapidly with neutron energy for energies between 10 ev. and 1000 ev. The resonance escape probability is a measure of the ability of a neutron to escape being absorbed while its energy is degraded by the moderation process to an energy below 10 ev.

A system, such as the one considered here, which has many types of nuclides present, some of which can absorb neutrons, is too complicated to solve analytically. From an asymptotic approximation for the slowing down density, $q(E)$, an expression for the resonance escape probability can be written in the form

$$p(E) = e^{-\frac{n_{Th}}{\Sigma_s}} \int_E^{E_o} \sigma_s \frac{\Sigma_a(E')\, dE'}{\xi(E')\,\Sigma_t(E')\, E'} \qquad (1.1)$$

where $\Sigma_a(E')$ = the macroscopic absorption cross section at E'.

$\Sigma_t(E')$ = the total macroscopic cross section at E'.

$\overline{\xi}(E')$ = an average logarithmic energy decrement for a mixture of nuclides.

σ_s = total scattering cross section for all the nuclides.

E_o = the source energy.

n_{Th} = the number of thorium atoms per unit volume.

Equation (1.1) is well discussed by Meghreblian and Holmes (12) along with versions for simpler systems. They define

$$p(E) = \frac{q(E)}{q(E_o)}$$

whence (1.1) results for

$$\overline{\xi} = \sum_i \xi_i \Sigma_{si} \Big/ \sum_i \Sigma_{si}$$

$$\xi_i = 1 + \frac{\alpha_i \ln \alpha_i}{1 - \alpha_i}$$

$$\alpha_i = \left(\frac{A_i - 1}{A_i + 1}\right)^2$$

A_i = the atomic mass number of the i^{th} target atom.

It is more convenient for our purposes to use a slightly different definition for p(E). We will define p(E) to be the ratio of the number of neutrons that reach energy E (which is in our case 10 ev.) from the resonance energy region to the number that enter that region from above 1000 ev. The resonance escape formulas are discussed more completely in section 5.1 and reference (12).

1.2 The Method

The Monte Carlo procedure when applied to physical phenomena becomes essentially a "theoretical experiment" in the sense that a hypothetical set of physical occurrences are imagined whose outcomes are decided deterministically or probabilistically from fairly well established physical theories. The "experiment" comes from allowing a series of many events to occur. The theoretical aspect comes from the use of physical theories to provide the distributions for the sampling procedures. The events considered in this paper are collisions between neutrons and atoms of the reactor system. In all such events the energy of the neutron relative to the atoms is high enough so that molecular collisions do not occur and hence a neutron interacts only with member nuclei separately.

The fundamental theorem of the Monte Carlo method for a continuous variable is as follows:

> Let $f(x)$ be a real, positive, single valued, continuous function of the variable x defined on the interval $-\infty < x < \infty$ such that
>
> $$\int_{-\infty}^{\infty} f(x)dx = 1.$$

If N_r is a random variable uniformly distributed on

the interval $0 \leq N_r \leq 1$, then the equation

$$N_r = \int_{-\infty}^{X_n} f(x)dx \qquad (1.2)$$

implies that X_n is a random variable with frequency function[1] $f(X_n)$.

A proof of this theorem appears in appendix I.

For the discrete case, where there are n mutually exclusive events available one of which is denoted by E_i with probability p_i, we say that event E_m occurs if for a selection of N_r we have

$$\sum_{i=1}^{m-1} p_i \leq N_r < \sum_{i=1}^{m} p_i \qquad (1.3)$$

where N_r is again a random number uniformly distributed on the interval $0 \leq N_r \leq 1$ and $\sum_{i=1}^{n} p_i = 1$. References (2), (9) and (10) provide good discussions of the Monte Carlo method and its applications.

It is not always easy to invert the integral in equation (1.2) so various tricks have been employed to

---

(1) Frequency function is often referred to as probability density function (9).

avoid excessive labor. One such trick is known as the rejection technique and is discussed by Kahn (9).

To apply equation (1.3) one subdivides the interval 0 to 1 into subintervals whose lengths correspond to the p_i of the events E_i. When a selection of N_r provides a value that lies in the m^{th} subinterval, equation (1.3) is satisfied and we say that event E_m occurs.

Large capacity high speed computers are needed in order to handle most Monte Carlo problems. The Virginia Polytechnic Institute has an IBM-650 on which we programmed the Monte Carlo model for the thorium resonance escape probability.

Our chief objective is to develop a Monte Carlo model which will provide a better description of the effect of resonance phenomena on the behavior of reactor systems than has been heretofore possible by analytical methods. It is conceded that the Monte Carlo approach is inefficient when compared to analytical methods but where the latter fails we turn to the former as a last resort. Analytical treatments of diffusion and transport phenomena are limited to special cases since there is a lack of knowledge about the transformation kernels appearing in the integral equations.

While waiting for development of the analytical methods it becomes necessary to turn to approximation and sampling procedures. Knowledge obtained in such a manner may lead to advances in the analytical techniques.

CHAPTER 2.

BACKGROUND AND LITERATURE REVIEW

Monte Carlo investigations of resonance escape probabilities have been done by several groups, who have concentrated on heterogeneous systems containing uranium as the resonance absorber. R. D. Richtmyer and collaborators (15), (16) developed a model for a heterogeneous symmetrical array of cylindrical U^{238} fuel rods contained in a water moderator.

As will be the case in this paper, Richtmyer considers neutron-nucleus scattering collisions, absorbing collisions and rectilinear motion between collisions as the possible events for description. Proceeding from the last neutron collision, Richtmyer determines the distance to the next collision by applying the expression

$$l(E) = -\lambda(E) \ln N_r$$

where $\lambda(E)$ = the mean free path at energy E

$l(E)$ = the distance from the last collision to the next at energy E

N_r = a random number distributed uniformly on (0,1) and selected by a standard random number algorithum in the computer.

The mean free path $\lambda(E)$ is determined from a knowledge of the total cross section by the relation

$$\lambda(E) = \frac{1}{\Sigma_t(E)}$$

where $\Sigma_t(E)$ = the total macroscopic cross section at energy E.

His first published resonance escape calculation in 1956 (15) employed the Doppler broadening function $\psi(x,t)$ for the uranium cross sections while in a later version in collaboration with Van Norton and Wolfe (16) he included a second Doppler broadening function which describes an interference effect in the cross section. See chapter 5 for definitions and discussions of these functions.

The Richtmyer code was written for an IBM-704 which has considerably more speed and storage than the IBM-650 for which our Monte Carlo was written. He, therefore, has been able to develop a rather flexible program to include some variation in geometry and composition of the reactor. His program employs a hexagonal unit cell parallel to the fuel rods.

Many investigations have been made of the resonance integral $\int \frac{\sigma(E)}{E} dE$ and the effective resonance integral

$$\int_{E}^{E_o} \frac{\sigma_a \Sigma_s(E')dE'}{\Sigma_t(E')\ E'} \qquad (2.1)$$

whose forms should be modified to include Doppler - broadening. A comparison between these investigations and the present one is difficult but possible provided we can accept the conditions concerning the resonance structure necessary for equation (1.1) to be valid. The origin of equation (1.1) and the conditions for validity are given in appendix IV. Dresner (6) has made some of the most extensive investigations of the resonance integral, and calculations based on his work are presented in section 6.5.

Safanov (of the Rand Corporation) (19) has made an investigation of resonance escape probabilities for water-natural uranium homogeneous mixtures with varying amounts of light and heavy water. The calculations for these systems are based on the Boltzmann equation with the diffusion approximation. A multi-energy group solution was carried out using 53 energies selected from the numerous noncoincident resonances of U^{235} and U^{238}. The IBM-701 provided solutions of the 53 simultaneous equations. The energy range 1 ev. to 1000 ev. is used as the resonance range and this interval required 42 of the groups. The

resonances were fit with histograms with only one block to a peak rather than a many block histogram or a Breit-Wigner expression. The definition of the resonance escape probability used by Safanov is the fraction of those neutrons living to energies less than 1000 ev. that survive to energies less than 1 ev. This is essentially the same definition that we use except our lower energy limit is 10 ev. Figure 3 of Safanov's paper displays the resonance escape probability as a function of the ratio of the number of moles of water to the number of moles of uranium. Our Monte Carlo with modifications to handle uranium cross sections should be able to reproduce the topmost curve of that figure if the two methods are compatible.

CHAPTER 3.

THE MONTE CARLO MODEL

3.1 Outline of the Model

Referring to the flow diagram exhibited in figure 1 we see that a neutron history begins by a reading of the source parameters into the machine storage. The energy is placed in a reference location and count boxes are set to zero. The sines and cosines of the velocity direction angles are computed and stored for future reference. The energy dependent mean free path $\lambda(E)$ is determined by the method outlined in section 3.3. The distance to the next (or first) collision is determined as follows:

The probability of a collision in dx at x, where x is the distance along a straight line, is given by

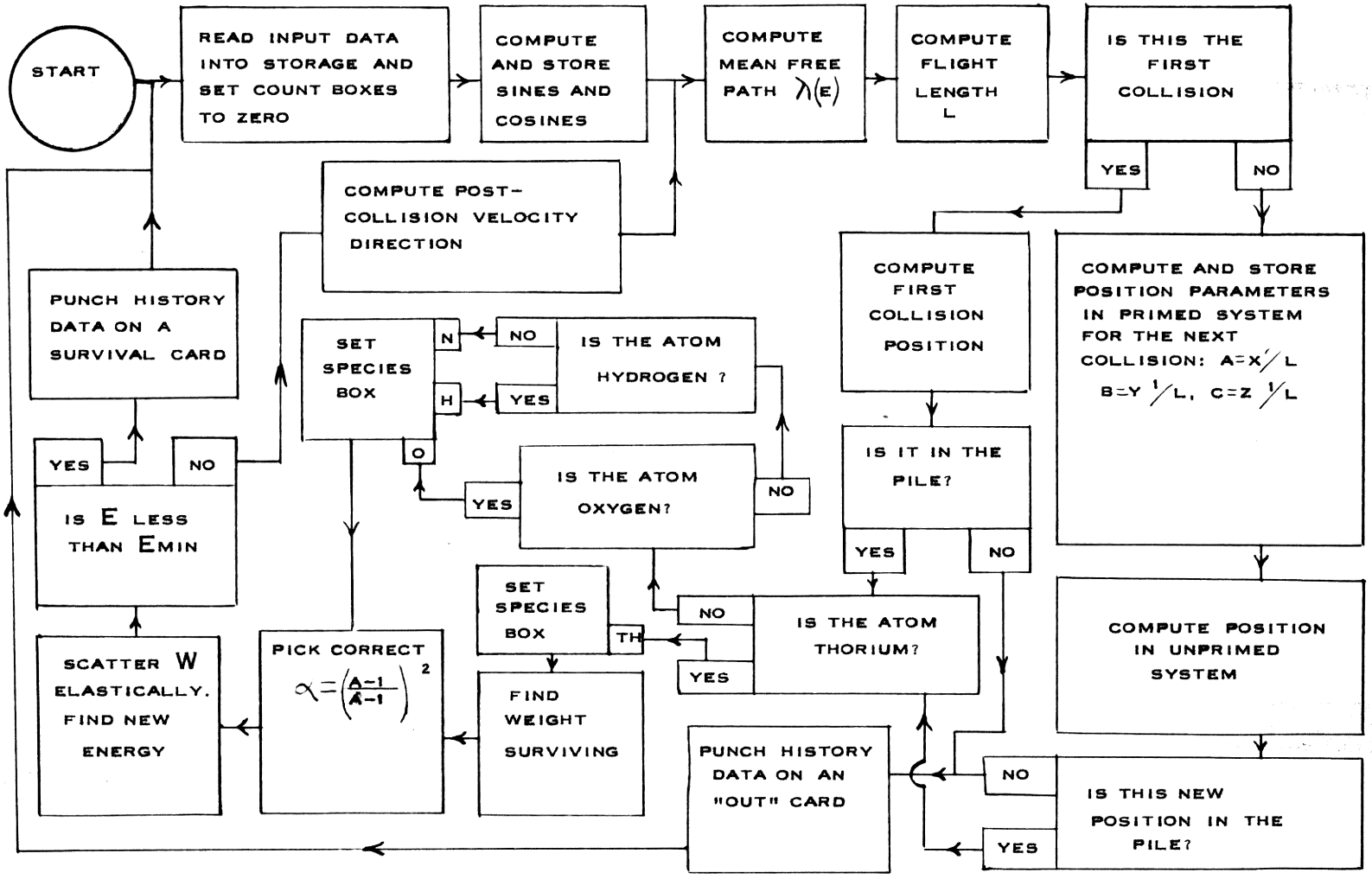
$$f(x)dx = \Sigma e^{-\Sigma x} dx$$

where $$\int_0^\infty f(x)dx = \int_0^\infty \Sigma e^{-\Sigma x} dx = 1$$

and f(x) = the probability density function (p.d.f.) for x.

We imagine another non-discrete random variable y that has a p.d.f. g(y) such that

$$g(y)dy = f(x)dx \qquad \text{where } g(y) = 1.$$



MONTE CARLO FLOW DIAGRAM FOR THORIUM RESONANCE ESCAPE PROBABILITY

FIG. — 1

We then say that the new variable is uniformly distributed and that

$$\int_0^{y(1)} g(y')dy' = \int_0^1 f(x)dx$$

or

$$y(1) = \int_0^1 \Sigma e^{-\Sigma x} dx$$

Since $f(x)$ is a p.d.f., $y(x) \leq 1$. We can therefore let

$$N_r = y(1)$$

i.e., both the random number and the new stochastic variable $y(1)$ are distributed uniformly on the interval $(0,1)$. Now we see that a selection of N_r will determine 1.

This brings in the Monte Carlo method of sampling a uniform distribution $g(y) = 1$ by selecting a random number between 0 and 1. We then have 1 in terms of the random number.

$$N_r = \int_0^1 \Sigma e^{-\Sigma x} dx = 1 - e^{-\Sigma 1}$$

$$e^{-\Sigma 1} = 1 - N_r$$

$$-\Sigma 1 = \ln(1-N_r)$$

$$1 = -\frac{1}{\Sigma} \ln(1-N_r)$$

$$1 = -\lambda \ln(N_r) \qquad (3.1)$$

We have, in the latter equation, used the fact that $1 - N_r$ has the same distribution as N_r (namely uniform on the interval (0,1)) so sampling N_r is equivalent to sampling $1 - N_r$.

The distance traveled from one position to the next collision will for each case be found by equation (3.1) employing a "machine" generated random number N_r.

In order to find the position of the collision one must know whether or not it is for the first collision. If it is for the first collision, the following equations give its coordinates (see figure 5).

$$x = x_o + l\sin\theta, \cos\varphi, \tag{3.2}$$

$$y = y_o + l\sin\theta, \sin\varphi, \tag{3.3}$$

$$z = z_o + l\cos\theta, \tag{3.4}$$

where x_o, y_o, z_o, θ,, φ, are the initial position and velocity direction coordinates.

If the collision is not the first we obtain the position by the equations

$$x' = x + l[(\sin\theta' \cos\varphi' \cos\theta + \cos\theta' \sin\theta) \cos\varphi - \sin\theta' \sin\varphi' \sin\varphi] \tag{3.5}$$

$$y' = y + l[(\sin\theta' \cos\varphi' \cos\theta + \cos\theta' \sin\theta) \sin\varphi + \sin\theta' \sin\varphi' \cos\varphi] \tag{3.6}$$

$$z' = z + l\cos\theta' \qquad (3.7)$$

where $\sin\theta'$, $\cos\theta'$, $\sin\varphi'$ and $\cos\theta'$ are determined by collision physics as discussed in subheadings 3.4 and 3.5.

After the collision position is determined a check is made whether it is still in the pile or not. If not, an "out" card is punched on which there is the initial weight, the final weight, the square of the final weight, and the numbers of collisions encountered with the various types of nuclei. If it remains in the pile at this new collision position, the type of target atom is determined. The following prescription is used to make the latter decision:

Let f_{Th}, f_O, f_H, and f_N stand for the probabilities of striking a thorium, oxygen, hydrogen or nitrogen atom respectively. Obviously they are conditional probabilities - conditional on there being a collision (the probability that there is a collision is one once we have determined l, the distance to the next collision). Then we have

$$f_{Th} + f_O + f_H + f_N = 1$$

and

$$f_{Th} = \frac{\Sigma_{Th}}{\Sigma} = \frac{n_{Th}\sigma_{Th}}{\sum_{i=1}^{4} n_i \sigma_i} \qquad (3.8)$$

$$f_O = \Sigma_O/\Sigma = n_O \sigma_O \left\{ \sum_{i=1}^{4} n_i \sigma_i \right\}^{-1} \qquad (3.9)$$

$$f_H = \Sigma_H/\Sigma = n_H \sigma_H \left\{ \sum_{i=1}^{4} n_i \sigma_i \right\}^{-1} \qquad (3.10)$$

$$f_N = \Sigma_N/\Sigma = n_N \sigma_N \left\{ \sum_{i=1}^{4} n_i \sigma_i \right\}^{-1} \qquad (3.11)$$

where all cross sections are determined for the incident neutron energy.

Now with a machine generated random number N_r we decide on an atom by using the Monte Carlo principle.

$0 \leq N_r < f_{Th}$	then thorium is the atom
$f_{Th} \leq N_r < f_{Th} + f_O$	then oxygen is the atom
$f_{Th} + f_O \leq N_r < f_{Th} + f_O + f_H$	then hydrogen is the atom
$f_{Th} + f_O + f_H \leq N_r \leq 1$	then nitrogen is the atom.

It is now convenient to treat one of two possibilities:

(1) The collision is not on thorium.

(2) The collision is on thorium.

Case 1

For this case the only possible reaction is elastic scattering since in the energy range under consideration (10 ev. to 1000 ev.) the absorption cross sections are essentially zero for oxygen, hydrogen and nitrogen. The energy of the neutron following such a collision is selected again by the device of sampling from the supply of random numbers using the equation

$$E_2 = -E_1(1 - \alpha)N_r + E_1 . \qquad (3.12)$$

This equation is based on the fact that all attainable energies following an elastic scattering are equally likely. See section 3.4, "The Collision", for the derivation of equation (3.12).

Case 2

If the collision occurs with thorium, the new weight* of the neutron is found by multiplying the pre-collision weight by the fraction scattered.

$$W_2 = W_1 \frac{\sigma_{sc}}{\sigma_{ab} + \sigma_{sc}} \qquad (3.13)$$

where W_1 = pre-collision neutron weight

W_2 = after-collision neutron weight.

---

* Weight is used here in a statistical sense. For example, if n neutrons collide with n absorbers where each colliding pair has the same relative energy then if N are absorbed $\frac{n-N}{n}$ will be the fraction that scatter. Rather than give up a history when an absorption occurs we assign the above probability for scattering as a "weight" and continue the history.

The quantity in parenthesis is the fraction scattered. The thorium cross sections are determined using the expressions (4.10) and (4.11) which are derived in appendix II. The pre-collision energy is examined to determine within which peak it lies and whether the tabular values of $\psi(x,t)$ and $\chi(x,t)$ are to be used or if the asymptotic calculations are appropriate.

The history proceeds by going back through case 1 for a thorium scattering and if the post-collision energy is below 10 ev. a low energy card is punched with the same information as on the "out" card referred to earlier. If $E_2 > 10$ ev., the laws of conservation of momentum and kinetic energy require that the new direction be given by

$$\cos\Theta' = \frac{1-A}{2}\sqrt{\frac{E_1}{E_2}} + \frac{1+A}{2}\sqrt{\frac{E_2}{E_1}} \quad . \qquad (3.14)$$

Subsection 3.4 with the subheading "The Collision" describes the latter equation and the energy selection in detail.

For the other velocity direction coordinate, φ', as defined in figure 5 of section 3.5 we use the assumption of a uniform distribution for φ' and therefore use the sampling technique with the equation

$$\varphi' = 2\pi N_r \quad . \qquad (3.15)$$

After the sines and cosines of Θ' and φ' are computed, the program returns to the computation of a new λ and ℓ. The position of the next collision is determined by the equations (3.5), (3.6), and (3.7). This cycle is continued until all the source cards have been read.

A data-extraction program is used to sum the weights of neutrons starting a history, the weights of neutrons leaving the pile, the weights going to low energy ($E < 10$ ev.), and the various collision counts.

The programming details are presented in appendix IV.

3.2 Beginning a Neutron History

The initial information needed to start a history was obtained from a Monte Carlo model of water moderation for a pulsed source (21). The neutrons being produced by $H^2(H^2,n)H^3_e$ reaction. This program provides on an output card from the IBM-650 the position, energy, weight, and the direction of the velocity vector for a neutron the first time that its energy falls into the 990 ev. energy range from 10 ev. to 1000 ev.

In an attempt to provide an analytical method for starting histories, the above data cards were analyzed to determine radial probability distributions for various

values of the z coordinate which is parallel to the deuteron beam. The position integrated energy distribution of "first arrivals" turned out to be uniform between 10 ev. and 1000 ev. Sampling the position distributions and the energy separately seemed to be a good approach, but storing the additional data and program instructions appeared to require more storage than was available. The card-read method therefore was used. This limits the calculation for a given concentration to about 4300 histories.

Figure 2 indicates that $\overline{E}(z)$, the average energy per slab located at z, is essentially uniform. Tables 1, 2 and 3 show the various data that must be stored in the machine for future reference.

3.3 The Mean Free Path

For neutron energies below 1000 ev. we have only two significant neutron reactions occurring. They are radiative capture (n,γ) and elastic scattering. Other types are not energetically possible. The lowest energy levels of thorium are too high to be excited by these relatively low energy neutrons. Therefore Σ_{ab} (the absorption cross section) is all due to radiative capture and Σ_{sc} (the scattering cross section) is due only to elastic

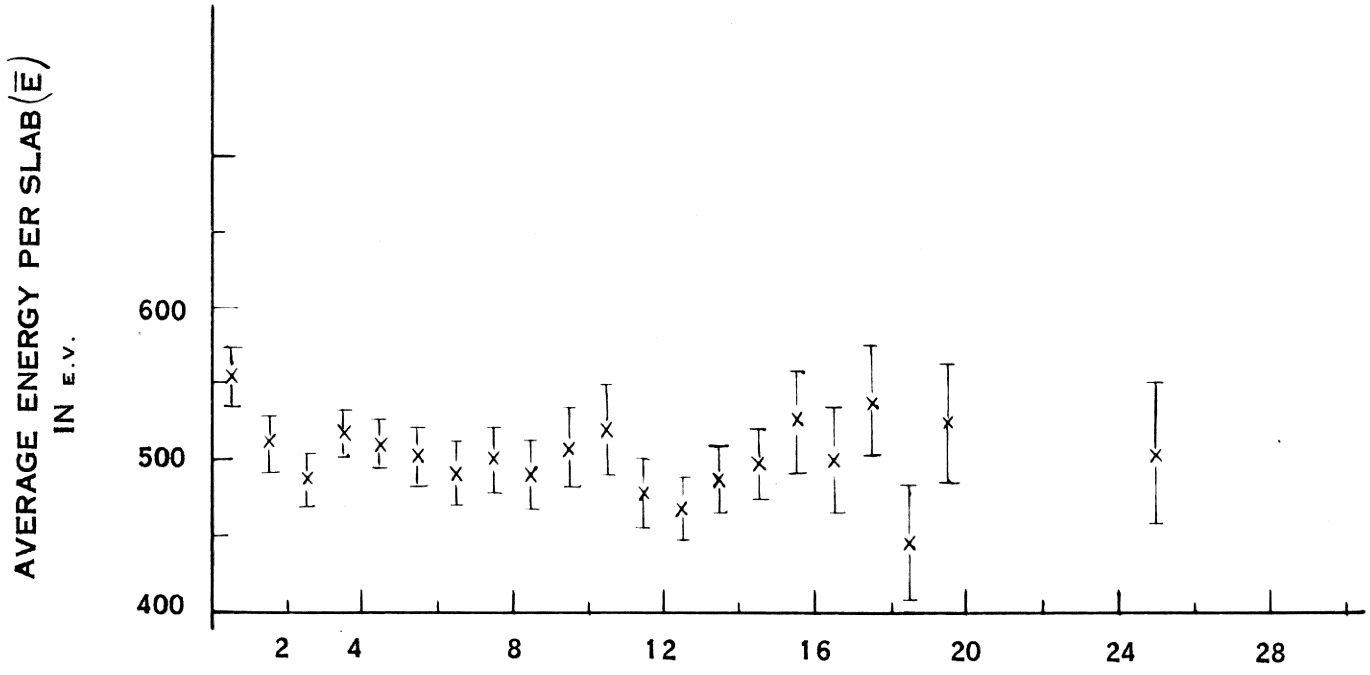


FIG. — 2

THE AVERAGE SOURCE ENERGY PER SLAB VERSUS Z

TABLE. 1

NUCLIDE NUMBER DENSITIES AND CROSSECTION FOR FIVE CONCENTRATIONS OF $TH(NO_3)_4$ IN WATER.

A/B	C	ρ IN GM/CM^3	$N_{TH} \times 10^{21}$ ATOMS/CM^3	$N_{OX} \times 10^{21}$ ATOMS/CM^3	$N_H \times 10^{21}$ ATOMS/CM^3	$N_N \times 10^{21}$ ATOMS/CM^3	σ_{ox} BARNS	σ_H BARNS	σ_N BARNS	Σ_{NOH} CM^{-1}
	64.00	1.915	1.5381	41.51	46.10	6.152	3.8	20.2	9.1	1.145
1.2	45.45	1.580	0.9013	39.64	57.64	3.605	3.8	20.2	9.1	1.348
1.85	35.09	1.415	0.6231	38.91	61.43	2.492	3.8	20.2	9.1	1.411
3.00	25.00	1.272	0.3991	36.69	63.81	1.596	3.8	20.2	9.1	1.443
5.00	16.67	1.166	0.2439	35.42	64.99	0.976	3.8	20.2	9.1	1.456

TABLE. 1 USES THE FOLLOWING NOTATION: ρ = SOLUTION DENSITY, C = CONCENTRATION, A = MASS OF WATER USED FOR SOLUTION, B = MASS OF SALT DISSOLVED, N_{TH} = NUMBER OF THORIUM ATOMS PER UNIT VOLUME (N_{OX}, N_H AND N ARE THE SAME QUANTITY FOR OXYGEN, HYDROGEN AND NITROGEN RESPECTIVELY) σ_{OX} = MICROSCOPIC CROSSECTION FOR NEUTRON INTERACTION WITH OXYGEN IN THE THORIUM RESONANCE REGION (σ_H AND σ_N ARE THE SAME QUANTITIES FOR HYDROGEN AND NITROGEN), $N_{OH} = N_{OX}\sigma_{OX} + M_H\sigma_H + N_N\sigma_N$.

scattering. The total macroscopic cross section would then be

$$\Sigma_t = \Sigma_{ab} + \Sigma_{sc} \tag{3.16}$$

with $$\Sigma_{ab} = \sum_{i=1}^{N=4} n_i(i\,\sigma_{ab}) \tag{3.17}$$

and $$\Sigma_{sc} = \sum_{i=1}^{N=4} n_i(i\,\sigma_{sc}). \tag{3.18}$$

Finally the mean free path becomes

$$\lambda = \frac{1}{\Sigma_t} = \frac{1}{\sum_{i=1}^{4} (n_i(i\,\sigma_{ab}) + n_i(i\,\sigma_{sc}))}. \tag{3.19}$$

The mean free path is energy-dependent because the cross sections are energy-dependent. It is therefore necessary to use the resonant behavior of thorium while computing λ.

As an example if one calculates λ for an "on resonance" thorium cross section and an "off resonance" value from peak 3 with $n_{Th} = 0.6231 \times 10^{21}$ atoms/cm^3 there results

$$\lambda_{off} = .704 \text{ cm}$$

$$\lambda_{on} = .198 \text{ cm}.$$

So the mean free path for off the peak is about 3.6 times as large as the value at the peak maximum.

3.4 The Collision

The commoner method of handling the collision routine is, first, to sample the direction of travel after the collision from the known angular distribution of the elastic collision and then to determine the energy from conservation laws. The order of this procedure has been reversed in this paper since for elastic scattering the energy distribution is simpler to sample from and the calculation of direction, once the energy is known, is easy to perform on the "machine". We therefore begin with the energy determination.

Let E_2 = the neutron energy after collision

E_1 = the neutron energy before collision

$\alpha = \left(\frac{A-1}{A+1}\right)^2$ where A is the atomic mass of the target nucleus.

Experiments show the neutron scattering at energies of less than several Mev is spherically symmetric in the center of mass system. Therefore the probability of a neutron proceeding from a collision into solid angle $d\Omega$ formed by a conical element of angle θ and angular width $d\theta$ (see figure 3) is uniform, i.e.

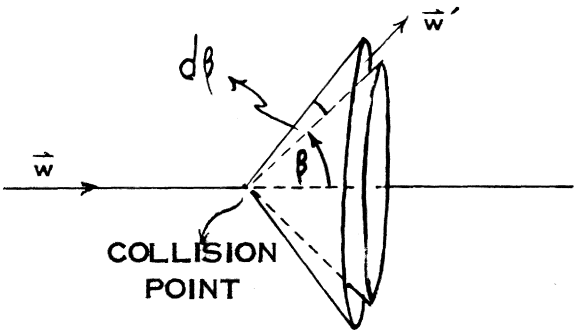


FIG. – 3. CENTER OF MASS COLLISION CONE.

$\vec{w}$ = THE CENTER OF MASS NEUTRON VELOCITY BEFORE COLLISION.

$\vec{w}'$ = THE CENTER OF MASS NEUTRON VELOCITY AFTER COLLISION.

β = THE CENTER OF MASS ANGLE OF ELASTIC SCATTERING.

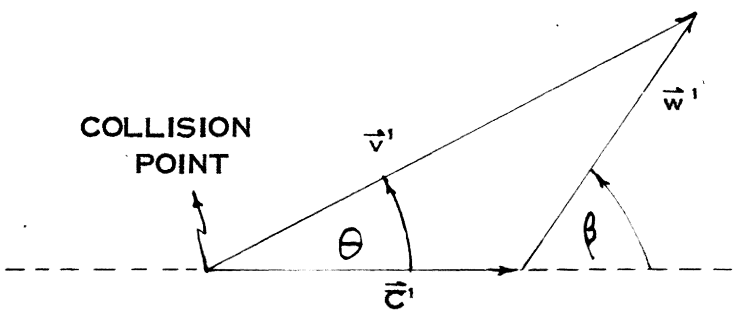


FIG. – 4. POST COLLISION NEUTRON VELOCITIES.

θ = THE LABORATORY ANGLE OF ELASTIC SCATTERING.

$\vec{v}^1$ = THE NEUTRON VELOCITY IN THE LABORATORY.

$\vec{w}^1$ = THE NEUTRON VELOCITY IN THE CENTER OF MASS.

$\vec{c}^1$ = THE CENTER OF MASS VELOCITY.

$$p(\beta)d\beta = \frac{d\Omega}{4\pi} = \frac{2\pi r \sin\beta \, r d\beta}{r^2}/4\pi$$

$$= \frac{2\pi \sin\beta}{4\pi} d\beta = \tfrac{1}{2}\sin\beta \, d\beta$$

$$\left|p(E_2)dE_2\right| = \left|p(\beta)\right| \left|\frac{d\beta}{dE_2}\right| \left|dE_2\right|$$

but $$\frac{E_2}{E_1} = \tfrac{1}{2}\left[(1+\alpha) + (1-\alpha)\cos\beta\right] \tag{3.20}$$

see reference (7) from which we obtain

$$\left|\frac{d\beta}{dE_2}\right| = \frac{2}{E_1(1-\alpha)\left|\sin\beta\right|}$$

and $$p(E_2)dE_2 = \frac{dE_2}{E_1(1-\alpha)}. \tag{3.21}$$

Since $p(E_2)$ is then energy independent the distribution of E_2 is uniform and all values of E_2 are equally likely.

Now let

$$N_r = F(E_2) = \int_{E_2}^{E_1} P(E_2^1)dE_2^1$$

where $\alpha E_1 \leq E_2 \leq E_1$

$$N_r = \frac{(E_1 - E_2)}{E_1(1-\alpha)}$$

$$\therefore \quad E_2 = E_1 - E_1(1-\alpha)N_r \tag{3.22}$$

where N_r is again a random number ($0 \leq N_r < 1$) to be selected by the machine.

To complete the collision we need to have Θ as a function of energy where Θ is the scattering angle in the laboratory system corresponding to β, the scattering angle in the center of mass system.

From conservation of momentum and conservation of kinetic energy we have the equations:

$$\cos\Theta = \frac{\frac{m}{M}\sqrt{\frac{2E_1}{m}} + \frac{A}{m}\sqrt{\frac{2E_1}{m}}\cos\beta}{\sqrt{\frac{2E_2}{m}}}, \quad M = m + A$$

and $$\cos\beta = \left(\frac{E_2}{E_1} - \frac{A^2+m^2}{(A+m)^2}\right)\left[\frac{2mA}{(A+m)^2}\right]^{-1}$$

which combine to give for $m = 1$

$$\cos\Theta = \frac{A+1}{2}\sqrt{\frac{E_2}{E_1}} - \frac{A-1}{2}\sqrt{\frac{E_1}{E_2}} \qquad (3.23)$$

where A = target mass given in atomic mass units in the latter equation

m = neutron mass which equals 1 in atomic mass units

E_2 = neutron energy after collision in the laboratory system

E_1 = neutron energy before collision in the laboratory system.

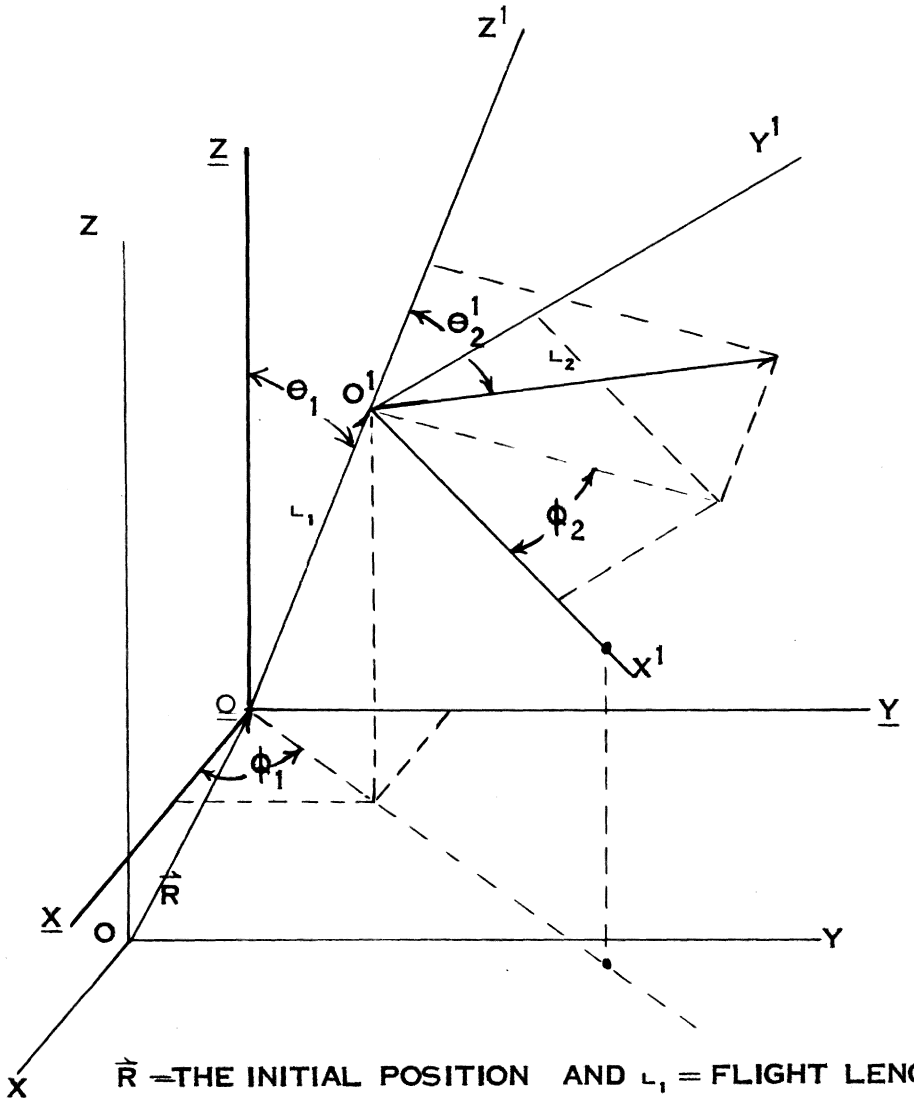
Figure 4 shows the scattering angles in the two systems.

3.5 Tracking the Position

The initial space coordinates (x, y, z) and the velocity direction coordinates (θ, φ), which are spherical coordinates with respect to the z axis as pole, are supplied as input data. The initial speed of the neutron is given indirectly by the neutron energy.

Referring to figure 5, the initial position which serves as origin for a second coordinate system ($\underline{x}$, $\underline{y}$, $\underline{z}$) parallel to (x, y,z) is given by the position vector $\bar{R}$. The initial flight direction is given by (θ_1, φ_1). Still another set of axes (x', y', z') called the primed system is formed by making the z' axis a continuation of the pre-collision flight line l_1. The x' axis is picked so as to be in the plane formed by $\underline{z}$ and z' while y' is perpendicular to that plane. To make the selection unique we further require that the positive x' axis never intersect the positive $\underline{z}$ axis.

Having calculated $\lambda(E)$ and l_1 by equations (3.19) and (3.1) we can find



$\vec{R}$ =THE INITIAL POSITION AND L_1 = FLIGHT LENGTH FOR INITIAL ENERGY.

FIG. — 5 —

TRACKING COORDINATES

$$\underline{x} = \Delta x_1 = l_1 \sin\theta_1 \cos\varphi_1$$

$$\underline{y} = \Delta y_1 = l_1 \sin\theta_1 \sin\varphi_1$$

$$\underline{z} = \Delta z_1 = l_1 \cos\theta_1 .$$

We now have the first collision position at O' given by

$$x_1 = x_o + \Delta x_1$$

$$y_1 = y_o + \Delta y_1$$

$$z_1 = z_o + \Delta z_1$$

where $\bar{R} = x_o \bar{i} + y_o \bar{j} + z_o \bar{k}$.

If the neutron at this new position is still in the pile, we proceed to find the position of the next collision. We have available both θ_2' and φ_2' by application of the Monte Carlo technique to the first collision. By application of equations (3.19) and (3.1) we obtain l_2 and then the primed coordinates become

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} l_2 \sin\theta_2' \cos\varphi_2' \\ l_2 \sin\theta_2' \sin\varphi_2' \\ l_2 \cos\theta_2' \end{pmatrix} .$$

Now by a coordinate rotation to the (x,y,z) system we have

$$\begin{pmatrix} \Delta x_2 \\ \Delta y_2 \\ \Delta z_2 \end{pmatrix} = \underline{M} \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} \tag{3.24}$$

where $$\underline{M} = \begin{pmatrix} \cos\theta_1\cos\varphi_1 & -\sin\varphi_1 & \sin\theta_1\cos\varphi_1 \\ \cos\theta_1\sin\varphi_1 & \cos\varphi_1 & \sin\theta_1\sin\varphi_1 \\ -\sin\theta_1 & 0 & \cos\theta_1 \end{pmatrix} .$$

The position of the second collision is then

$$\begin{aligned} x_2 &= x_1 + \Delta x_2 \\ y_2 &= y_1 + \Delta y_2 \\ z_2 &= z_1 + \Delta z_2 \quad . \end{aligned}$$

A small saving in computer time due to leakage can be obtained if one waits until out checking starts before multiplying by l_2. We, therefore, divide (3.24) by l_2 and define $A = \Delta x_2/l_2$, $B = \Delta y_2/l_2$, $C = \Delta z_2/l_2$, $a = x'/l_2$, $b = y'/l_2$, $c = z'/l_2$ to obtain

$$\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \underline{M} \begin{pmatrix} a \\ b \\ c \end{pmatrix} . \qquad (3.25)$$

The new collision location is then given by

$$(x_2, y_2, z_2) = (x_1 + l_2 A, y_1 + l_2 B, z_1 + l_2 C). \qquad (3.26)$$

The direction angles are then given by

$$\cos\theta_2 = C$$

$$\sin\theta_2 = \sqrt{1-C^2}$$

$$\cos\varphi_2 = A/\sqrt{A^2+B^2}$$

$$\sin\varphi_2 = B/\sqrt{A^2+B^2} .$$

Since most of the leakage neutrons leave through the entrance face at z=0, the calculation for x_2 and y_2 may often be omitted if z is checked first. Hence, two multiplications are often saved, namely $l_2 A$ and $l_2 B$.

CHAPTER 4.

NEUTRON-NUCLEUS CROSS SECTIONS

In order to determine the fraction of the incident neutron weight that is scattered in a thorium encounter we must have some physical information to provide the probabilities of scattering and absorption. A common procedure is to describe the resonance cross section peaks by single level Doppler-Broadened Breit-Wigner equations which seem to apply quite well to thorium resonances. Cast in this form the cross sections are given by:

$$\sigma_{Th} = \sqrt{\frac{E_o'}{E}}\sigma_{or}\psi(x,t) + 4\pi R^2 + \sigma_{os}\psi(x,t) + \sqrt{\sigma_{pot}\sigma_{os}}\chi(xt) \tag{4.1}$$

where $$\psi(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} \frac{e^{-(x-y)^2/4t}}{1+y^2}\, dy \tag{4.2}$$

$$\chi(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} \frac{2ye^{-(x-y)^2/4t}}{1+y^2}\, dy \tag{4.3}$$

$$x = \frac{2}{\Gamma}(E-E_o), \qquad y = \frac{2}{\Gamma}(E'-E_o) \tag{4.4} \quad (4.5)$$

$$t = \frac{4kTE_o}{A\Gamma^2} = 4.34\frac{E_o}{\Gamma^2} \times 10^{-2} \quad . \tag{4.6}$$

$$\sigma_{or} = \frac{4\pi}{k_o^2} \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} = \frac{2.6 \times 10^6}{E_o} \frac{\Gamma_n \Gamma_\gamma}{\Gamma^2} \qquad (4.7)$$

is the natural peak resonant absorption maximum cross section

$$\sigma_{os} = \frac{4\pi}{k_o^2} \frac{\Gamma_n^2}{\Gamma^2} = \frac{2.6 \times 10^6}{E_o} \frac{\Gamma_n^2}{\Gamma^2} \text{ ev. bns} \qquad (4.8)$$

is the natural peak resonant scattering maximum cross section

$$\sigma_{pot} = 4\pi R^2 \qquad (4.9)$$

is the hard sphere potential scattering cross section. The other symbols used are defined as follows:

E_o = Energy corresponding to the maximum cross section for the resonance in ev.

R = effective nuclear radius

k = neutron wave number or propagation number corresponding to energy E

T = the temperature of the target particles or moderator nuclei

Γ_n = neutron level width

Γ_γ = radiation level width

Γ = total natural level width

k_o = propagation constant for E_o neutron of energy E_o

$$= \frac{p_o}{\hbar} = \frac{2\pi}{\lambda_o} .$$

The first term in equation (4.1) gives the resonant absorption cross section for the Doppler-broadened peak, and the next three terms together comprise the Doppler-broadened scattering cross section. Therefore we can write:

$$\sigma_{ab} = \sqrt{\frac{E_o}{E}}\, \sigma_{or} \psi(x,t) \qquad (4.10)$$

for the thorium absorption cross section and

$$\sigma_{sc} = \sigma_{pot} + \sigma_{os} \psi(x,t) + \sqrt{\sigma_{pot}\, \sigma_{os}}\, \chi(x,t) \qquad (4.11)$$

for the thorium scattering cross section.

The last two terms of the last expression form the resonant scattering cross section. The last term is often referred to as the interference term between the hard sphere (potential) scattering and the resonance scattering. For a more detailed development of equations (4.1) through (4.11) refer to appendix II.

The $\log \sigma$ vs. $\log E$ thorium resonance curves that appear in BNL-325 (reference 8) proved to be inadequate for the purposes of this paper. L. M. Bollinger (1) provided

the raw data, on which the above were based, in a form much easier to examine. These data were obtained at the Argonne National Laboratory with a fast chopper neutron spectrometer. Figures 6, 7, and 8 show portions of that data. The resolution for all measurements was about .09 usec/m which translates to 0.26 ev. for the lowest energy peak which is shown in figure 6. The theoretical fit at room temperature shown by the solid line is within the stated resolution as is the case for fits on the other peaks. The fits referred to were obtained by programming the IBM-650 to calculate equation (4.1). It is fortuitous that methods for extracting level parameters from transmission data have been developed that are independent of the detailed shape of the yield curve. Rosen (16) has used one such method known as area analysis to provide the thorium resonance parameters. His results corroborate those of Bollinger. With no available evidence to refute the Breit-Wigner peak shape detail we proceeded to apply equation (4.1) with Rosen's parameters for the lowest eight peaks. The function $\chi(x,t)$ was obtained by means of the relation

$$\chi(x,t) = 4t \frac{\partial \psi(x,t)}{\partial x} + 2x\psi(x,t) \qquad (4.12)$$

where the derivative was taken graphically.

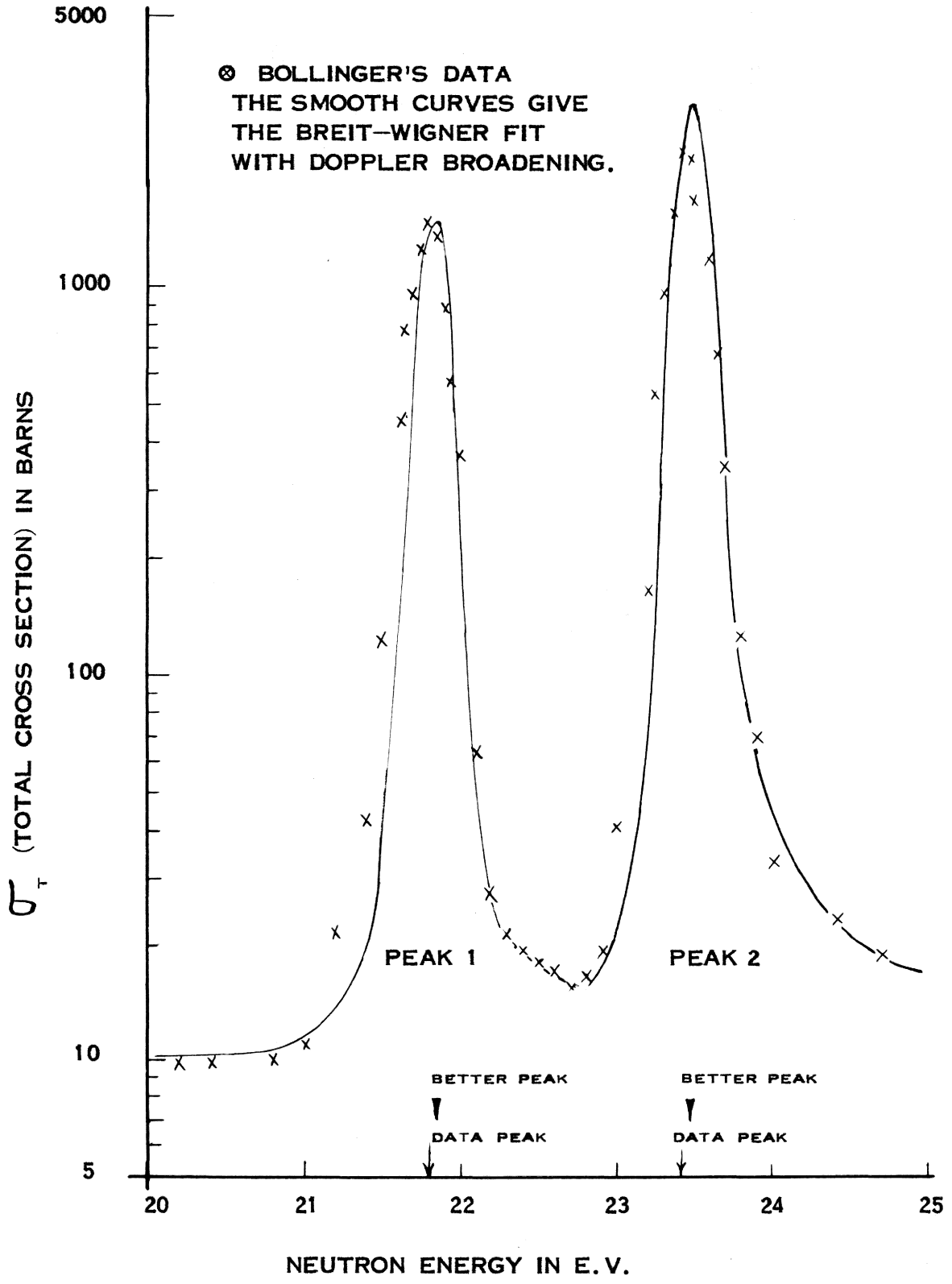


FIG. — 6
THORIUM RESONANCE PEAKS 1 AND 2.

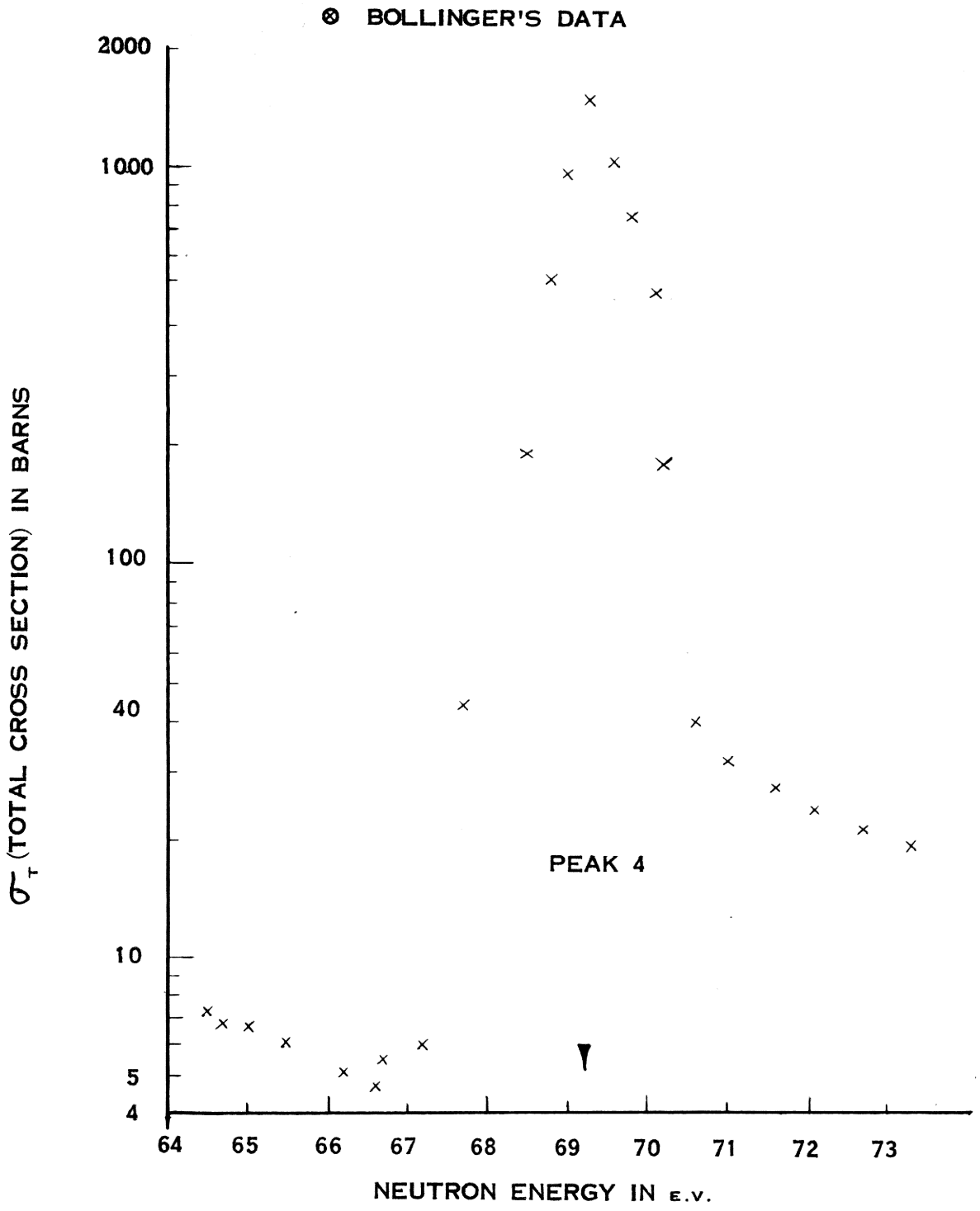


FIG. — 7

THORIUM RESONANCE PEAK 4.

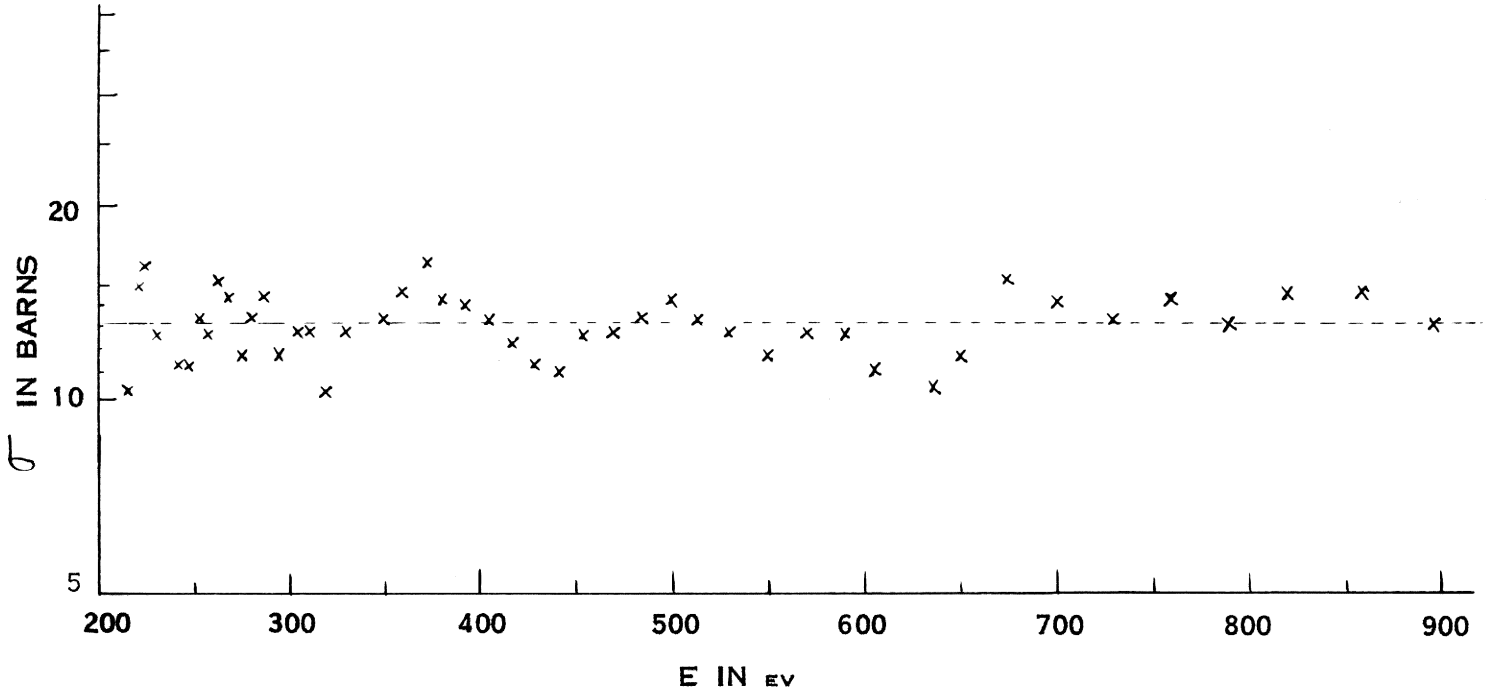


FIG. — 8. CROSS SECTIONS IN THE UNRESOLVED REGION.

To avoid excessively large machine storage tables of the functions $\psi(x,t)$ and $\chi(x,t)$, asymptotic equations (given below) were used out in the wings of a resonance where $x^2 >> t$. This compressed the tables down to about twenty entries per peak. The tabular procedure replaces the analytic function by a step function with what amounts to many steps over the peak. The asymptotic expressions used were:

$$\psi(x,t) \simeq \frac{1}{1+x^2}\left[1 + \frac{2t(3x^2-1)}{(1+x^2)^2} + \ldots\right] \qquad (4.13)$$

$$\chi(x,t) \simeq \frac{2x}{1+x^2}\left[1 + \frac{2t(x^2-3)}{(1+x^2)^2} + \ldots\right] . \qquad (4.14)$$

If more confidence could be placed in the available thorium cross section data, it would become reasonable to use smaller increments of x over the peak in order to approximate more closely the analytic function for the resonance. One must keep in mind however that this refinement coupled with a machine-generated source routine may well overload the IBM-650 storage capacity making access to a larger machine necessary. Also, there are resonances of small magnitude above the eight peaks treated, but their structure is not clear enough to incorporate in this calculation. An average value was used for these peaks. When

this structure is more accurately analyzed experimentally, one can easily add the corresponding parameters and functions to the program provided that sufficient machine storage is available. The variation of these higher energy peaks about the chosen average is very small and in most cases will contribute very little absorption. After all, ψ asymptotic is smaller than χ asymptotic so that σ_{sc} (resonance) is the largest contributor to the total cross section for energies far out in the wings. For the larger t's of these high energy peaks, $\chi(x,t)$ is larger relative to $\psi(x,t)$ and hence the persistence of σ above σ_{pot} is largely due to the interference term of σ_{sc}.

CHAPTER 5.

COMPUTATIONS AND RESULTS

5.1 Resonance Escape

The theory of neutron slowing down processes for a homogeneous mixture of nuclides with hydrogen as the primary moderator leads to an expression for the slowing down density that contains the factor

$$\exp\left\{-\frac{N_{Th}}{\xi\Sigma_s}\int_E^{E_o}\frac{\sigma_a(E')\Sigma_s(E')}{\Sigma_s(E')+\Sigma_a(E')}\frac{dE'}{E'}\right\} .$$

If one defines a resonance escape probability by the relation:

$$p(E:E_o) = \frac{q(E)}{q(E_o)} \qquad (5.1)$$

where $q(E)$ = the slowing down density at energy E

$q(E_o)$ = the number of neutrons leaving the source at energy E_o per cm^3 per sec

then $$p(E,E_o) = \exp\left\{-\frac{N_{Th}}{\xi\Sigma_s} I_{eff}\right\} \qquad (5.2)$$

where $$I_{eff} = \int_E^{E_o}\frac{\sigma_a(E')\Sigma_s(E')}{\Sigma_s(E')+\Sigma_a(E')}\frac{dE'}{E'} . \qquad (5.3)$$

A more complete discussion of these relations appears in reference (12).

If there is no absorption for $E \geq E_1$, where the resonance region is defined by $E_2 \leq E \leq E_1$, then

$$P(E_2:E_1) = P(E_2:E_o) = \frac{q(E_2)}{q(E_o)} . \qquad (5.4)$$

When hydrogen is present in the mixture the possibility exists that a neutron can skip the resonance region with one collision on hydrogen. Definition (5.4) counts such events in both $q(E_2)$ and $q(E_1)$. We wish to exclude such events from our probability as implied by the definition offered in the introduction where the number of neutrons skipping is deleted from both $q(E_2)$ and $q(E_1)$ by the phrases "...from the resonance region..." and "...enter that region from above 1000 ev.".

The probability excluding "skipping" will be reported as REP_∞ and REP_g for the infinite and finite geometry cases respectively. The probability including "skipping" will be reported as REP'_∞ and REP'_g for the same two geometry cases.

The following information can be obtained as output data for a complete calculation:

W_1 = the sum of the weights attaining low energy from the resonance energy region

W_{in} = the sum of the weights of the source neutrons each of which starts with energy in the resonance region

W_o = the sum of the neutron weights that leak through the walls of the container and go out of the pile.

The quantity W_s (the sum of the weights skipping the resonance region) is obtained from the first stage Monte Carlo developed by Settles (21). It then follows that we have

$$REP_g = \frac{W_1}{W_{in}} , \qquad REP'_g = \frac{W_1+W_s}{W_{in}+W_s} \qquad (5.5), (5.6)$$

$$REP_\infty \simeq \frac{W_1}{W_{in}-W_o} , \qquad REP'_\infty \simeq \frac{W_1+W_s}{W_{in}-W_o+W_s} . \qquad (5.7), (5.8)$$

Equation (5.8) should come closest to providing a value of

$$P(E_2:E_1) = \exp\left\{ - \frac{M_{Th}}{\xi \Sigma_s} I_{eff} \right\} .$$

Equation (5.7) comes about because

$$REP_\infty \simeq \frac{W_1+(REP_\infty)W_o}{W_{in}} .$$

Reference to tables 4 and 5 will show the escape probabilities determined by the Monte Carlo program for

TABLE. 4.

DATA FROM OUTPUT CARDS									
N_{TH} $\times 10^{21}$ ATOMS/CM^3	$W_{IN} = \sum_i W_{IN}$	$W_{LOW} = \sum_i W_{LOW}$	$\sum_i W_{LOW}^2$	$W_{OUT} = \sum_i W_{OUT}$	N_N	N_C	N_H	N_{OX}	N_{TH}
1.5381	4317.475	3836.553	3787.629	258.012	1082	23533	18656	3121	674
.9013	4316.475	3940.634	3908.280	230.550	550	22230	18852	2466	362
.6231	4315.480	4008.910	3985.000	214.129	390	21741	18882	2232	237
.3991	4212.490[1]	3941.890	3922.120	194.750	252	21152	18617	2111	172
.2439	4316.480	4073.150	4062.830	198.750	141	21381	19091	2038	103

[1] 104 OUTPUT CARDS WERE ACCIDENTLY LOST. THEREFORE WITH $\frac{21152}{4213} = 5.02$ COLLISIONS PER CARD AN ADDITIONAL 104 CARDS AUGHT TO INCREASE N_C BY $104 \times 5.02 = 523$ COLLISIONS SO THAT $N_C = 21675$ COLLISIONS. THIS MAINTAINS THE INCREASE OF N_C WITH N_{TH}.

TABLE. 5

PROBABILITY RESULTS										
$N_{TH} \times 10^{21}$ ATOMS/CM^3	REP_G	REP_∞	REP'_G	REP'_∞	P_{OX}	P_H	P_N	P_{TH}	P_{AB}	P_{AB}
.2439	.9436	.9892	.9443	.9893	.0953	.8929	.0066	.0048	.437	.4260
.3991	.9358	.9811	.9366	.9814	.0998	.8802	.0119	.0081	.441	.4535
.6231	.9290	.9775	.9298	.9778	.1027	.8685	.0179	.0109	.390	.3945
.9013	.9129	.9644	.9140	.9649	.1109	.8480	.0247	.0165	.4014	.4130
1.5381	.8886	.9451	.8900	.9458	.1326	.7932	.0460	.0286	.3298	.3285

various thorium number densities. Figure 10 displays these results graphically.

A five point least squares fit to a straight line was made for the REP_∞' curve with the result that

$$P = REP_\infty' = 1 - .0367n \qquad (5.9)$$

where n is the thorium number density in atoms per cm^3. The closeness of the fit can be seen by comparing the observed data points to those calculated by equation (5.9) as listed in table 13.

To decide whether the data is sufficiently well fit by a straight line rather than by a higher degree polynomial a quadratic fit was made giving the equation

$$P = 1 - .03669n + .005095n^2 \qquad (5.10)$$

A test to measure improvement employs the F statistic given by

$$F(K,n-k) = \frac{\sum_{i=1}^{n} {}_1e_i^2 - \sum_{i=1}^{n} {}_q e_i^2}{\frac{\sum_{i=1}^{n} {}_q e_i^2}{n-k}}$$

where ${}_1e_i$ = the deviation of the i^{th} data point from the linear curve

${}_q e_i$ = the deviation of the i^{th} data point from the quadratic curve

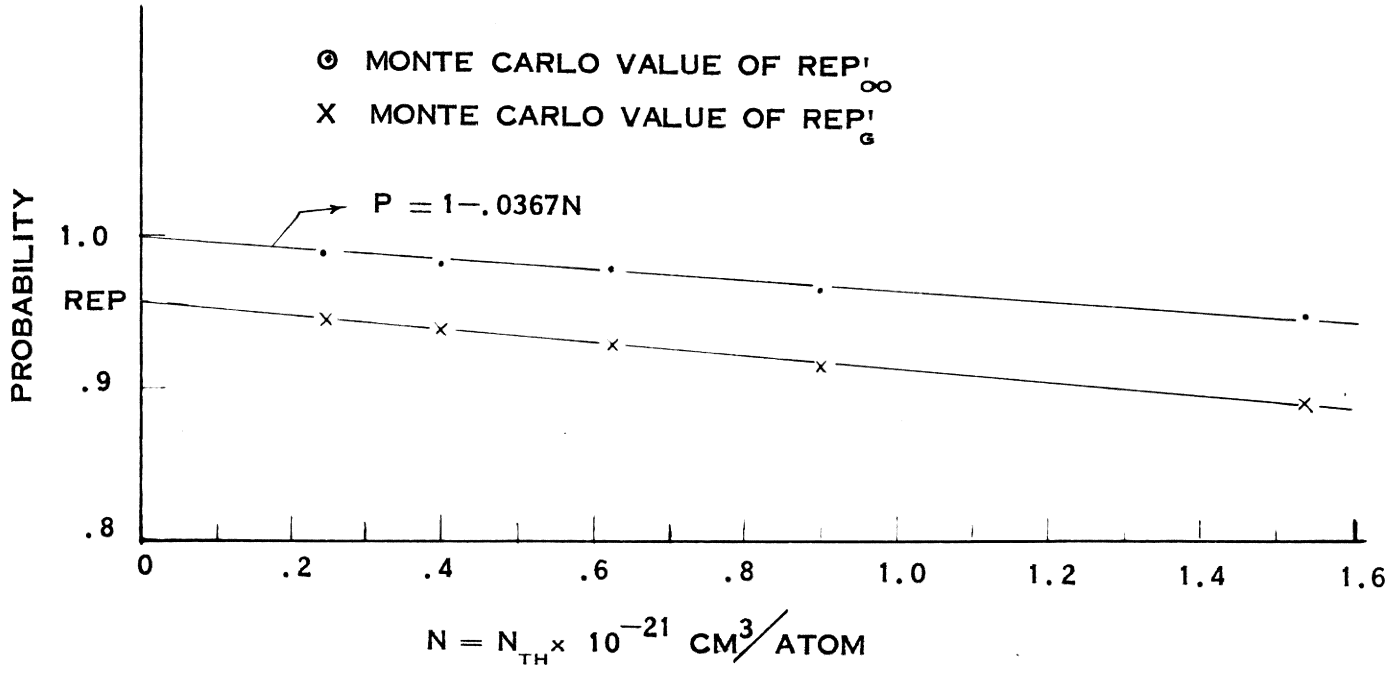


FIG. — 10

RESONANCE ESCAPE PROBABILITY AS A FUNCTION OF THORIUM NUMBER DENSITY

n = the number of data points
k = the number of degrees of freedom in the quadratic case
K = the number of degrees of freedom in the linear case.

For our problem n = 5, k = 2, K = 1, and F(1,3) = 3.85. From a table of the F distribution we find

$$F_{.10}(1,3) = 5.54 > 3.85$$
$$F_{.05}(1,3) = 10.13 > 3.85$$
$$F_{.01}(1,3) = 34.12 > 3.85.*$$

We conclude, therefore, that at all levels of significance the linear model fits the data and that the error reduction due to the quadratic term is insignificant. Equation (5.9) gives the functional dependence of P on n sufficiently well.

The separate contributions to the reduction of the resonance escape probability by the effects of leakage and absorption are displayed for comparison in table 6. The increase in the leakage effect with larger n_{Th} is to be expected since, with the addition of more $Th(NO_3)_4$, the

---

* This notation means that the chance for F > 5.54 is 0.1 or the fraction of the area under the F frequency function beyond F = 5.54, i.e.,

$$\text{for} \quad \int_0^\infty f(F)dF = 1 \qquad 0.1 = \int_{5.54}^\infty f(F)dF.$$

TABLE. 6

COMPARISON OF LEAKAGE AND ABSORPTION

$N_{TH} \times 10^{-21}$ ATOMS/CM^3	% LEAKAGE $(REP_\infty - REP_G)$	% ABSORPTION $(1 - REP_\infty)$
.2439	4.26	1.08
.3991	4.53	1.89
.6231	4.85	2.25
.9013	5.15	3.56
1.5381	5.65	5.49

TABLE. 7

NUCLIDE POPULATION CONTROL OF Σ_{NOH}

$N_{TH} \times 10^{21}$ ATOMS/CM^3	$N_{OX} \times 10^{21}$ ATOMS/CM^3	$N_H \times 10^{21}$ ATOMS/CM^3	Σ_{NOH} IN CM^{-1}
.2439	35.42	64.99	1.456
.3991	36.69	63.81	1.433
.6231	38.91	61.43	1.409
.9013	39.64	57.64	1.348
1.5381	41.51	46.10	1.145

relative number density of hydrogen will be less. With the heaviest contribution to the total macroscopic cross section coming from hydrogen we expect that cross section to reduce along with the hydrogen number density and therefore produce larger mean free paths.

$$\lambda = \frac{1}{n_{Th}\sigma_{Th}+n_{ox}\sigma_{ox}+n_{N}\sigma_{N}+n_{H}\sigma_{H}} \quad . \qquad (5.10)$$

We have values of the sum

$$\Sigma_{NoH} = \Sigma_{ox} + \Sigma_{N} + \Sigma_{H} \qquad (5.11)$$

for the five values of n_{Th}. We see from table 7 that they decrease with increasing n_{Th}.

5.2 Collision Probabilities

We notice that the last point for each graph of figure 11 deviates from the approximate linear pattern set by the points for small n_{Th}. We can expect relatively more collisions with thorium because of multiple collisions that are infrequent on the smaller samplings of thorium collisions, but we would expect to see some multiple collisions on the larger samplings that go with larger n_{Th}.

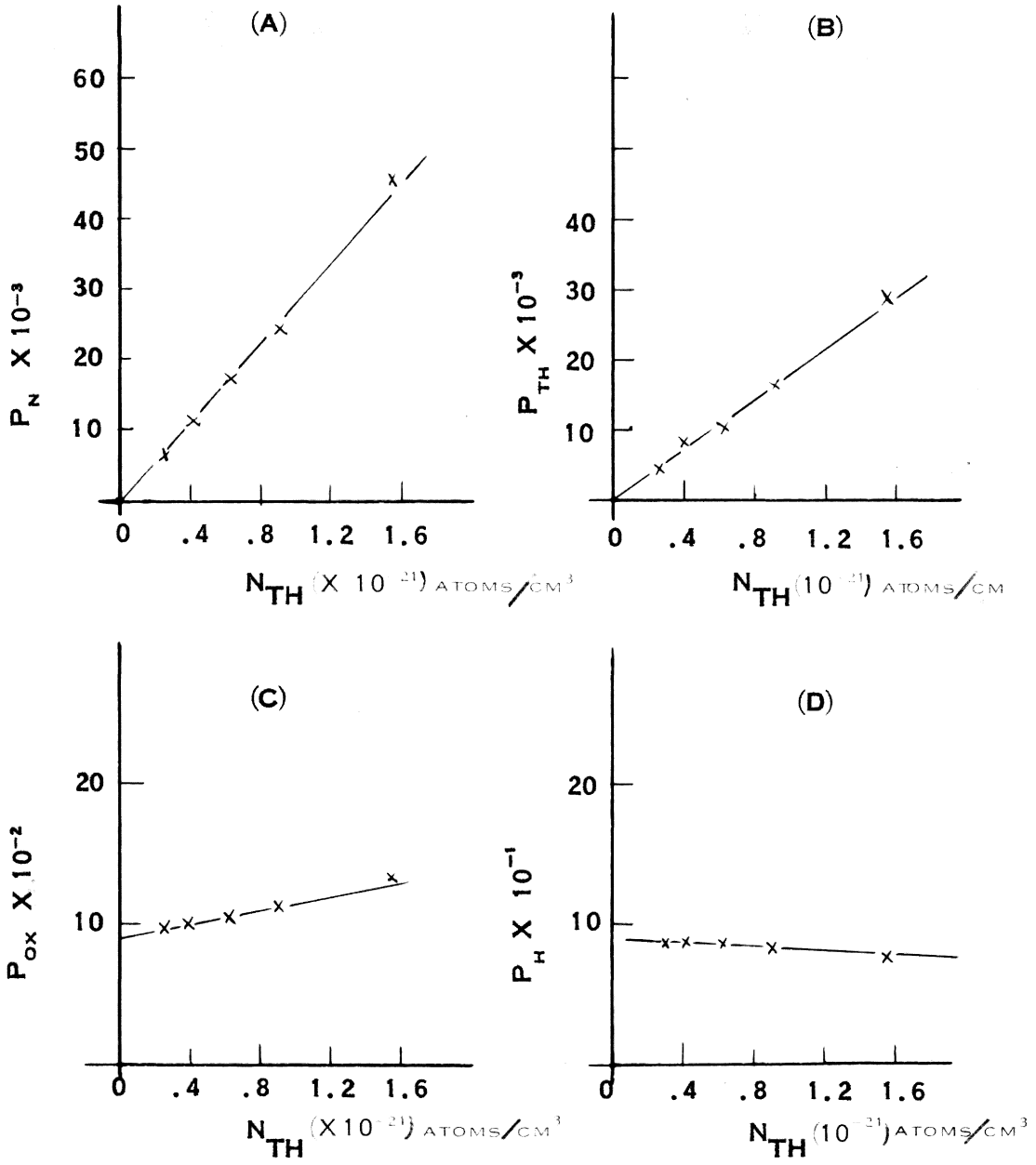


FIG. — 11

ATOMIC COLLISION FREQUENCIES
(A) NITROGEN (B) THORIUM (C) OXYGEN (D) HYDROGEN

Whereas, n_N and n_{ox} increase faster than linear with a linear increase of n_{Th} making possible a faster than linear increase of their collision frequencies. Accompanied with this, we get a faster than linear decrease in n_H making possible a faster than linear decrease in its collision frequency with n_{Th}. These latter effects are due to the non-linearity shown in figure 12. See equations in appendix III.

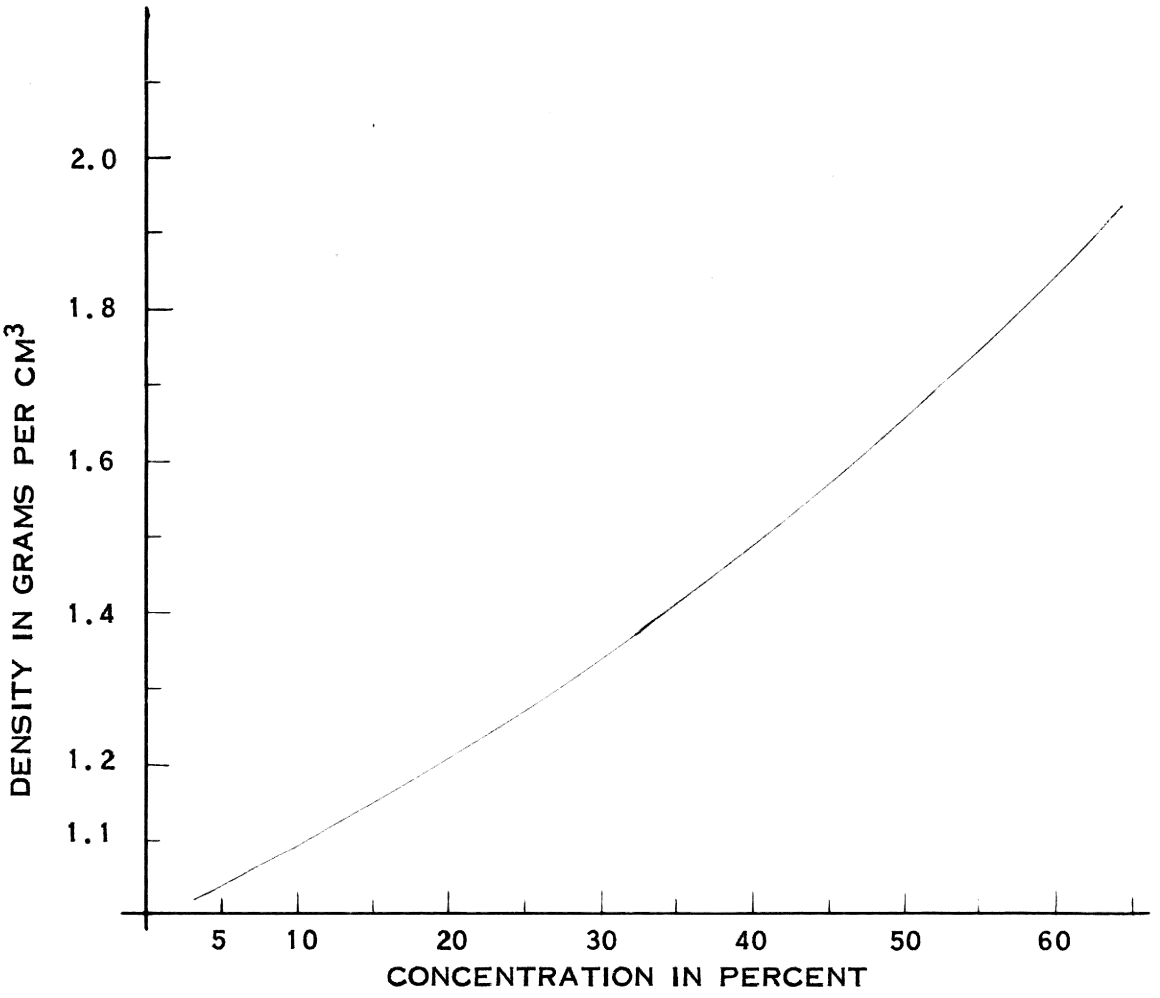


FIG. — 12

DENSITY AT 20°C OF $TH(NO_3)_4$ AQUEOUS SOLUTION AS A FUNCTION OF CONCENTRATION

CHAPTER 6.

ERROR ANALYSIS AND CONCLUSIONS

6.1 Monte Carlo Statistics

The random error or measure of statistical variation can be estimated by means of the central limit theorem which for the case of weighted events takes the form

$$P\left(\left|\frac{M}{N} - a\right| < \epsilon\right) = \operatorname{erf}\left(\frac{t}{\sqrt{2}}\right) + \rho_N \qquad (6.1)$$

where $t = \epsilon\sqrt{\frac{N}{b}}$ and $\rho_N \to 0$ as $N \to \infty$

b = the dispersion

$\frac{M}{N}$ = the ratio of the number of histories surviving to below 10 ev. to the number of histories begun

a = true value of the escape probability.

We take as an estimator of b the quantity β which is given by:

$$\beta = \sum_{i=1}^{N} \frac{(W_{1i})^2}{W_{in}} - \left(\frac{W_1}{W_{in}}\right)^2$$

$$\beta = \overline{W^2} - \overline{W}^2 \quad . \qquad (6.2)$$

The error function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-x'^2}\, dx' \qquad (6.3)$$

is well tabulated.

If we wish to specify a probability of 0.5 that the computed REP be within $\pm \epsilon$ of the correct value a we must then pick an $\epsilon > 0$ such that $\mathrm{erf}\left(\frac{t}{\sqrt{2}}\right)$ is about 0.5. We will refer to such an ϵ as the probable error. For this to be true $\frac{t}{\sqrt{2}} \simeq .5$ hence $\epsilon\sqrt{\frac{W_{in}}{2b}} = .5$

or $$\epsilon = \frac{1}{2}\sqrt{\frac{2b}{W_{in}}} \quad .$$

Now $$\overline{W} = \frac{\sum_i W_{in,i} W_{1,i}}{\sum_i W_{in,i}}$$

however a very good estimator of this number is

$$\overline{W} = \frac{W_1}{N}$$

since all $W_{in,i}$ are about equal to unity. We then have

$$\beta = \frac{\sum_{i=1}^{N} (W_{1,i})^2}{N} - \left(\frac{W_1}{N}\right)^2 . \qquad (6.4)$$

The results with ϵ displayed as the probable error are given in table 8.

TABLE. 8

RESULTS INCLUDING MONTE CARLO STATISTICAL PROBABLE ERRORS

$N_{TH} \times 10^{-21}$ ATOMS/CM^3	REP_{∞}'	PROBABLE ERROR	PERCENT ERROR
1.5381	.9458	.0026	.27
.9013	.9649	.0018	.19
.6231	.9778	.0014	.14
.3991	.9814	.0013	.13
.2439	.9893	.0010	.10

6.2 Probable Error for the Slope of Equation (5.9)

We wish to estimate the probable error of the slope of the equation

$$P = 1 - .0367n \ .$$

Assume an equation

$$P = 1 + an \ . \tag{6.5}$$

The following procedure leads to the normal equations of a least squares fit:

$$v_i = P_i - (1+an_i)$$

$$\sum_i^N v_i^2 = \sum_i^N \left[P_i - (1+an_i) \right]^2$$

$$\frac{\partial \sum_i^N v_i^2}{\partial a} = 0 = \sum_i^N 2\left[P_i - (1+an_i) \right](-n_i)$$

$$\text{or} \quad \sum_i^N \left[P_i - (1+an_i) \right] n_i = 0 \ . \tag{6.6}$$

This last set of equations is the normal equations.

$$(P_1 n_1 - n_1 - a n_1^2) + (P_2 n_2 - n_2 - a n_2^2) + \ldots = 0$$

hence $$\sum_{i=1}^{5} P_i n_i - \sum_{i=1}^{5} n_i = a \sum_{i=1}^{5} n_i^2$$

or $$a = \frac{\sum P_i n_i - \sum n_i}{\sum n_i^2} . \qquad (6.7)$$

If one considers the n_i fixed constants and the P_i variables then we can write an equation for the probable error.

$$\epsilon_a = \sqrt{\sum_{i=1}^{N} \left(\frac{\partial a}{\partial P_i} \epsilon_{P_i} \right)^2} \qquad (6.8)$$

or $$\epsilon_a = \frac{\sqrt{\sum_{i=1}^{5} (n_i \epsilon_{P_i})^2}}{\sum n_i^2} . \qquad (6.9)$$

For the Monte Carlo results we have the values listed in table 9 whence we obtain

$$\epsilon_a = \frac{\sqrt{19.7118 \times 10^{-6}}}{3.7698} = \frac{4.4398 \times 10^{-3}}{3.7698} = 1.1777 \times 10^{-3}$$

and we then have

$$a = -(.0367 \pm .0012)$$
$$= -.0367(1 \pm .033) .$$

TABLE. 9

QUANTITIES FOR SLOPE PROBABLE ERROR

N_I	N^2	$\epsilon_{PI} \times 10^3$	$N_I \epsilon_{PI} \times 10^2$	$(N \epsilon_P)^2 \times 10^{-8}$
1.5381	2.3504	2.6	4.00	1600.00
.9013	0.8123	1.8	1.62	262.44
.6231	0.3883	1.4	8.72	76.04
.3991	0.1593	1.3	5.19	26.94
.2439	0.0595	1.0	2.40	5.76

6.3 Built-In Systematic Errors

The model provides no absorption in the energy region where the cross section is fit with the exponential function

$$\sigma_{Th} = 33.78\, e^{-0.01113E} \qquad (6.10)$$

where $76 \text{ ev.} < E \leq 105 \text{ ev.}$

This is a very good approximation since the resonance absorption due to the 69.20 ev. resonance drops off much more rapidly than the resonance scattering for that peak, i.e., the interference term in σ_{Th} controls the variation in the interval in question.

The model also neglects absorption in the interval $185.5 \text{ ev.} \leq E \leq 1000 \text{ ev.}$ where an average of 13.2 barns has been used. This latter number came from Bollinger's raw data (1) parts of which are displayed graphically in figures 6, 7, and 8. The resonance structure of the region is neglected since the data is quite uncertain and the contributions from absorption are very small in general compared to the total of potential scattering, resonant scattering, and interference. The interference and potential terms are completely dominant in the wings of these relatively weak and poorly resolved resonances since $\chi(x,t)$ decreases more slowly than the function $\psi(x,t)$ which controls the resonant absorption and scattering.

6.4 Discussion of the Results

Probably the most striking feature of the Monte Carlo results is the "goodness of fit" to a straight line for resonance escape probability as a function of thorium number density. In view of the very small probable errors for each REP determination we conclude that more than a sufficient number of histories were processed to provide "good statistics".

Although we might expect no change in the probability for an absorption (given that a thorium interaction occurs) from density to density, nevertheless, the data seen in table 5 and figure 13 for P_{ab}, show considerable fluctuations on top of a general downward trend with increasing n_{Th}. We do, of course, expect the variation since the statistics (in this case the total weight absorbed) are much poorer than for the REP calculations. One would have to process about twenty times as many histories to provide similarly precise data for P_{ab},. We might explain the downward trend of P_{ab}, with increasing n_{Th} on the basis that Σ_{Th}/Σ increases. One recalls that it is this ratio which, according to the Monte Carlo prescription of section 3.1, controls the selection of thorium for a collision. For the first collision of a history, the probability of

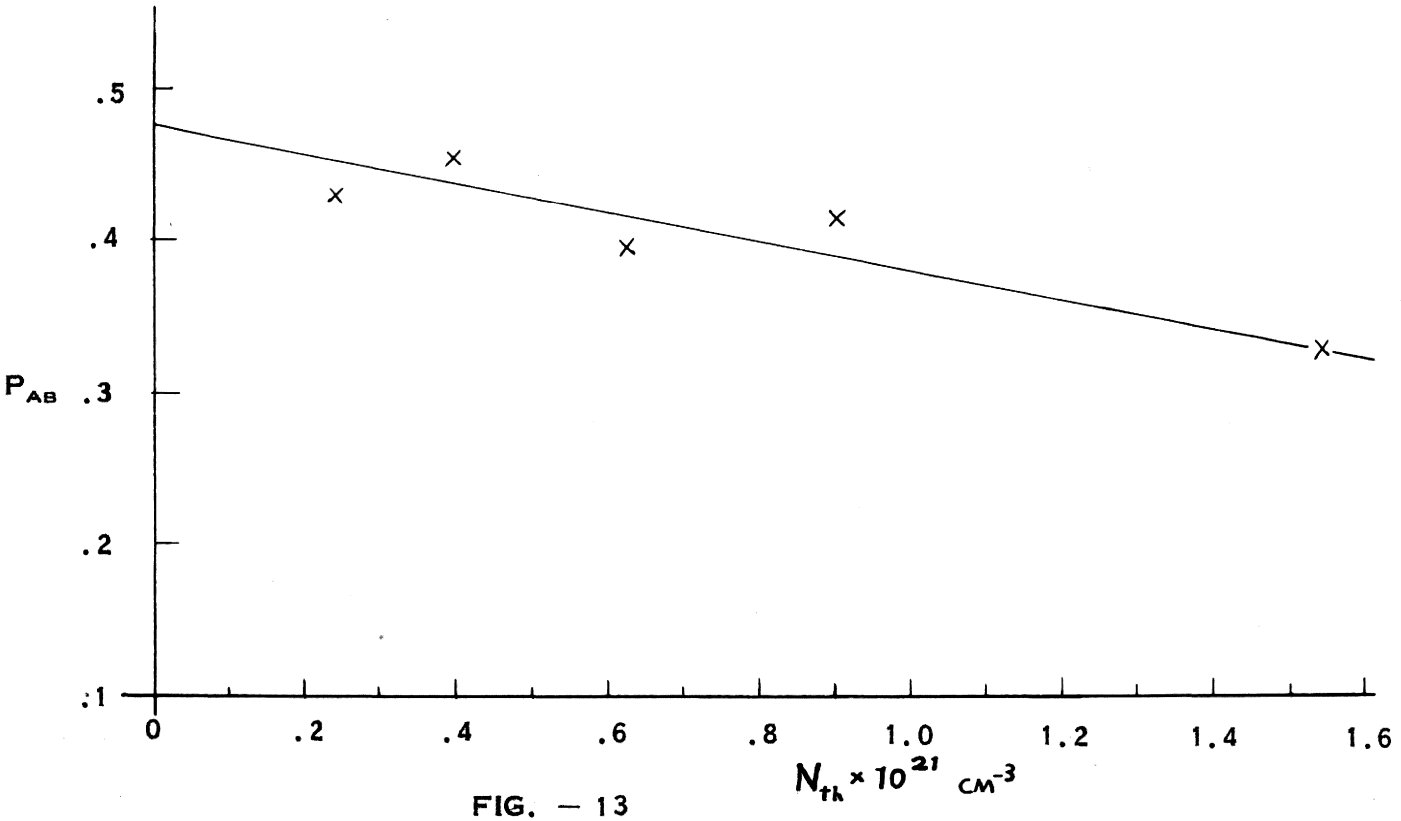


FIG. — 13

PROBABILITY FOR AN ABSORPTION GIVEN A THORIUM COLLISION

a thorium collision will be larger if Σ_{Th}/Σ is larger. Since

$$\frac{\Sigma_{Th}}{\Sigma} = \frac{1}{1+\frac{\Sigma_{NoH}}{\Sigma_{Th}}}$$

we can examine $\frac{\Sigma_{NoH}}{\Sigma_{Th}}$ for the answer. We note in table 5 that Σ_{NoH} decreases with increasing n_{Th} and that $\Sigma_{Th} = n_{Th}\sigma_{Th}$ is in general larger for larger n_{Th}. Therefore the ratio Σ_{NoH}/Σ_{Th} is smaller, making the ratio Σ_{Th}/Σ larger. This means that for a run with larger n_{Th} relatively more thorium collisions occur at higher neutron energies where the absorption cross sections are smaller. This reduces the amount of absorption per thorium collision on the average.

The percentage of leakage increases with n_{Th} indicating longer mean free paths in general. Since

$$\Sigma = \Sigma_{Th} + \Sigma_{NoH} ,$$

we conclude that the decrease in Σ_{NoH} is not compensated by the increase in Σ_{Th}. The reduction of Σ_{NoH} may appear to be at odds with the idea that a more dense solution should increase its value. However, the element of highest cross section is hydrogen and its density decreases with increasing concentration by enough to reduce the overall value of Σ_{NoH}.

6.5 Comparisons to Analytical Calculations

The analytical evaluation of REP is very difficult for the whole resonance region as one problem. Calculating a REP for even one resonance can be quite laborious. A qualitative discussion of the problem is useful.

It is important to distinguish between wide resonances and narrow resonances by stating a criterion for the classification. It may seem paradoxical but a resonance with a width large compared to another can be classified narrower by use of the criterion. For example, with a criterion that $\Gamma_i << E_1(1-\alpha)$ where E_1 is an energy above the i^{th} resonance, there will be fewer neutron reactions in the resonance, i.e., the width is narrow compared to the energy change that can accompany a scattering. The figure 14 indicates the concept. $\Delta E_{max} = E_1(1-\alpha)$ and the smaller is $\Gamma/\Delta E_{max}$, the narrower is the peak.

If E_o is large then $E_1 \simeq E_o$ and $\Delta E_{max} \simeq E_o(1-\alpha)$. For a specific example let us try to decide which is the wider of two thorium resonances. We shall pick the E_o = 21.84 ev. and the E_o = 170.80 ev. resonances from table 2 where they are labeled peak 1 and peak 8.

$$\Gamma_1 = \frac{2.00}{55.55} \text{ ev.} = .036 \text{ ev.}, \quad \Gamma_8 = \frac{2.00}{18.87} \text{ ev.} = .106$$

$$= 36 \text{ mv} \qquad\qquad = 106 \text{ mv}.$$

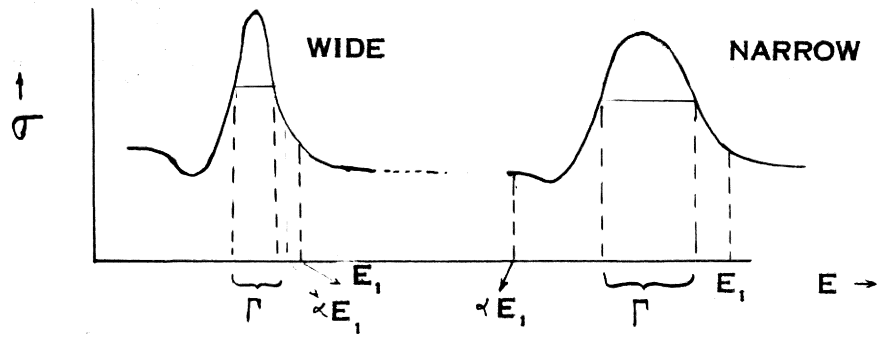


FIG. — 14. PICTORIAL CONCEPT OF NARROW RESONANCE

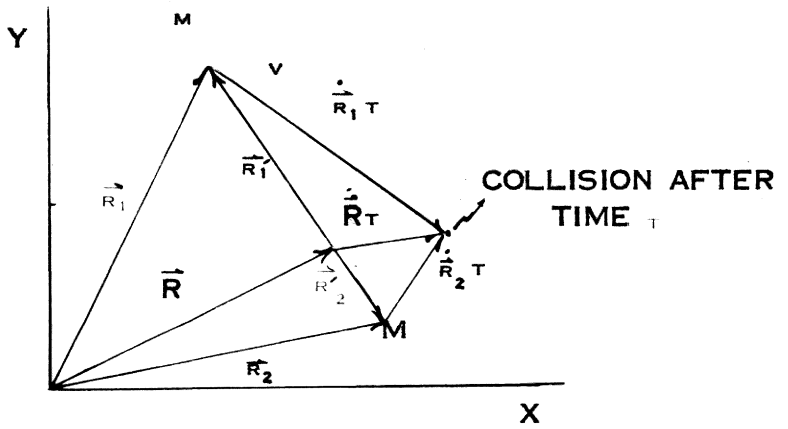


FIG. — 15. POSITION VECTORS

From the point of view of resonance widths peak 8 is wider than peak 1. Continuing, we have

$$\alpha = \left(\frac{A-1}{A+1}\right)^2 = \left(\frac{231}{233}\right)^2 = .983$$

and $$(\Delta E_1)_{max} = (1-.983)21.84 \text{ ev.} = .37 \text{ ev.},$$

$$(\Delta E_2)_{max} = (1-.983)(170.8 \text{ ev.}) = 2.9 \text{ ev.}$$

Since .036 ev. << .37 ev. and since .106 << 2.9 ev. we conclude by our criteria that both resonances are narrow as is the case for all of the thorium resonances included in table 2. However

$$\frac{\Gamma}{\Delta E_{max}} = \frac{36}{370} = .0973 \quad \text{and} \quad \frac{106.0}{2900} = .0366$$

which means that peak 8 satisfies narrowness more strongly than peak 1 yet $\Gamma_8 > \Gamma_1$. This, of course, occurs because E_o for peak 8 is so much larger than E_o for peak 1. If a neutron appears with energy $E_1 > E_o$ and scatters from thorium it has a greater chance of reducing its energy to below E_o for peak 8 than for peak 1 and therefore less chance for suffering a second or third collision in thorium assuming that scattering occurs rather than capture in each case.

The low lying 6.7 ev. peak of U^{238} has $\Gamma = 26.5$ mv. and $\alpha = .9833$.

$$E_1 \simeq E_o = 6.7 \text{ ev. then } (\Delta E)_{max} = (.0167)6.7$$

$$= .1119$$

and

$$\frac{\Gamma}{\Delta E_{max}} = .207.$$

This peak is much wider than either of the thorium peaks. In all three cases the addition of the Doppler-broadening will weaken the narrowness criterion; this brings the lowest lying peaks out of the narrow classification.

Analytic evaluation of the resonance integral is more easily obtained for the narrower resonances of the higher energy region, and thorium should prove easier than uranium in this respect. See reference (19) for additional details.

Presumably we can arrive at an estimate of REP_∞' by calculating the value of the resonance integral for each of the eight peaks and adding them to get an effective resonance integral I. Then

$$REP_\infty' = \exp\left\{ - \frac{I n_{Th}}{\xi \Sigma_p} \right\} .$$

The calculations leading to the values in table 10 are based on the curves of figure 3-3 of reference (5) and equation (31-3) of the same reference.

$$I = \sigma_p \frac{\Gamma_\gamma}{E_o} \int_o^\infty \frac{\psi(x,\theta)}{\psi(x,\theta)+\beta} dx \quad . \tag{6.11}$$

We will now present a calculation for the REP' based on the analytical expressions valid for the narrow resonance approximation in homogeneous mixtures. The following equations will be employed where REP' is replaced by P:

$$P = e^{-\left\{\sum_{i=1}^{8} I_i \frac{n_{Th}}{\bar{f}\,\Sigma_p}\right\}} \tag{6.12}$$

$$I_i = \frac{\sigma_p \Gamma_\gamma}{E_o} J_i(\theta,\beta) \tag{6.13}$$

$$J_i(\theta,\beta) = \int_o^\infty \frac{\psi(x,\theta_i)}{\psi(x,\theta_i)+\beta_i} dx \tag{6.14}$$

$$\bar{f} = \sum_{i=1}^{4} f_i c_i \quad , \quad c_i = \frac{\Sigma_{si}}{\sum_{i=1}^{4} \Sigma_{si}} \tag{6.15} \tag{6.16}$$

$$\sigma_p = \frac{\Sigma_p}{n_{Th}} \tag{6.17}$$

TABLE. 10

SAMPLE DATA AND RESULTS FOR AN ANALYTICAL CALCULATION WITH $N_{TH} = .9013 \times 10^{21}$ ATOMS CM^3

PEAK NUMBER	E_0 IN E.V.	Γ_r IN M V	$\theta = \frac{1}{\sqrt{t}}$	$\frac{\sigma_p \Gamma_r}{E_0}$ IN BARNS	$\beta = \frac{\sigma_p}{\sigma_0}$	$j(\beta)$	$J(\theta,\beta)$ CM^{-1}	$I_i(\theta,\beta)$ IN BARNS	$\sigma_0 = \frac{\Gamma_r}{\Gamma} \sigma_{or}$ BARNS
1	21.84	34	.3691	2.344	.2058	14.33	4.9	11.49	7316
2	23.48	39	.4252	2.501	.1366	13.74	5.1	12.76	11026
3	59.55	21	.1615	.531	.1950	14.25	6.0	3.19	7720
4	69.20	43	.4725	.934	.0842	16.36	7.0	6.54	17887
5	113.15	42	.2388	.559	.3157	14.95	3.5	1.96	4770
6	121.00	41	.2614	.510	.2250	14.46	4.6	2.35	6690
7	129.40	41	.1854	.471	1.0649	16.70	1.3	.61	1414
8	170.80	48	.3887	.423	.1808	14.14	4.9	2.07	8325

FOR THIS TABLE $\sigma_p = 1505$ BNS, $J = .875$, $\Sigma_p = 1.3572\,cm^{-1}$ AND $REP_0^1 = .9689$.

$$\Sigma_p = n_{Th}\sigma_{pa} + \Sigma_{NoH} \qquad (6.18)$$

$$\beta = \frac{\sigma_p}{\sigma_o} \qquad (6.19)$$

$$\sigma_o = \frac{4\pi}{k^2}\frac{\Gamma_n}{\Gamma} = \frac{2.6\times10^6}{E_o}\frac{\Gamma_n}{\Gamma} = \frac{\Gamma}{\Gamma_n}\sigma_{os} \qquad (6.20)$$

$$\xi_i = 1 + \frac{\alpha_i \ln\alpha_i}{1-\alpha_i} \quad \text{(See pp. 81-83 of reference 12)} \qquad (6.2.)$$

$$\xi_i \simeq \frac{2}{A_i + 2/3} \quad \text{for } A_i > 10 \qquad (6.22)$$

where σ_{pa} is the potential scattering cross section of the absorber which is thorium. These equations and the necessary data are found in reference (5). Reference is also made to tables 1 and 2 for the necessary peak parameters. Assuming $n_{Th} = .6231 \times 10^{21}$ atoms/cm^3 we have

$$\Sigma_{NoH} = 1.41 \text{ cm}^{-1}$$

$$\Sigma_p = n_{Th}\sigma_{pa} + \Sigma_{NoH}$$

$$= (.6231\times10^{21})10.5\times10^{-24}\text{cm}^{-1} + 1.4114 \text{ cm}^{-1}$$

$$= 1.418 \text{ cm}^{-1}.$$

$$\bar{\xi} = \frac{\xi_{Th}\Sigma_{Th} + \xi_o\Sigma_o + \xi_N\Sigma_N + \quad H \quad H}{1.418}$$

$$\xi_{Th} \simeq \frac{2}{232.67} = .0086$$

$$\xi_o \simeq \frac{2}{16.67} = .1200$$

$$\xi_N \simeq \frac{2}{14.67} = .1363$$

$$\xi_H = 1$$

$$\Sigma_o = (38.91\text{x}10^{21})(3.8\text{x}10^{-24}) = .14786 \text{ cm}^{-1}$$

$$\Sigma_N = 2.492(9.1)\text{x}10^{-3} = .02268 \text{ cm}^{-1}$$

$$\Sigma_H = (61.43)(20.2)\text{x}10^{-3} = 1.24089 \text{ cm}^{-1}$$

$$\bar{\xi} = \frac{(.0086)(.0665)+(.12)(.148)+(.136)(.0227)+(1.241)}{1.418} =$$

.890

$$\sigma_p = 10.5 \text{ bns} + \frac{1.411}{.6231} \text{ x } 10^3 \text{ bns} = 2270.3 \text{ bns}$$

$$\beta = \frac{\sigma_p}{\sigma_o} .$$

To proceed with the calculation we refer to figure 3-3 and table 3-3 of reference 5[1], where $J(\theta,\beta)$ is given as a function of j.

$$\beta = 2^j \times 10^5 \quad \text{so that}$$

$$j = \frac{5 + \log \beta}{\log 2} \ .$$

Table 10 gives the data and resonance integral values from each peak for $n_{Th} = .9013 \times 10^{21}$ atom/cm^3. Proceeding for $n_{Th} = .6231 \times 10^{21}$ atoms/cm^3 we obtain

$$\sum_{i=1}^{8} I_i = 35.34 \text{ bns.}$$

The separate I_i's are obtained from equation (6.13). Finally, applying equation (6.12) we obtain P = .9827 which is 0.5% higher than the value calculated by the Monte Carlo.

It should be noted in table 10 that over one half of the total absorption contribution comes from the first

---

(1) The same figure and table appear in volume 1 of Nuclear Science and Engineering p. 74 and 76 (1956) where the figure is larger.

two peaks. Peak 4 is the largest in magnitude including the Doppler peak reduction and yet does not contribute as much as either 1 or 2. This means that peak 4 is narrower than peaks 1 and 2 by our criteria. Similarly for peak 6. It is interesting to note that the first peak of uranium (6.7 ev.) contributes over 78% of the absorption. This means that it must not only be large in magnitude but very wide by our criteria.

Table 11 gives the comparison between Monte Carlo and analytical calculations.

We now refer to figure 3 on page 78 of the reference listed in footnote (1) where the effective integral for Th^{232} is given as a function of σ_p. In the range of σ_p from 400 bns. to 2000 bns. there are two measurements that fall somewhat below the theoretical resonance integral values for 300 ^{o}K. The first two entries of table 12 have σ_p in the same range and the corresponding effective resonance integral falls below the experimental points. Several explanations of these differences are as follows:

1. Table 12 lists I_{eff} calculated by Dresner's method but using only the lowest eight resonances while Dresner used fifteen taken from Hughes and Harvey (8).

2. Several parameters (particularly σ_o) that Dresner used are in doubt. The σ_o reported in reference (5) is too large in several cases.

TABLE. 11

COMPARISON OF MONTE CARLO AND ANALYTICAL VALUES FOR REP_∞^1

N_{TH} $\times 10^{21}$ CM^{-3}	REP BY MONTE CARLO	$\frac{N_{TH}}{\bar{\xi}\Sigma_\rho}\left(\sum_{i=1}^{8} I_i\right)$	NR $e^{-\frac{N_{TH}}{\bar{\xi}\Sigma_\rho}\left(\sum_i I\right)}$	$\bar{\xi}$	Σ_ρ	% DIFFERENCE COLUMNS 2 AND 4	NR $1-\frac{N_{TH}}{\bar{\xi}\Sigma_\rho}\left(\sum_{i=1}^{8} I_i\right)$	% DIFFERENCE COLUMNS 2 AND 8	σ_ρ
.2439	.9893	.01345	.9865	.912	1.459	.28	.9865	.28	5981.4
.3991	.9814	.01805	.9838	.904	1.447	.24	.9837	.23	3625.9
.6231	.9778	.02471	.9827	.890	1.418	0.50	.9826	.49	2270.3
.9013	.9649	.03349	.9694	.875	1.357	0.46	.9689	.41	1505.9
1.5381	.9458	.05143	.9569	.825	1.161	1.16	.9560	1.07	754.9

TABLE. 12.

EFFECTIVE RESONANCE INTEGRALS

$N_{TH} \times 10^{21}$ ATOMS/CM^3	σ_p IN BARNS	I_{EFF} IN BARNS
1.5891	754.9	27.41
.9013	1505.9	40.95
.6231	2270.3	35.34
.3991	3625.9	53.56
.2439	5981.4	73.37

3. Dresner's calculations indicate that the unresolved resonances may contribute as much as 30% of the total value of the effective resonance integral. If 30% is added to the high concentration value in table 12, I_{eff} falls in line with the measured value. For higher concentrations, larger percentages due to the unresolved resonances are expected because of self shielding of the resolved resonances.

It appears that Dresner's theoretical calculations are too high because the data he uses (8) give values of σ_o and Γ_n that are too large. The data used in this paper comes from Bollinger and Cote' (1) and Rosen (18). It is believed that these sources of the resonance parameters for thorium are more reliable with the latter being the most recent.

6.6 Conclusions

The Monte Carlo calculation gives the following contributions to the resonance escape problem:

1. It indicates the geometric effect on the resonance escape probability allowing calculations for finite and rather small reactors.

2. It gives the relative contributions of thorium absorption and geometric leakage as a function of concentration.

3. It provides an analog calculation of the thorium resonance escape probability independent of the theoretical assumptions leading to equation (6.12).

4. If this Monte Carlo program were translated from IBM-650 language to the IBM-704 language the whole problem could be run in less than two hours. On the IBM-650 it takes about 65 hours.

CHAPTER 7.

SUGGESTED EXTENSIONS

A series of radial (off the beam axis) distributions for sixteen values of z (the coordinate along the beam axis) have been determined by least squares fitting with a function of the form

$$f(r,z) = a(z)r^{b(z)}e^{-c(z)r} \qquad (7.1)$$

to the position distributions obtained from the water moderated Monte Carlo which was used as the source for the REP Monte Carlo (21). These distributions coupled with the uniformly distributed "first arrival" energies and the assumption of an isotropically directed set of "first arrival" initial velocity vectors may well provide a sufficient basis for Monte Carlo sampling to initiate a history. This would replace the card-read source routine used in this paper. It may well happen that the programming of this new source routine may overtax the storage of a "bare" IBM-650 in which case a larger computer would be necessary. Since "reading" is very slow, we might anticipate an overall speed up of the computations allowing more statistics in a shorter running time. This would

help remove the large statistical fluctuations implied in the results for such quantities as P_{ab}'.

It should prove interesting to modify the program to provide a check for Safanov's water-uranium curve (19).

A larger computer would provide more storage to allow more definitive tabular histograms with which to approximate the resonance cross sections.

When data with better resolution becomes available the higher energy resonances could be included with more precision. All that need be done to the program is to increase the number of energy gaps tested and expand the number of ψ and χ tables correspondingly. The basic structure of the program would thus be unaltered. This refinement will not likely improve the results significantly.

With a faster computer one could examine the effects of temperature variation on the REP. This can be done by using different Doppler widths which provide the source of temperature dependence of REP.

ACKNOWLEDGMENTS

I wish to thank Dr. Wilbur Payne for the initial ideas to this research and for his consultation during its progress.

My thanks go also to Dr. D. Willard who ably advised me during the major portion of the project.

I am indebted to Mr. for providing valuable data by altering his Monte Carlo program for water moderation.

Dr. R. E. Bargmann gave valuable help with programming and statistical analysis.

Others who have contributed time and energy are Mrs. with the IBM equipment, Mr. for tabulating services, Mr. for the lettering of tables and figures and Mrs. for her masterful typing of the manuscript.

A special note of thanks goes to my wife, , who has known not a few sacrifices throughout the pursuit of this goal.

The research presented in this paper was sponsored by the United States Atomic Energy Commission.

BIBLIOGRAPHY

Literature Cited

1. Bollinger, L. M. and Cote'c R. E., "Thorium Resonance Data", Argonne National Laboratory, 1956, Private Communication.
2. Cashwell, E. D. and Everett, C. J., "A Practical Manual on the Monte Carlo Method for Random Walk Processes", Pergamon Press, pp. 4-10, (1959).
3. ibid, pp. 27-29.
4. ibid, pp. 128-133.
5. Dresner, L., Resonance Absorption in Nuclear Reactors, Pergamon Press, pp. 6-37, (1960).
6. ibid, pp. 115-123.
7. Glasstone, S., and Edlund, M., The Elements of Nuclear Reactor Theory, pp. 136-168, Van Nostrand (1952).
8. Hughes, D. J. and Harvey, J. A., BNL-325 Second Edition (1958).
9. Kahn, Herman, "Application of Monte Carlo", Rand Corporation, AECU-3259, pp. 3-19, 83-88 (1954).
10. Kahn, Herman, "Random Sampling Techniques in Neutron Attenuation Problems - I", Nucleonics, Volume 6, pp. 27-33, (1950).

11. Hughes, D. J., and Eggler, C., Resonance Absorption of Thorium, CP 3093, July (1945).

12. Meghreblian, R. V., and Holmes, D. K., Reactor Analysis, McGraw-Hill, (1960).

13. Morton, K. W., "A Calculation of Resonance Escape Probability by Monte Carlo Methods", Second International Conference on the Peaceful Uses of Atomic Energy, A/CONF.15/P/19 United Kingdom, 21 May 1958.

14. Neumann, H., "Resonance Escape Probability in Reactor Lattices", Proceedings of the Brookhaven Conference on Resonance Absorption of Neutrons in Nuclear Reactors, pp. 110-115 (1956).

15. Richtmyer, R. D., "Resonance Capture Calculations for Lattices by the Monte Carlo Method", Proceedings of the Brookhaven Conference on Resonance Absorption of Neutrons in Nuclear Reactors, pp. 82-89 (1956).

16. Richtmyer, R. D., Van Norton, R., Wolfe A., "The Monte Carlo Calculation of Resonance Capture in Reactor Lattices", Second United Nations International Conference on the Peaceful Uses of Atomic Energy, A/CONF.15/P/2489, USA, 8 August 1958.

17. Rose, M. E., et. al., "A Table of the Integral $\psi(x,t)$", AEC WAPD-SR-506, Vol. II, Oct. (1954).

18. Rosen, J., Thorium Level Parameters, Columbia Nevis Cyclotron Laboratory, Private Communication, Sept. (1960).

19. Safanov, G., "Resonance Escape Probability in Natural Uranium and Light and Heavy Water Mixtures", Rand Corporation, Proceedings of the Brookhaven Conference on Resonance Absorption of Neutrons in Nuclear Reactors, pp. 79-81 (1956).

20. Sampson, J. B., and Chernick, J., Resonance Escape Probability in Thermal Reactors, Progress in Nuclear Energy, Series I, Physics and Mathematics Volume II, Pergamon Press, pp. 223-270 (1958).

21. Settles, R., M. S. Thesis, Virginia Polytechnic Institute, (1961).

22. Spinney, K. T., "Resonance Absorption in Homogeneous Mixtures", Proceedings of the Brookhaven Conference on Resonance Absorption of Neutrons in Nuclear Reactors, BNL 433 (C-24) (1956).

Literature Examined

1. Egelstaff, P. A. and Hughes, D. J. "Resonance Structure of U^{233}, U^{235} and $P_u{}^{239}$", Progress in Nuclear Energy, Series I, Physics and Mathematics, Volume 1, McGraw-Hill, pp. 55-68 (1956).
2. Goertzel, G. and Kalos, M. H., "Monte Carlo Methods in Transport Problems", Progress in Nuclear Energy, Series I, Physics and Mathematics, Volume II, McGraw-Hill, pp. 315-369 (1958).
3. Dresner, L., "The Effective Resonance Integrals of U-238 and Th-232", Nuclear Science and Engineering, Volume 1 (1956).
4. Meyer, H. A., Symposium on Monte Carlo Methods, pp. 146-190, an article by Kahn, H., pp. 249-264, an article by Butler, J. W., John Wiley and Sons (1954).
5. Harvey, J. A. and Schwartz, R. B., "Thermal and Resonance Nutron Cross Sections of Heavy Nuclei", Progress in Nuclear Energy, Series I, Physics and Mathematics, Volume II, pp. 51-90 (1958).
6. Spanier, J., "Monte Carlo Methods and Their Application to Neutron Transport Problems", Bettis Atomic Power Laboratory, Pittsburgh, Pa., WAPD 195: A wealth of material with mathematical rigor (1959).

7. Spanier, J., Kuehn, H., Guilinger, W., "Tut-15 - A Two Dimensional Monte Carlo Calculation of Capture Probabilities for the IBM-704", Bettis Atomic Power Laboratory, Pittsburgh, Pa., WAPD-TM-125, Nov. (1959).

The vita has been removed from the scanned document

APPENDIX I

The Fundamental Theorem of Monte Carlo

The primary question to be answered in a Monte Carlo problem is how to select the value of a variable from many possible values where the possibilities are described by a frequency function or probability density function. The answer to that question is provided by the following theorem.

Theorem: Given a random number N_r uniformly distributed on the interval $(0,1)$ and a real, positive, single valued, continuous function $f(x)$ defined on the interval $-\infty$ to ∞ such that

$$\int_{-\infty}^{\infty} f(x)dx = 1 .$$

Then for $N_r = \int_{0}^{X} f(x)dx$ we have that X is a random variable with frequency function $f(x)$.

Proof: The indefinite integral

$$F(x) = \int_{-\infty}^{x} f(x')dx' \quad \text{exists} \qquad (1)$$

because of the given conditions on $f(x)$.

$$\lim_{x\to\infty} F(x) = \int_{-\infty}^{\infty} f(x')dx' = 1$$

$$\lim_{x\to-\infty} F(x) = \int_{-\infty}^{-\infty} f(x')dx' = 0 \quad .$$

$F(x_1) < F(x_2)$ for $x_1 < x_2$ since $f(x) > 0$ for all x. We then recognize F(x) as a monitonically increasing function so

$$F_{max} = F(\infty) = 1$$

and

$$F_{min} = F(-\infty) = 0$$

$$0 < F(x) \leq 1 .$$

From equation (1) and the fundamental theorem of integral calculus

$$\frac{dF}{dx} = f(x), \quad \text{or} \quad dF = f(x)dx . \qquad (2)$$

This is of the form $g(F)dF = f(x)dx$ where $g(F) = 1$. We thus say that f(x) in (x,f) space maps into g(F) in (F,g) space. Since $g(F) = 1$, F is uniformly distributed in (F,g) space on (0,1). F then satisfies the conditions for being N_r and we can write $F(x) = N_r$ or $x = F^{-1}(N_r)$. Since a function of a random variable is also a random variable we conclude that x is a random variable and by (2) its frequency function is f(x).

F(x) is called the distribution function of x and gives the probability that $x' < x$, i.e.,

$$F(x) = P(x' < x) = \int_{-\infty}^{x} f(x')dx' .$$

APPENDIX II

1. Cross Section Formulas*

In the present paper the neutron energies for all collisions is so low that only interactions for $l = 0$ occur.

The cross sections for absorption and scattering in terms of l are given by

$$\sigma_{ab,l} = \frac{\pi}{k^2} \sum_l (2l+1)(1 - |\eta_l|^2) \qquad (1)$$

$$\sigma_{sc,l} = \frac{\pi}{k^2} \sum_l (2l+1) |1 - \eta_l|^2 \qquad (2)$$

where k = the neutron wave number in the center of mass

$$= \sqrt{\frac{2\mu E}{\hbar^2}}$$

and l = the orbital angular momentum quantum number.

η_l is a factor giving the phase shift and amplitude change in the scattered partial wave.

For $l = 0$ the equations (1) and (2) become

---

* The equations (1) to (12) are derived in the book, "Theoretical Nuclear Physics" by Blatt and Weisskopf.

$$\sigma_{ab,o} = \frac{\pi}{k^2}(1-|\eta_o|)^2 \tag{3}$$

$$\sigma_{sc,o} = \frac{\pi}{k^2}|1-\eta_o|^2 \quad . \tag{4}$$

Introduction of the quantity

$$f_o = R\left(\frac{dU_o}{dr}\ \frac{1}{U_o}\right)_{r=R} \tag{5}$$

where U_o is the radial wave function for $l = 0$ and R is the nuclear radius gives

$$\sigma_{ab,o} = \frac{\pi}{k^2}\frac{-4(\mathrm{Im}f_o)kR}{(\mathrm{Re}f_o)^2+(\mathrm{Im}f_o-kR)^2} \tag{6}$$

$$\sigma_{sc,o} = \frac{\pi}{k^2}\left|A_{pot} + A_{res}\right|^2 \tag{7}$$

where $A_{pot} = e^{i2kR}-1$ (8)

$$A_{res} = \frac{-2ikR}{f_o-ikR} \quad . \tag{9}$$

With the introduction of resonance level widths Γ_n, Γ_γ and Γ

where Γ_n = neutron level width

Γ_γ = radiative capture level width

$$\Gamma = \Gamma_n + \Gamma_\gamma \tag{10}$$

we obtain with suitable approximations and algebraic manipulations

$$\sigma_{ab,o} = \frac{\pi}{k^2} \frac{\Gamma_\gamma \Gamma_n}{(E - E_o)^2 + \frac{\Gamma^2}{4}} \tag{11}$$

$$\sigma_{sc,o} = \frac{\pi}{k^2} \frac{\Gamma_n^2}{(E-E_o)^2+\frac{\Gamma^2}{4}} + \frac{4\pi R}{k} \frac{n(E-E_o)}{(E-E_o)^2+\frac{\Gamma^2}{4}} + 4\pi R^2 \,. \tag{12}$$

E and E_o are the center of mass neutron energies "off resonance" and "on resonance" respectively. Equations (11) and (12) are the single level Breit-Wigner formulas for an l=0, I=0 interaction. The nuclear spin I is zero for thorium.

2. The Doppler Broadening Effect

We wish to include in our description of the resonance cross sections the effect of the motion of the target nuclei. To do this we use a relative energy formulation.

Define $E_{relative} \equiv E_{center\ of\ mass} \equiv E'$

then $E' = \frac{1}{2}\mu\dot{\bar{r}}^2$ where $\mu = \frac{mM}{m+M}$

m = neutron mass

M = target nucleus mass

$\dot{\bar{r}}$ = relative velocity

$\bar{r} = \bar{r}_1 - \bar{r}_2$ (see figure 15)

$E' = \frac{1}{2}\mu\dot{\bar{r}}^2$

$= \frac{1}{2}\mu(\dot{\bar{r}}_1 - \dot{\bar{r}}_2)^2$.

Let $\dot{\bar{r}}_1 = \hat{v}v$ then we have

$$E' = \tfrac{1}{2}\mu(v^2 - 2\hat{v}\cdot v\dot{\bar{r}}_2 + \dot{\bar{r}}_2^{\,2}) = \mu v^2\left(\tfrac{1}{2} - \frac{\hat{v}\cdot\dot{\bar{r}}_2}{v} + \tfrac{1}{2}\frac{\dot{\bar{r}}_2^{\,2}}{v^2}\right)$$

now for $v \gg |\dot{\bar{r}}_2|$

$$E' \simeq \mu v^2\left(\tfrac{1}{2} - \hat{v}\cdot\frac{\dot{\bar{r}}_2}{v}\right) \qquad \text{but } \hat{v}\cdot\dot{\bar{r}}_2 = U_x$$

where U_x is the component of the target atom velocity in the $\hat{v}$ direction. This becomes

$$E' \simeq \tfrac{1}{2}\mu v^2\left(1 - \frac{2U_x}{v}\right) . \qquad (1)$$

We define $E'_0 \equiv \frac{1}{2}\mu v^2$ called the relative energy of m and M for M at rest.

Then $v = \sqrt{\frac{2E'_o}{\mu}}$ and $\mu v = \sqrt{2\mu E'_o}$

so that equation (1) becomes

$$E' \simeq E'_o - \sqrt{2\mu E'_o}\ U_x \qquad (2)$$

and $$dE' = -\sqrt{2\mu E'_o}\ dU_x . \qquad (3)$$

If we assume the speeds of the target atoms to have a Maxwellian distribution and that the system contains isotropic motion (no direction preferred) only, we can write the one dimensional distribution for U_x by the expression

$$f(U_x)dU_x = \sqrt{\frac{M}{2\pi kT}}\ e^{-\frac{M}{2kT}U_x^2}\ dU_x \qquad (4)$$

but $f(U_x)dU_x = f(E')dE'$.

Therefore substituting equations (2) and (3) into equation (4) we have

$$f(E')dE' = \sqrt{\frac{M}{4\pi\mu\tau E'_o}}\ e^{-\frac{M}{4\mu\tau E'_o}(E'_o-E')^2}\ dE' \qquad (5)$$

where $\tau = kT$.

We now wish to use this distribution to calculate an effective cross section. The function f(E') is actually a probability density function since it has been normalized $(\int_0^\infty f(E')dE' = 1)$

therefore $$\sigma_{(E_o',T)} = \int_0^\infty \sigma_{(E')} f(E')dE' \ . \qquad (6)$$

$\sigma_{Total,l} = \sigma_{ab,l} + \sigma_{sc,l}$ and for $l = 0$

which is our case, since the neutron energies are too small to have larger angular momenta, we would have

$$\sigma_{T,o} = \sigma_{ab,o} + \sigma_{sc,o} \ .$$

For future ease of writing we will drop the zero getting the form

$$\sigma_T = \sigma_{ab} + \sigma_{sc} \qquad (7)$$

which is more explicitly given by the Breit-Wigner equation as

$$\sigma_T = g(s)\frac{\pi}{k^2}\frac{\Gamma_n \Gamma_\sigma}{(E-E_o)^2+\frac{\Gamma^2}{4}} + g(s)\frac{\pi}{k^2}\left|\frac{i\Gamma_n}{(E-E_o)+i\frac{\Gamma}{2}} + e^{2ikR} - 1\right|^2$$

$$+ (1-g(s))\, 4\pi R^2 \qquad (8)$$

where $g(s) = \frac{2s+1}{2(2I+1)}$, $\quad s = I+\frac{1}{2},\ I-\frac{1}{2}$ (9)

but for thorium (I=0) $g(s) = \frac{2}{2} = 1$

so equation (8) becomes

$$\sigma_T = \frac{\pi}{k^2} \frac{\Gamma_n \Gamma_\gamma}{(E-E_o)^2+\frac{\Gamma^2}{4}} + \frac{\pi}{k^2} \left| \frac{i\Gamma_n}{(E-E_o)+i\frac{\Gamma}{2}} + e^{2ikR}-1 \right|^2 . \quad (10)$$

Expanding the second term gives

$$\sigma_T = \frac{\pi}{k^2} \frac{\Gamma_n \Gamma_\gamma}{(E-E_o)^2+\frac{\Gamma^2}{4}} + \frac{\pi}{k^2} \frac{\Gamma_n^2}{(E-E_o^2)+\frac{\Gamma^2}{4}} + \frac{4\pi R}{k} \frac{\Gamma_n(E-E_o)}{(E-E_o)^2+\frac{\Gamma^2}{4}}$$

$$+ 4\pi R^2 \quad (11)$$

where the first term is σ_{ab} and the sum of the rest is σ_{sc}.

Let $\sigma_{ab,max.} = \sigma_{or}$, $\sigma_{sc,max} - 4\pi R^2 = \sigma_{os}$ (12) (13)

and $\sigma_{pot} = 4\pi R^2$. (14)

Since the neutron width is proportional to E' with the reduced width being the proportionality constant we have

$$\frac{\Gamma_n}{{}_o\Gamma_n} = \frac{\sqrt{E'}\Gamma_n^o}{\sqrt{E_o}\Gamma_n} \quad (15)$$

where Γ_n^o = reduced width

$${}_o\Gamma_n = \Gamma_n \text{ at resonance.}$$

Then $\sigma_{or} = \frac{4\pi}{k_o^2}\frac{{}_o\Gamma_n\Gamma_\gamma}{\Gamma^2}$ and $\sigma_{os} = \frac{4\pi}{k_o^2}\left(\frac{{}_o\Gamma_n}{\Gamma}\right)^2$. (16) (17)

We can now rewrite equation (6).

$$\sigma_{(E_o',t)} = \int_o^\infty \sigma_T(E')f(E')dE' = \int_o^\infty \sigma_{ab}(E')f(E')dE' + \int_o^\infty \sigma_{sc}(E')f(E')dE'. \quad (18)$$

We proceed to reduce the first term by use of equations (11) to (17).

$$\sigma_{ab}(E_o',T) = \frac{\sigma_{or}}{\sqrt{\pi}}\int_o^\infty \frac{k_o^2}{k^2}\sqrt{\frac{E'}{E_o}}\frac{e^{-(E_o'-E'^2)/4\frac{\mu}{M}\gamma E_o'}}{2\sqrt{\frac{\mu}{M}\gamma E_o'}\left(\frac{(E'-E_o)^2}{\Gamma^2/4}+1\right)}\,dE'. \quad (19)$$

We can use the expressions in energy for the k's as follows

$$\frac{k_o^2}{k^2} = \frac{2E_o\mu/\hbar^2}{2E'\mu/\hbar^2} = \frac{E_o}{E'}.$$

It is convenient here to introduce the following definitions

$$x = \frac{E'-E_o}{\Gamma/2}\,, \quad y = \frac{E'-E_o}{\Gamma/2}\,, \quad \Delta = 2\sqrt{\frac{m}{M}\,\gamma\,E'_o} \qquad (20)\ (21)\ (22)$$

where E_o is the energy at resonance

$$\theta \equiv \Gamma/\Delta \quad \text{and} \quad dy = \frac{2}{\Gamma}\,dE'\,. \qquad (23)\ (24)$$

In equation (19) $2\sqrt{\frac{m}{M}\,\gamma\,E'_o} \simeq 2\sqrt{\frac{m}{M}\,\gamma\,E_o}$

for $|E'_o-E_o| << E_o$ and so equation (19) becomes

$$\sigma_{ab}(E'_o,T) \simeq \frac{\sigma_{or}}{\sqrt{\pi}} \int_{-E_o/\frac{\Gamma}{2}}^{\infty} \sqrt{\frac{E_o}{E'}}\; \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{(y^2+1)}\,\Gamma/2\,dy$$

$$\sigma_{ab}(E'_o,T) = \sigma_{or}\,\frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \sqrt{\frac{E_o}{E'}}\; \frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2}\,dy, \quad E_o >> \Gamma. \qquad (25)$$

For $|y| >> |x|$ the integrand is very small and if one stays away from the pole at E'=0 the only contributions that are significant come for $E' \simeq E'_o$. Another way of saying this is that the function $\sqrt{E_o/E'}$ is very slowly

varying compared to $\frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2}$ which drives the integrand to zero long before a noticeable change in $\sqrt{E_o/E'}$ can occur. This allows us to write

$$\sigma_{ab}(E',T) = \sqrt{\frac{E_o}{E'_o}}\,\sigma_{or}\psi(x,\theta) \tag{26}$$

$$\text{where } \psi(x,\theta) = \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2}\,dy\ . \tag{27}$$

We now reduce the second term of equation (18) using equations (11) to (17) and (5) where (5) can now be given in the form

$$f(E')dE' = f(y),dy = \frac{\theta}{2\sqrt{\pi}}\,e^{-\frac{\theta^2}{4}(x-y)^2}\,dy$$

$$\sigma_{sc}(E'_o,T) = \frac{\theta\,\sigma_{os}}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{e^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2} + \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{4\pi R}{k}\,\frac{\Gamma_n(E'-E_o)/\Gamma^2}{\frac{4}{1+y^2}}\,e^{\frac{-\theta^2}{4}(x-y)^2}\,dy$$

$$+\ \sigma_{pot}$$

$$= \sigma_{os}\psi(x,\theta) + \sigma_{pot} + \frac{\theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}(2\sqrt{\pi}R)\,2\sqrt{\pi}\,\frac{2}{\Gamma}\,\frac{\Gamma_n}{k}\,\frac{y}{1+y^2}\,e^{\frac{-\theta^2}{4}(x-y)^2}\,dy\ .$$

The last term becomes

$$\frac{\Theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\sqrt{\sigma_{pot}}\sqrt{\frac{4\pi}{k^2}\left(\frac{\Gamma_n}{\Gamma}\right)^2\frac{2y}{1+y^2}}\; e^{-\frac{\Theta^2}{4}(x-y)^2}\, dy$$

$$\frac{\Gamma_n}{k} = \frac{\Gamma_n^o\sqrt{E'}}{\{2E'\mu\}^{\frac{1}{2}}} = \frac{\Gamma_n^o}{\{2\mu\}^{\frac{1}{2}}} \text{ and } \frac{{}_o\Gamma_n}{k_o} = \frac{\Gamma_n^o\sqrt{E_o}}{\{2E_o\mu\}^{\frac{1}{2}}} = \frac{1}{k}\frac{\Gamma_n^o}{\{2\mu\}^{\frac{1}{2}}}$$

$$\therefore \quad \frac{\Gamma_n}{k} = \frac{{}_o\Gamma_n}{k_o} \; .$$

Finally,

$$\sigma_{sc}(E'_o,T) = \sigma_{os}\psi(x,\Theta) + \sigma_{pot} + \sqrt{\sigma_{pot}\sigma_{os}}\,\frac{\Theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{2y\; e^{-\frac{\Theta^2}{4}(x-y)^2}}{1+y^2}\, dy \; . \qquad (28)$$

By defining

$$\chi(x,\Theta) \equiv \frac{\Theta}{2\sqrt{\pi}}\int_{-\infty}^{\infty}\frac{2y\; e^{-\frac{\Theta^2}{4}(x-y)^2}}{1+y^2}\, dy \qquad (29)$$

we obtain

$$\sigma_{sc}(E'_o,T) = \sigma_{os}\psi(x,\Theta) + \sqrt{\sigma_{pot}\sigma_{os}}\,\chi(x,\Theta) + \sigma_{pot} \; . \qquad (30)$$

Since $$\sigma_T(E'_o,T) = \sigma_{ab}(E'_o,T) + \sigma_{sc}(E'_o,T) \qquad (31)$$

we have

$$\sigma_T(E'_o,T) = \sqrt{\frac{E_o}{E'_o}}\,\sigma_{or}\psi(x,\theta) + \sigma_{os}\psi(x,\theta) + \sqrt{\sigma_{pot}\,\sigma_{os}}\,\chi(x,\theta) + \sigma_{pot} \quad . \qquad (32)$$

To express this in laboratory energies we recall that

$$E'_o = \tfrac{1}{2}\mu v^2 = \frac{M}{m+M} E_1 \qquad (33)$$

where E_1 is the neutron energy in the laboratory system. From equation (22) the Doppler width becomes

$$\Delta \simeq 2\sqrt{\frac{mM}{M(m+M)}\gamma E'_o} \simeq 2\sqrt{\frac{mM}{(m+M)^2}\,\gamma_o E_1} \quad ,$$

where ${}_oE_1$ is the neutron energy in the laboratory at resonance. If we let the neutron mass m be equal to one and the target mass M be the isotopic mass number A, we have

$$\Delta = \sqrt{\frac{4\gamma_o E_1}{(1+A)\,\frac{1+A}{A}}} = \frac{1}{1+\frac{1}{A}}\sqrt{\frac{4\gamma_o E_1}{A}} \quad \text{and for } A >> 1$$

$$\Delta \simeq \sqrt{\frac{4\gamma_o E_1}{A}} \quad . \qquad (34)$$

The cross section equations given use center of mass energies. If we wish to use laboratory energies we must multiply each energy including level widths by the factor $\frac{m+M}{m}$ or $\frac{1+A}{A}$ in our case. Since only energy ratios appear in the formulas we can use laboratory energies directly. In computing Θ, we use equation (34) with no significant error.

3. Properties of $\psi(x,t)$ and $\chi(x,t)$: where $t = 1/\theta^2$

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

$$\chi(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} \frac{2ye^{-\frac{(x-y)^2}{4t}}}{1+y^2}\, dy = \frac{\theta}{2\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{2ye^{-\frac{\theta^2}{4}(x-y)^2}}{1+y^2}\, dy \qquad (2)$$

$$\chi(x,t) = 2x\psi + 4t\frac{\psi}{x}. \qquad (3)$$

which can be derived simply by taking the derivative of ψ with respect to x and re-using (1) and (2).

We wish to obtain asymptotic expressions for ψ and χ that will afford ease in machine computation for x beyond a value that provides only a small error. For smaller values of x numerical integrations are available in tabular form (16).

The asymptotic solution for $\psi(x,t)$ can be obtained as follows:

Expand the factor $1/1+y^2$ of the integrand of equations (1) and (2) in a Taylor series about y = x to obtain

$$\frac{1}{1+y^2} = \frac{1}{1+x^2} + (y-x)\left\{\frac{-2x}{(1+x^2)^2}\right\} + \frac{(y-x)^2}{2}\left\{-\frac{2}{(1+x^2)^2} + \frac{8x^2}{(1+x^2)^3}\right\}$$

$$+ \frac{(y-x)^3}{3}\left\{\frac{24x}{(1+x^2)^3} - \frac{48x^3}{(1+x^2)^4}\right\} + \frac{(y-x)^4}{4}\left\{\frac{24}{(1+x^2)^3} - \frac{288x^2}{(1+x^2)^4}\right.$$

$$\left. + \frac{384x^4}{(1+x^2)^5}\right\} + \ldots \qquad (4)$$

Upon substitution of equation (4) into (1) and (2) we obtain

$$\Psi_{\text{asymptotic}} = \frac{1}{1+x^2}\left[1 + 2t\frac{3x^2-1}{(1+x^2)^2} + \frac{12t^2}{(1+x^2)^4}\left(1-10x^2+5x^4\right)+\ldots\right] \qquad (5)$$

$$\chi_{\text{asymptotic}} = \frac{2x}{1+x^2}\left[1 + \frac{2t(x^2-3)}{(1+x^2)^2} + \frac{12t^2}{(1+x^2)^4}\left(5-10x^2+x^4\right)+\ldots\right]. \qquad (6)$$

In order to neglect the third term in equation (5) we require that

$$2t\frac{3x^2-1}{(1+x^2)^2} >> \frac{12t^2}{(1+x^2)^4}\left(1 - 10x^2 + 5x^4\right)$$

which becomes

$$(1+x^2)\,\frac{3 + 2/x^2 - 1/x^4}{5 - 10/x^2 + 1/x^4} >> 6t$$

and for large x

$$\frac{3}{5}x^2 >> 6t \quad \text{or} \quad x^2 >> 10t\ .$$

Neglect of the third term in equation (6) by similar reasoning requires $x^2 >> 6t$.

APPENDIX III

Nuclide Number Densities

We shall define the following symbols:

c = concentration of reactor solution

ρ = density of the reactor solution in gm/cm^3

n_{Th} = number of thorium atoms per cm^3

n_{ox} = number of oxygen atoms per cm^3

n_N = number of nitrogen atoms per cm^3

n_H = number of hydrogen atoms per cm^3.

One can show for a $Th(NO_3)_4$ aqueous solution that

$$n_{Th} = 1.255 \times 10^{21}\, c$$

$$n_N = 5.020 \times 10^{21}\, c$$

$$n_{ox} = 12 n_{Th} + 26.64\left(\frac{1}{c} - 1\right) n_{Th}$$

$$n_H = 53.29\left(\frac{1}{c} - 1\right) n_{Th} .$$

Using the density vs. concentration curve one can, for a specified c, calculate the number densities from the above equations.

APPENDIX IV

The Programs

1. Input and Output Data.

(a) Input Data:

The initial parameters for beginning a neutron history are fed into the IBM-650 by reading punch cards that contain eight 10-digit words. We have the following arrangement of data:

Word	Columns	Quantity	Decimal Point
1	1 - 10	(irrelevant)	-
2	11 - 20	x	4 - 6
3	21 - 30	y	4 - 6
4	31 - 40	z	4 - 6
5	41 - 50	E	8 - 2
6	51 - 60	W	1 - 9
7	61 - 70	θ	1 - 9
8	71 - 80	Φ	1 - 9

E is the first energy the neutron has below 1000 ev. and W is its statistical weight at that energy. W is essentially one, but due to the inclusion of very small absorption during the water moderation some neutrons have a weight slightly less than one.

(b) Output Data:

An output card contains the following information concerning the neutron history:

Word	Column	Quantity	Decimal
1	1 - 10	initial weight, W_{in}	1 - 9
2	11 - 20	final weight, W	1 - 9
3	21 - 30	W^2	2 - 8
4	31 - 40	$\sum_{i=1}^{N=4317} i W_{in}$	1 - 9
5	41 - 50	N , the total number of collisions per history	6 - 4
6	51 - 60	$N_{H,i}$ the number of hydrogen collisions on the i^{th} card	6 - 4
7	61 - 70	$N_{ox,i}$, the number of oxygen collisions...	6 - 4
8	72 and 73	90 means out 01 means low	
	74 - 80	$N_{Th,i}$, the number of thorium collisions...	8 - 2

2. The Data Extraction Program.

This program adds the words on the output cards to provide the following quantities:

$W_1 = \sum_{i=1}^{k} W_{1i}$, the sum of weights for neutrons surviving to energies less than 10 ev. where k is the number of histories producing an energy less than 10 ev.

W_{in} = the sum of initial weights from all source cards.

W_o = the sum of weights that escape from the pile before an energy less than 10 ev. is attained.

$W_1^2 = \sum_{i=1}^{k} W_{1i}^2$

$N = \sum_{i=1}^{K+k} N_{c,i}$ K = number of histories resulting in escape from the pile.

$N_H = \sum_{i=1}^{K+k} N_{H,i}$.

$N_{ox} = \sum_{i=1}^{K+k} N_{ox,i}$

$N_{Th} = \sum_{i=1}^{K+k} N_{Th,i}$.

THE MAIN PROGRAM

	Soap Language			Machine Language			
START	RCD	R0001		0300	70	0351	0301
	RAL	R0006		0301	65	0356	0311
	STL	WS		0311	20	0315	0318
	SRD	0004		0318	31	0004	0331
	ALO	SUMWI		0331	15	0334	0339
	STL	SUMWI		0339	20	0334	0337
	LDD	R0005		0337	69	0355	0308
	STD	ETWO		0308	24	0361	0314
	RAU	ZEROP		0314	60	0317	0321
	STU	COLLB		0321	21	0326	0329
	STU	COLHY		0329	21	0434	0387
	STU	COLOX		0387	21	0342	0345
	STU	COLTH		0345	21	0350	0303
	RAU	R0007		0303	60	0357	0411
	LDD	EXIT1	0000	0411	69	0364	0000
EXIT1	STL	SINA1		0364	20	0319	0322
	RAU	R0007		0322	60	0357	0461
	LDD	EXIT2	0049	0461	69	0414	0049
EXIT2	STL	COSA1		0414	20	0369	0372
	RAU	R0008		0372	60	0358	0313
	LDD	EXIT3	0000	0313	69	0316	0000
EXIT3	STL	SINC1		0316	20	0371	0324
	RAU	R0008		0324	60	0358	0363
	LDD	EXIT4	0049	0363	69	0366	0049
EXIT4	STL	COSB1	MEANF	0366	20	0421	0374
MEANF	RAU	ETWO		0374	60	0361	0365
	SUP	NINTN		0365	11	0368	0323
	BMI	GAP1	PEAK1	0323	46	0376	0327
GAP1	RAU	NTH		0376	60	0429	0333
	MPY	SIG1		0333	19	0336	0306
	SRD	0006		0306	31	0006	0373
	STL	SIGTH	LOOP	0373	20	0427	0330
LOOP	ALO	SINOH		0330	15	0433	0437
	STL	SIG		0437	20	0341	0344
	RAL	ONE		0344	65	0347	0401
	SLT	0002		0401	35	0002	0307
	DVR	SIG		0307	64	0341	0302

```
                SRD     0002                    0302    31  0002    0511
                STL     LAMBD . NR              0511    20  0415    0418
PEAK1           RAU     PEAK                    0327    60  0430    0335
                SUP      8003                   0335    11  8003    0343
                STU     PEAK                    0343    21  0430    0483
                RAU     PEAK                    0483    60  0430    0435
                AUP     ONE                     0435    10  0347    0451
                STU     PEAK                    0451    21  0430    0533
                RAU     ETWO                    0533    60  0361    0465
                SUP     TWO27                   0465    11  0468    0423
                BMI     EQU     PEAK2           0423    46  0426    0477
PEAK2           RAU     PEAK                    0477    60  0430    0485
                AUP     ONE                     0485    10  0347    0501
                STU     PEAK                    0501    21  0430    0583
                RAU     ETWO                    0583    60  0361    0515
                SUP     TWO8                    0515    11  0518    0473
                BMI     EQU     GAP4            0473    46  0426    0527
GAP4            RAU     ETWO                    0527    60  0361    0565
                SUP     FIVE2                   0565    11  0568    0523
                BMI     NEG     PEAK3           0523    46  0476    0577
NEG             RAU     NTH                     0476    60  0429    0633
                MPY     SIG2                    0633    19  0436    0406
                SRD      0006                   0406    31  0006    0573
                STL     SIGTH   LOOP            0573    20  0427    0330
PEAK3           RAU     PEAK                    0577    60  0430    0535
                AUP     ONE                     0535    10  0347    0551
                STU     PEAK                    0551    21  0430    0683
                RAU     ETWO                    0683    60  0361    0615
                SUP     SIX4                    0615    11  0618    0623
                BMI     EQU     PEAK4           0623    46  0426    0627
PEAK4           RAU     PEAK                    0627    60  0430    0585
                AUP     ONE                     0585    10  0347    0601
                STU     PEAK                    0601    21  0430    0733
                RAU     ETWO                    0733    60  0361    0665
                SUP     SEV6                    0665    11  0668    0673
                BMI     EQU     GAP7            0673    46  0426    0677
GAP7            RAU     ETWO                    0677    60  0361    0715
                SUP     TEN5                    0715    11  0718    0723
                BMI     EXPON   PEAK5           0723    46  0526    0727
EXPON           RAU     ETWO                    0526    60  0361    0765
                MPY     ONE11                   0765    19  0768    0338
                SLT      0009                   0338    35  0009    0309
                SLO      8002                   0309    16  8002    0367
                SLO     FIVEB                   0367    16  0320    0325
                LDD     NEXT1    1600           0325    69  0328    1600
NEXT1           RAU      8002                   0328    60  8002    0487
                MPY     THRE3                   0487    19  0340    0310
                SLO      8002                   0310    16  8002    0419
                MPY     NTH                     0419    19  0429    0400
```

```
                RAL     8003                    0400    65  8003    0407
                STL     SIGTH   LOOP            0407    20  0427    0330
PEAK5           RAU     PEAK                    0727    60  0430    0635
                AUP     ONE                     0635    10  0347    0651
                STU     PEAK                    0651    21  0430    0783
                RAU     ETWO                    0783    60  0361    0815
                SUP     ELEV8                   0815    11  0818    0773
                BMI     EQU     PEAK6           0773    46  0426    0777
PEAK6           RAU     PEAK                    0777    60  0430    0685
                AUP     ONE                     0685    10  0347    0701
                STU     PEAK                    0701    21  0430    0833
                RAU     ETWO                    0833    60  0361    0865
                SUP     ONE25                   0865    11  0868    0823
                BMI     EQU     PEAK7           0823    46  0426    0827
PEAK7           RAU     PEAK                    0827    60  0430    0735
                AUP     ONE                     0735    10  0347    0751
                STU     PEAK                    0751    21  0430    0883
                RAU     ETWO                    0883    60  0361    0915
                SUP     ONE40                   0915    11  0918    0873
                BMI     EQU     PEAK8           0873    46  0426    0877
PEAK8           RAU     PEAK                    0877    60  0430    0785
                AUP     ONE                     0785    10  0347    0801
                STU     PEAK                    0801    21  0430    0933
                RAU     ETWO                    0933    60  0361    0965
                SUP     ONE85                   0965    11  0968    0923
                BMI     EQU     GAP13           0923    46  0426    0927
GAP13           RAU     NTH                     0927    60  0429    0983
                MPY     ONE32                   0983    19  0486    0456
                RAL     8003                    0456    65  8003    0413
                STL     SIGTH   LOOP            0413    20  0427    0330
EQU             RAL     ZEROP                   0426    65  0317    0471
                LDD     PEAK                    0471    69  0430    1033
                TLU     1900                    1033    84  1900    0305
                ALO     VALUE   8002            0305    15  0408    8002
VALUE           RAU     0000    ACT             0408    60  0000    0405
ACT             SUP     PEAK    STEP            0405    11  0430    0835
STEP            STU     0181                    0835    21  0181    0484
                RAU     STEP                    0484    60  0835    0389
                AUP     ONEC                    0389    10  0392    0397
                STU     STEP                    0397    21  0835    0388
                RAU     PEAK                    0388    60  0430    0885
                AUP     ONEB                    0885    10  0438    0393
                STU     PEAK                    0393    21  0430    1083
                SLT     0004                    1083    35  0004    0443
                SUP     FIVE                    0443    11  0346    0851
                NZU     EQU     XGAP            0851    44  0426    0506
XGAP            RAU     STEP                    0506    60  0835    0439
                SUP     FIVEB                   0439    11  0320    0375
                STU     STEP                    0375    21  0835    0488
```

```
                RAU   ETWO                  0488  60  0361  1015
                SUP    0181                .1015  11  0181  0935
                MPY    0185                0935  19  0185  0556
                SRD    0003                0556  31  0003  0417
                STL   XDELE                0417  20  0521  0424
                RAM   XDELE                0424  67  0521  0425
                SLO    0182                0425  16  0182  0537
                BMI   TAB2    ASYMP        0537  46  0390  0391
ASYMP           RAU   XDELE                0391  60  0521  0475
                MPY   XDELE                0475  19  0521  0442
                STL   XSQAR                0442  20  0447  0450
                ALO   ONED                 0450  15  0403  0457
                SRD    0002                0457  31  0002  1065
                STL   DIV                  1065  20  0469  0422
                RAU   XSQAR                0422  60  0447  0901
                MPY   THREE                0901  19  0304  0474
                SLO   ONED                 0474  16  0403  0507
                RAU    8002                0507  60  8002  1115
                MPY    0186                1115  19  0186  0606
                SRD    0002                0606  31  0002  1165
                DVR   DIV                  1165  64  0469  0480
                SLT    0003                0480  35  0003  0489
                DVR   DIV                  0489  64  0469  0530
                ALO   ONEB                 0530  15  0438  0493
                SLT    0003                0493  35  0003  0951
                DVR   DIV                  0951  64  0469  0580
                SRD    0003                0580  31  0003  0441
                STL   PSI                  0441  20  0395  0348
                RAL   XSQAR                0348  65  0447  1001
                SLO   THREB                1001  16  0404  0409
                SLT    0001                0409  35  0001  1215
                DVR   DIV                  1215  64  0469  0630
                RAU    8002                0630  60  8002  0539
                MPY    0186                0539  19  0186  0656
                DVR   DIV                  0656  64  0469  0680
                ALO   ONEB                 0680  15  0438  0543
                RAU    8002                0543  60  8002  1051
                MPY   TWO                  1051  19  0454  0524
                RAU    8002                0524  60  8002  1133
                MPY   XDELE                1133  19  0521  0492
                SRD    0001                0492  31  0001  0349
                DVR   DIV                  0349  64  0469  0730
                STL   CHI     COMP         0730  20  0985  0538
TAB2            RAU    0182                0390  60  0182  0587
                STU   XMODT                0587  21  0542  0445
                RAU   PEAK                 0445  60  0430  1035
                SRT    0006                1035  30  0006  0399
                SLO    8002                0399  16  8002  0557
                SLT    0009                0557  35  0009  0977
```

```
                STU     ARG2                    0977    21  0332    1085
                RAU     XMODT                   1085    60  0542    0497
                SUP     SPLIT                   0497    11  0500    0455
                BMI     MIN     POS             0455    46  0458    0459
MIN             RAU     DEL1                    0458    60  0561    1265
                STU     DELTA   SCAN            1265    21  0370    0973
POS             RAU     DEL2                    0459    60  0312    0467
                STU     DELTA   SCAN            0467    21  0370    0973
SCAN            RAU     XDELE                   0973    60  0521    0525
                BMI     DOWN    UP              0525    46  0428    0479
DOWN            RAU     XMODT   DOWN2           0428    60  0542    0547
DOWN2           AUP     XDELE                   0547    10  0521    0575
                SUP     DELTA                   0575    11  0370    0625
                BMI     TABLE   YET             0625    46  0478    0529
YET             RAU     ARG2                    0529    60  0332    0637
                AUP     ONEE                    0637    10  0440    0495
                STU     ARG2                    0495    21  0332    1135
                RAU     XMODT                   1135    60  0542    0597
                SUP     DELTA                   0597    11  0370    0675
                STU     XMODT   DOWN2           0675    21  0542    0547
UP              RAU     XMODT   UP2             0479    60  0542    0647
UP2             SUP     XDELE                   0647    11  0521    0725
                SUP     DELTA                   0725    11  0370    0775
                BMI     TABLE   YET2            0775    46  0478    0579
YET2            RAU     ARG2                    0579    60  0332    0687
                AUP     ONEE                    0687    10  0440    0545
                STU     ARG2                    0545    21  0332    1185
                RAU     XMODT                   1185    60  0542    0697
                SUP     DELTA                   0697    11  0370    0825
                STU     XMODT   UP2             0825    21  0542    0647
TABLE           RAU     ARG2                    0478    60  0332    0737
                AUP     ONEE                    0737    10  0440    0595
                STU     ARG2                    0595    21  0332    1235
                LDD      8003                   1235    69  8003    0592
                TLU      1700                   0592    84  1700    0505
                ALO     PEET     8002           0505    15  0508    8002
PEET            RAU      0000   TERSE           0508    60  0000    0555
TERSE           SLT      0003                   0555    35  0003    0463
                SRT      0006                   0463    30  0006    1027
                STU     PSI                     1027    21  0395    0398
                SUP      8003                   0398    11  8003    0605
                SLT      0005                   0605    35  0005    0517
                STU     CHI                     0517    21  0985    0588
                RAU     XDELE                   0588    60  0521    0875
                BMI     NEGIT   SHIFT           0875    46  0528    0629
NEGIT           RAU     CHI                     0528    60  0985    0589
                MPY     NEG1                    0589    19  0642    0362
                STL     CHI     SHIFT           0362    20  0985    0629
SHIFT           RAU     PSI                     0629    60  0395    0449
```

```
            SLT     0001                    0449  35  0001  0655
            STU     PSI     COMP            0655  21  0395  0538
COMP        RAL     0181                    0538  65  0181  1285
            SLT     0004                    1285  35  0004  0645
            DVR     ETWO                    0645  64  0361  0472
            LDD     GOON    0110            0472  69  0925  0110
GOON        SRD     0003                    0925  31  0003  1335
            RAU     8002                    1335  60  8002  0593
            MPY     0183                    0593  19  0183  0504
            RAU     8002                    0504  60  8002  0513
            MPY     PSI                     0513  19  0395  0416
            SRD     0007                    0416  31  0007  1385
            STL     SIGAB                   1385  20  0639  0692
            RAU     PSI                     0692  60  0395  0499
            MPY     0184                    0499  19  0184  0554
            SRD     0003                    0554  31  0003  1315
            STL     TEMP                    1315  20  0519  0522
            RAU     SPOT                    0522  60  0975  0679
            MPY     0184                    0679  19  0184  0604
            LDD     AFT     0110            0604  69  0607  0110
AFT         SRD     0004                    0607  31  0004  0569
            RAU     8002                    0569  60  8002  1077
            MPY     CHI                     1077  19  0985  0706
            SRD     0005                    0706  31  0005  0571
            ALO     SPOT                    0571  15  0975  0729
            ALO     TEMP                    0729  15  0519  1023
            STL     SIGSC                   1023  20  1127  0780
            ALO     SIGAB                   0780  15  0639  0643
            RAU     8002                    0643  60  8002  1101
            STU     THSIG                   1101  21  0756  0509
            MPY     NTH                     0509  19  0429  0550
            SRD     0006                    0550  31  0006  0567
            STL     SIGTH   LOOP            0567  20  0427  0330
NR          LDD     AFTNR   0150            0418  69  0621  0150
AFTNR       RAL     8001                    0621  65  8001  0779
            SRD     0005                    0779  31  0005  0693
            RAU     8002                    0693  60  8002  1151
            NZU     NON     NR              1151  44  0705  0418
NON         LDD     POSTL   0214            0705  69  0558  0214
POSTL       RAU     8003                    0558  60  8003  1365
            MPY     LAMBD                   1365  19  0415  0536
            SRD     0006                    0536  31  0006  0453
            STL     D12                     0453  20  0657  0410
            RAU     COLLB                   0410  60  0326  0431
            NZU     CAL2    ZERO            0431  44  1435  0586
ZERO        RAM     D12                     0586  67  0657  0611
            RAU     8002                    0611  60  8002  0619
            MPY     COSA1                   0619  19  0369  0490
            SRD     0007                    0490  31  0007  0559
```

```
                ALO     R0004                   0559    15  0354    0609
                STL     ZEE                     0609    20  0563    0466
                RAM     D12                     0466    67  0657    0661
                RAU      8002                   0661    60  8002    0669
                MPY     SINA1                   0669    19  0319    0540
                SLT      0004                   0540    35  0004    1201
                SLO      8002                   1201    16  8002    0659
                MPY     COSB1                   0659    19  0421    0742
                AUP     R0002                   0742    10  0352    0707
                STU     X                       0707    21  0412    1415
                RAM     D12                     1415    67  0657    0711
                RAU      8002                   0711    60  8002    0719
                MPY     SINA1                   0719    19  0319    0590
                SLT      0004                   0590    35  0004    1251
                SLO      8002                   1251    16  8002    0709
                MPY     SINC1                   0709    19  0371    0792
                AUP     R0003                   0792    10  0353    0757
                STU     Y                       0757    21  0462    1465
                RAU     ZEE     OUTZ            1465    60  0563    0617
OUTZ            BMI     POUT    ZOUT            0617    46  0420    0671
ZOUT            RAM     ZEE                     0671    67  0563    0667
                SLO     ZMAX                    0667    16  0470    1025
                BMI     XOUT    POUT            1025    46  0578    0420
POUT            RAU     NINE                    0420    60  1073    1177
                AUP     COLTH                   1177    10  0350    0755
                STU     P0008                   0755    21  0384    0787
                RAU     COLLB                   0787    60  0326    0481
                STU     P0005                   0481    21  0381    0534
                LDD     COLHY                   0534    69  0434    0837
                STD     P0006                   0837    24  0382    1485
                LDD     COLOX                   1485    69  0342    0695
                STD     P0007                   0695    24  0383    0636
                RAU     WS                      0636    60  0315    0769
                STU     P0002                   0769    21  0378    0531
                MPY      8003                   0531    19  8003    0806
                STU     P0003                   0806    21  0379    0432
                RAU     R0006                   0432    60  0356    0761
                STU     P0001                   0761    21  0377    0830
                LDD     SUMWI                   0830    69  0334    0887
                STD     P0004                   0887    24  0380    1183
                PCH     P0001   START           1183    71  0377    0300
XOUT            RAM     X                       0578    67  0412    0717
                SLO     XMAX                    0717    16  0520    1075
                BMI     YOUT    POUT            1075    46  0628    0420
YOUT            RAM     Y                       0628    67  0462    0767
                SLO     YMAX                    0767    16  0570    1125
                BMI     THOR    POUT            1125    46  0678    0420
THOR            LDD     AFTER    0150           0678    69  0581    0150
AFTER           STL     NR2                     0581    20  1535    0638
```

```
        RAL     SIGTH                   0638    65    0427    0631
        SLT      0006                   0631    35    0006    0745
        DVR     SIG                     0745    64    0341    0402
        SLT      0004                   0402    35    0004    0613
        STL     FTH                     0613    20    0817    0620
        SLO     NR2                     0620    16    1535    0689
        BMI     NOTH    YESTH           0689    46    0842    0743
NOTH    RAL     SIGOX                   0842    65    0795    0549
        SLT      0006                   0549    35    0006    0663
        DVR     SIG                     0663    64    0341    0452
        SLT      0004                   0452    35    0004    0713
        STL     FOX                     0713    20    0867    0670
        ALO     FTH                     0670    15    0817    0721
        SLO     NR2                     0721    16    1535    0739
        BMI     NOOX    YESOX           0739    46    0892    0793
NOOX    RAL     SIGHY                   0892    65    0845    0599
        SLT      0006                   0599    35    0006    0763
        DVR     SIG                     0763    64    0341    0502
        SLT      0004                   0502    35    0004    0813
        STL     FHY                     0813    20    0917    0720
        ALO     FTH                     0720    15    0817    0771
        ALO     FOX                     0771    15    0867    0821
        SLO     NR2                     0821    16    1535    0789
        BMI     NOHY    YESHY           0789    46    0942    0843
NOHY    RAU     FOUR                    0942    60    0895    0649
        SLT      0005                   0649    35    0005    0811
        STU     ID      COLL            0811    21    0516    0819
YESHY   RAU     THREE                   0843    60    0304    0759
        SLT      0005                   0759    35    0005    0871
        STU     ID                      0871    21    0516    0869
        RAU     COLHY                   0869    60    0434    0839
        AUP     ONED                    0839    10    0403    0807
        STU     COLHY   COLL            0807    21    0434    0819
YESOX   RAU     TWO                     0793    60    0454    0809
        SLT      0005                   0809    35    0005    0921
        STU     ID                      0921    21    0516    0919
        RAU     COLOX                   0919    60    0342    0747
        AUP     ONED                    0747    10    0403    0857
        STU     COLOX   COLL            0857    21    0342    0819
YESTH   RAU     ONEB                    0743    60    0438    0893
        STU     ID                      0893    21    0516    0969
        RAU     COLTH                   0969    60    0350    0805
        AUP     ONED                    0805    10    0403    0907
        STU     COLTH   WATE            0907    21    0350    0503
WATE    RAU     WS                      0503    60    0315    1019
        MPY     SIGSC                   1019    19    1127    0448
        DVR     THSIG                   0448    64    0756    0566
        STL     WS      COLL            0566    20    0315    0819
COLL    RAU     COLLB                   0819    60    0326    0681
```

```
                AUP     ONED                    0681    10  0403    0957
                STU     COLLB                   0957    21  0326    0829
                LDD     ID                      0829    69  0516    1069
                TLU      1850                   1069    84  1850    0855
                ALO     VALU        8002        0855    15  0608    8002
VALU            RAU      0000       ACT2        0608    60  0000    0905
ACT2            SLT      0005                   0905    35  0005    0967
                SRT      0005                   0967    30  0005    0879
                STU     MASS                    0879    21  0584    0937
                LDD     AFR         0150        0937    69  0640    0150
AFR             STD     ENR                     0640    24  0943    0396
                RAU     ONED                    0396    60  0403    1007
                SRT      0002                   1007    30  0002    0863
                AUP     MASS                    0863    10  0584    0889
                STU     AONE                    0889    21  0394    0797
                RAU     MASS                    0797    60  0584    0939
                SLT      0002                   0939    35  0002    0945
                SUP     ONED                    0945    11  0403    1057
                SRT      0002                   1057    30  0002    0913
                DVR     AONE                    0913    64  0394    0654
                RAU      8002                   0654    60  8002    0963
                MPY      8003                   0963    19  8003    0688
                SRT      0004                   0688    30  0004    0699
                STU     ALPHA                   0699    21  0704    1107
                SLO      8002                   1107    16  8002    1515
                RAU     ONE                     1515    60  0347    1301
                SUP     ALPHA                   1301    11  0704    0859
                MPY     ENR                     0859    19  0943    0464
                SRD      0009                   0464    31  0009    0987
                AUP     ONEE                    0987    10  0440    0995
                SUP      8002                   0995    11  8002    0553
                SLO      8002                   0553    16  8002    0861
                MPY     ETWO                    0861    19  0361    0482
                STD     EONE                    0482    24  1585    0738
                SRD      0007                   0738    31  0007    1157
                STL     ETWO                    1157    20  0361    0514
                SLO     EMIN                    0514    16  1017    0971
                BMI     LOW         ESCAT       0971    46  0574    1175
LOW             RAU     R0006                   0574    60  0356    0911
                STU     P0001                   0911    21  0377    0880
                RAU     COLLB                   0880    60  0326    0731
                STU     P0005                   0731    21  0381    0634
                LDD     COLHY                   0634    69  0434    1037
                STD     P0006                   1037    24  0382    1685
                LDD     COLOX                   1685    69  0342    1045
                STD     P0007                   1045    24  0383    0686
                RAU     ONE                     0686    60  0347    1351
                AUP     COLTH                   1351    10  0350    0955
                STU     P0008                   0955    21  0384    1087
```

```
                RAU     WS                      1087    60  0315    1119
                STU     P0002                   1119    21  0378    0781
                MPY      8003                   0781    19  8003    0856
                STU     P0003                   0856    21  0379    0532
                LDD     SUMWI                   0532    69  0334    1137
                STD     P0004                   1137    24  0380    1233
                PCH     P0001   START           1233    71  0377    0300
ESCAT           RAU     ETWO                    1175    60  0361    1565
                SRT      0002                   1565    30  0002    1021
                DVR     EONE                    1021    64  1585    0446
                LDD     NXT     0110            0446    69  0749    0110
NXT             SRD      0005                   0749    31  0005    1013
                STL     AID                     1013    20  1067    0770
                RAL     ALPHA                   0770    65  0704    0909
                SLT      0004                   0909    35  0004    1169
                LDD     AUX     0110            1169    69  0572    0110
AUX             SRD      0002                   0572    31  0002    0831
                DVR     AID                     0831    64  1067    0728
                AUP     AID                     0728    10  1067    1071
                SUP      8002                   1071    11  8002    0929
                SLO      8002                   0929    16  8002    1187
                MPY     AONE                    1187    19  0394    0564
                RAU      8002                   0564    60  8002    1123
                MPY     FIVE                    1123    19  0346    0616
                SRD      0005                   0616    31  0005    0881
                STL     COSAP                   0881    20  1885    0788
                RAU      8002                   0788    60  8002    0847
                MPY      8003                   0847    19  8003    0622
                SLT      0001                   0622    35  0001    0979
                STU     AID                     0979    21  1067    0820
                RAU     ONED                    0820    60  0403    1207
                SRT      0003                   1207    30  0003    1865
                SLO     AID                     1865    16  1067    1121
                SLT      0001                   1121    35  0001    1227
                NZU     NON2    NX              1227    44  0931    0582
NX              LDD     SQ       0110           0582    69  1985    0110
SQ              SRD      0001                   1985    31  0001    0491
                STL     SINAP   AZMTH           0491    20  1095    0498
NON2            SRD      0001                   0931    31  0001    1237
                STL     SINAP   AZMTH           1237    20  1095    0498
AZMTH           LDD     NXNR     0150           0498    69  1401    0150
NXNR            RAU      8002                   1401    60  8002    0959
                MPY     TPI                     0959    19  0512    0632
                SLT      0005                   0632    35  0005    1145
                STU     AID                     1145    21  1067    0870
                SLO      8002                   0870    16  8002    1029
                LDD     AFPHI   0000            1029    69  0682    0000
AFPHI           STL     SINBP                   0682    20  1287    0690
                RAU     AID                     0690    60  1067    1171
```

```
            LDD     AFCOS    0049      1171   69   0624   0049
AFCOS       STL     COSBP    MEANF     0624   20   1079   0374
CAL2        RAU     SINAP              1435   60   1095   0799
            MPY     COSBP              0799   19   1079   0600
            SRT      0002              0600   30   0002   1257
            STU     XPOND              1257   21   0562   0666
            RAU     SINAP              0666   60   1095   0849
            MPY     SINBP              0849   19   1287   0658
            SRT      0002              0658   30   0002   0716
            STU     YPOND              0716   21   0920   1173
            RAU     COSAP              1173   60   1885   0989
            SRT      0003              0989   30   0003   0897
            STU     ZPOND              0897   21   0552   1005
            RAU     YPOND              1005   60   0920   1225
            MPY     SINC1              1225   19   0371   0992
            SLT      0001              0992   35   0001   0899
            STU     AID                0899   21   1067   0970
            RAU     XPOND              0970   60   0562   1117
            MPY     COSA1              1117   19   0369   0740
            SLT      0001              0740   35   0001   0947
            STU     STORE              0947   21   0602   1055
            RAU     ZPOND              1055   60   0552   1307
            MPY     SINA1              1307   19   0319   0790
            SLT      0001              0790   35   0001   0997
            AUP     STORE              0997   10   0602   1357
            STU     STORE              1357   21   0602   1105
            SLO      8002              1105   16   8002   1063
            MPY     COSB1              1063   19   0421   1042
            SLT      0001              1042   35   0001   0949
            SUP     AID                0949   11   1067   1221
            STU     DELXD              1221   21   0576   1129
            RAU     YPOND              1129   60   0920   1275
            MPY     COSB1              1275   19   0421   1092
            SLT      0001              1092   35   0001   0999
            STU     AID                0999   21   1067   1020
            RAU     STORE              1020   60   0602   1407
            MPY     SINC1              1407   19   0371   1142
            SLT      0001              1142   35   0001   1049
            AUP     AID                1049   10   1067   1271
            STU     DELYD              1271   21   0626   1179
            RAU     XPOND              1179   60   0562   1167
            MPY     SINA1              1167   19   0319   0840
            SLT      0001              0840   35   0001   1047
            STU     AID                1047   21   1067   1070
            RAU     ZPOND              1070   60   0552   1457
            MPY     COSA1              1457   19   0369   0890
            SLT      0001              0890   35   0001   1097
            SUP     AID                1097   11   1067   1321
            SLT      0003              1321   35   0003   1229
```

```
                STU     COSA1                   1229    21  0369    0672
                RAU     DELXD                   0672    60  0576    0981
                MPY      8003                   0981    19  8003    0906
                SLT      0006                   0906    35  0006    1371
                STU     AID                     1371    21  1067    1120
                RAU     DELYD                   1120    60  0626    1031
                MPY      8003                   1031    19  8003    0956
                SLT      0006                   0956    35  0006    1421
                AUP     AID                     1421    10  1067    1471
                RAL      8003                   1471    65  8003    1279
                LDD     B       0110            1279    69  0732    0110
B               STL     SINA1                   0732    20  0319    0722
                RAU     DELXD                   0722    60  0576    1081
                SRT      0001                   1081    30  0001    1337
                DVR     SINA1                   1337    64  0319    0930
                SLT      0002                   0930    35  0002    1387
                STL     COSB1                   1387    20  0421    0674
                RAU     DELYD                   0674    60  0626    1131
                DVR     SINA1                   1131    64  0319    0980
                SLT      0002                   0980    35  0002    1437
                STL     SINC1                   1437    20  0371    0724
                RAM     D12                     0724    67  0657    0961
                STL     D12                     0961    20  0657    0460
                RAU      8002                   0460    60  8002    1219
                MPY     COSA1                   1219    19  0369    0940
                SLT      0003                   0940    35  0003    1099
                AUP     ZEE                     1099    10  0563    1217
                STU     ZEE                     1217    21  0563    0766
                BMI     POUT    ZIN             0766    46  0420    1170
ZIN             RAU     DELXD                   1170    60  0576    1181
                MPY     D12                     1181    19  0657    0778
                SRD      0004                   0778    31  0004    0541
                ALO     X                       0541    15  0412    1267
                STL     X                       1267    20  0412    0816
                RAM     X                       0816    67  0412    1317
                SLO     XMAX                    1317    16  0520    1325
                BMI     XIN     POUT            1325    46  0828    0420
XIN             RAU     DELYD                   0828    60  0626    1231
                MPY     D12                     1231    19  0657    0878
                SRD      0004                   0878    31  0004    0591
                ALO     Y                       0591    15  0462    1367
                STL     Y                       1367    20  0462    0866
                RAM     Y                       0866    67  0462    1417
                SLO     YMAX                    1417    16  0570    1375
                BMI     THOR    POUT            1375    46  0678    0420
NTH             00       0006    2500           0429    00  0006    2500
SINOH           00       0001    5276           0433    00  0001    5276
NINTN           00       0000    1900           0368    00  0000    1900
SIG1            00       0000    1150           0336    00  0000    1150
```

TWO8	00	0000	2800	0518	00	0000	2800
FIVE2	00	0000	5200	0568	00	0000	5200
SIG2	00	0000	1180	0436	00	0000	1180
SIX4	00	0000	6400	0618	00	0000	6400
SEV6	00	0000	7600	0668	00	0000	7600
TEN5	00	0001	0500	0718	00	0001	0500
ONE11	00	0111	3000	0768	00	0111	3000
ELEV8	00	0001	1800	0818	00	0001	1800
ONE25	00	0001	2500	0868	00	0001	2500
ONE40	00	0001	4000	0918	00	0001	4000
ONE85	00	0001	8550	0968	00	0001	8550
ONE32	00	1320	0000	0486	00	1320	0000
THRE3	03	3780	0000	0340	03	3780	0000
TWO27	00	0000	2270	0468	00	0000	2270
SIXTY	60	0000	0000	0650	60	0000	0000
ONE	00	0100	0000	0347	00	0100	0000
ONEB	00	0010	0000	0438	00	0010	0000
FIVE	50	0000	0000	0346	50	0000	0000
ONEC	00	0001	0000	0392	00	0001	0000
DEL1	00	0000	0010	0561	00	0000	0010
DEL2	00	0000	0020	0312	00	0000	0020
SPLIT	00	2000	0000	0500	00	2000	0000
ZMAX	00	3700	0000	0470	00	3700	0000
XMAX	00	3650	0000	0520	00	3650	0000
YMAX	00	3650	0000	0570	00	3650	0000
NINE	00	9000	0000	1073	00	9000	0000
SIGOX	00	0000	1554	0795	00	0000	1554
SIGHY	00	0001	3439	0845	00	0001	3439
SIGNI	00	0000	0228	0700	00	0000	0228
EMIN	00	0000	1000	1017	00	0000	1000
TPI	00	0006	2832	0512	00	0006	2832
FOUR	00	0000	0004	0895	00	0000	0004
ONEE	00	1000	0000	0440	00	1000	0000
THREB	00	0000	0300	0404	00	0000	0300
TWO	00	0000	0002	0454	00	0000	0002
THREE	00	0000	0003	0304	00	0000	0003
ONED	00	0000	0100	0403	00	0000	0100
FIVEB	00	0005	0000	0320	00	0005	0000
ZEROP	00	0000	00 0	317	00	0000	0000
SPOT	00	0000	1050	0975	00	0000	1050
				470	00	3300	0000
				520	00	3100	0000
				570	00	3100	0000
				429	00	0015	3813
				795	00	0000	1577
				845	00	0000	9312
				700	00	0000	0560
				433	00	0001	1449

TABLE LOOKUP FOR PEAK PARAMETERS

The data for each peak is given by a group of six words. The last 5 digits of each gives the particular parameter value.

Position	Argument	Function
1900	00010	02184
1901	00011	00190
1902	00012	06871
1903	00013	00445
1904	00014	05555
1905	00015	01468
1906	00020	02348
1907	00021	00170
1908	00022	09340
1909	00023	00957
1910	00024	04651
1911	00025	01106
1912	00030	05955
1913	00031	00440
1914	00032	06235
1915	00033	01365
1916	00034	07692
1917	00035	07668
1918	00040	06920
1919	00041	00150
1920	00042	09380
1921	00043	08500
1922	00044	02439
1923	00045	00896
1924	00050	11315
1925	00051	00300
1926	00052	03780
1927	00053	00989
1928	00054	03774
1929	00055	03506
1930	00060	12100
1931	00061	00280
1932	00062	04610
1933	00063	02079
1934	00064	03333
1935	00065	02926
1936	00070	12940

1937	00071	00380
1938	00072	01318
1939	00073	00100
1940	00074	04545
1941	00075	05818
1942	00080	17080
1943	00081	00190
1944	00082	03770
1945	00083	04560
1946	00084	01887
1947	00085	01324

TABLE LOOKUP FOR $\psi(x,t)$ AND $\chi(x,t)$

For a given 10 digit word, digits 4 through 7 carry the value of $\psi(x,t)$ and digits 8 through 10 carry the corresponding value of $\chi(x,t)$. The values are 0-4 and 0-3 numbers respectively. The first digit gives the peak number

1700	10100	35058
1701	10200	40061
1702	10300	46065
1703	10400	55074
1704	10500	67079
1705	10600	84084
1706	10701	10091
1707	10801	50099
1708	10902	11110
1709	11003	03125
1710	11104	39141
1711	11206	30151
1712	11308	82153
1713	11411	95157
1714	11515	51147
1715	11619	22138
1716	11722	63125
1717	11825	27068
1718	11926	71042
1719	20100	50069
1720	20200	59074
1721	20300	72081
1722	20400	90087
1723	20501	17097

1724	20601	59109
1725	20702	27119
1726	20803	35132
1727	20905	02158
1728	21007	46171
1729	21110	79176
1730	21214	94180
1731	21319	59163
1732	21424	14137
1733	21527	82088
1734	21629	88030
1735	30100	06025
1736	30200	07026
1737	30300	08027
1738	30400	09029
1739	30500	11031
1740	30600	14034
1741	30700	18036
1742	30800	24041
1743	30900	34045
1744	31000	50050
1745	31100	74055
1746	31201	14061
1747	31301	70071
1750	31402	50077
1751	31503	55078
1752	31604	88078
1753	31706	43076
1754	31808	12074
1755	31909	80069
1756	32011	31057
1757	32112	44040
1758	32213	04017
1759	40100	56074
1760	40200	67079
1761	40300	82087
1762	40401	03095
1763	40501	36106
1764	40601	88119
1765	40702	75135
1766	40804	17152
1767	40906	41180
1768	41009	72189
1769	41114	19205
1770	41219	54280
1771	41325	07144
1772	41429	72069
1773	41532	41032
1774	50100	14036

1775	50200	17040
1776	50300	21044
1777	50400	26049
1778	50500	36052
1779	50600	54060
1780	50700	88072
1781	50801	51080
1782	50902	62103
1783	51004	40110
1784	51106	97106
1785	51210	19117
1786	51313	65087
1787	51416	63071
1788	51518	37024
1789	60100	16039
1790	60200	19043
1791	60300	24047
1792	60400	32052
1793	60500	45060
1794	60600	69070
1795	60701	18082
1796	60802	11097
1797	60903	76116
1800	61006	36132
1801	61109	91123
1802	61213	96118
1803	61317	63109
1804	61419	82042
1805	70100	09029
1806	70200	10032
1807	70300	12036
1808	70400	14038
1809	70500	17042
1810	70600	23048
1811	70700	32058
1812	70800	47072
1813	70900	73090
1814	71001	15121
1815	71101	82158
1816	71202	80200
1817	71304	17249
1818	71405	92238
1819	71507	99305
1820	71610	19311
1821	71712	25290
1822	71813	87176
1823	71914	76006
1824	80100	34057
1825	80200	39060

1826	80300	45065
1827	80400	53070
1828	80500	63075
1829	80600	79082
1830	80701	01090
1831	80801	35097
1832	80901	89110
1833	81002	72123
1834	81103	98138
1835	81205	82147
1836	81308	34163
1837	81411	57179
1838	81515	36151
1839	81619	40132
1840	81723	21123
1841	81826	20087
1842	81927	84016
1600	24160	31606
1606	16800	21665
1665	24166	81621
1621	19162	41660
1660	10166	31620
1620	31000	81641
1641	16800	21649
1649	24160	21605

TABLE LOOKUP FOR ATOMIC MASSES

The mass is given by the last five digits.

1850	00001	00232
1851	00002	00016
1852	00003	00001
1853	00004	00014

SUBROUTINE exp{-x}

Position	Operation	Data Address	Instruction Address
1605	30	0001	1662
1662	11	8003	1669
1669	35	0001	1626
1626	15	8001	1631
1631	35	0004	1642
1642	10	1645	1650
1650	11	8003	1608
1608	24	1661	1664
1664	18	1668	1623
1623	45	1676	1679
1676	46	1629	1630
1630	69	1633	1637
1629	69	1632	1637
1679	69	1634	1637
1637	22	1643	1647
1647	60	1602	1607
1607	11	1663	1667
1667	30	0001	1674
1674	16	8002	1635
1635	19	8003	1658
1619	89	1250	9381
1658	24	1673	1627
1627	65	8003	1636
1636	31	0002	1646
1646	15	1601	1655
1655	10	1609	1666
1666	16	8002	1625
1625	30	0001	1638
1638	64	8001	1644
1644	16	1648	1653
1653	35	0001	1659
1659	10	8002	1670
1670	15	1673	1677
1677	11	8001	1639
1639	16	8002	1651
1651	30	0001	1657
1657	64	8001	1652

Position	Operation	Data Address	Instruction Address	
1652	60	8002	1661	
1661	19	0000	1671	
1671	31	0009	1643	
1643	00	0000	1603	
1624	43	4294	4819	
1663	50	0000	0000	
1645	19	1610	1671	
1633	35	0000	1603	SUBROUTINE
1632	31	0000	1603	
1634	00	0000	1603	exp {-x}
1601	11	3167	0182	(continued)
1609	49	1478	1154	
1648	52	1153	3783	
1610	11	2201	8454	
1611	14	1253	7545	
1612	17	7827	9410	
1613	22	3872	1139	
1614	28	1838	2931	
1615	35	4813	3892	
1616	44	6683	5922	
1617	56	2341	3252	
1618	70	7945	7844	
1619	89	1250	9381	

SUBROUTINE FOR SINE AND COSINE

49	24	0003	0006
6	10	0009	0013
13	46	0025	0017
17	11	0020	0025
	24	0003	0025
25	46	0028	0029
28	10	0032	0037
29	11	0032	0037
37	21	0042	0045
45	46	0048	0099
48	10	0002	0007
99	11	0002	0007

7	21	0012	0015
15	46	0018	0019
18	10	0022	0027
19	11	0022	0027
27	21	0082	0035
35	68	8003	0043
43	15	0046	0001
1	35	0001	0057
57	20	0011	0014
14	60	8001	0021
21	19	8001	0005
5	21	0056	0059
59	60	0012	0069
69	46	0072	0073
72	60	0082	0087
87	46	0092	0050
73	60	0082	0038
38	46	0050	0092
92	61	0095	0051
51	19	0056	0030
30	10	0091	0096
96	61	8003	0053
53	19	0056	0041
41	10	0089	0094
94	61	8003	0052
52	19	0056	0044
44	10	0085	0090
90	61	8003	0098
98	19	0056	0054
54	10	0034	0040
40	61	8003	0047
47	19	0056	0055
55	10	0093	0097
97	60	8003	0008
8	19	0011	0031
31	21	0036	0039
39	65	0042	0004
4	46	0070	0071
70	65	0036	0003
71	66	0036	0003
50	61	0056	0064
64	24	0079	0033
33	19	0086	0058
58	10	0063	0068
68	61	8003	0026
26	19	0079	0074
74	10	0062	0067
67	61	8003	0076
76	19	0079	0078

78	10	0061	0016
16	61	8003	0075
75	19	0079	0088
88	10	0010	0066
66	61	8003	0024
24	19	0079	0080
80	10	0060	0065
65	61	8003	0023
23	19	0079	0083
83	10	0093	0031
9	15	7079	6327
20	62	8318	5307
32	31	4159	2654
2	15	7079	6327
22	07	8539	8163
46	07	8539	8163
95	00	0000	0025
91	00	0000	2756
89	00	0019	8413
85	00	0833	3333
34	01	6666	6667
93	10	0000	0000
86	00	0000	0002
63	00	0000	0276
62	00	0002	4802
61	00	0138	8889
10	00	4166	6667
60	05	0000	0000

SUBROUTINE FOR RANDOM NUMBER

110	45	0114	8001
114	24	0118	0121
121	20	0127	0106
106	65	0109	0113
113	10	8001	0122
122	19	0127	0115
115	65	8003	0124

124	10	0127	0131
131	16	8002	0139
139	64	8001	0130
130	16	8001	0138
138	46	0100	0108
100	15	8001	0107
107	15	8001	0116
116	10	0119	0123
123	30	0001	0129
129	16	8002	0137
137	19	8001	0124
108	15	8001	0118
109	50	0000	0000
119	00	0000	0050
156	60	0159	0163
150	24	0153	0156
163	19	0166	0160
160	20	0166	0169
169	21	0174	0177
177	60	0180	0151
151	19	0154	0152
152	15	0174	0179
179	20	0154	0153
159	11	6226	1467
180	11	6226	1467
154	01	3508	5171
166	76	7299	2089

SUBROUTINE FOR NATURAL LOG

224	24	0227	0280
280	69	0231	0285
285	24	0288	0291
214	24	0227	0221
221	69	0232	0285
291	46	0299	0295
295	45	0298	0299
299	01	9999	9999

298	36	0000	0223
223	20	0277	0281
281	65	8003	0230
230	15	0233	0238
238	31	0001	0245
245	20	0249	0202
202	35	0001	0209
209	16	0212	0217
217	16	8001	0225
225	35	0209	0246
246	64	0249	0239
239	20	0244	0247
247	60	8001	0206
206	19	8001	0237
237	31	0000	0215
231	10	0000	0000
232	23	0258	5093
215	20	0222	0228
228	60	8001	0235
235	19	0240	0236
236	10	0243	0201
201	60	8003	0216
216	19	0222	0200
200	10	0203	0210
210	60	8003	0218
218	19	0222	0204
204	10	0207	0211
211	60	8003	0219
219	19	0222	0226
226	10	0229	0234
234	60	8003	0241
241	19	0244	0205
205	10	0208	0213
213	30	0001	0220
220	15	8001	0278
229	86	8591	7180
207	28	9335	5240
203	17	7522	0710
243	09	4376	4760
240	19	1337	7140
212	31	6227	7660
233	31	6227	7660
208	50	0000	0000
278	21	0282	0286
286	61	0277	0283
283	10	0287	0292
287	00	0000	0004
292	30	0001	0279
279	60	8002	0242

```
242     10   0282   0289
289     19   0288   0227
```

DATA EXTRACTION PROGRAM

After reading the output cards into this program locations 277, 278, 281, 282, 283, 284, 285, 286, 287, 288, 289, and 290 will contain the necessary results.

```
405     00   0100   0000
 60     70   0251   0065
 65     60   0331   0070
 70     10   0405   0075
 75     21   0331   0080
 80     60   0258   0085
 85     44   0410   0090
 90     60   0251   0092
 92     31   0003   0095
 95     10   0277   0100
100     21   0277   0105
105     60   0252   0107
107     31   0003   0110
110     10   0278   0115
115     21   0278   0120
120     60   0281   0125
125     10   0255   0130
130     21   0281   0135
135     60   0282   0140
140     10   0256   0145
145     21   0282   0150
150     60   0283   0155
155     10   0257   0160
160     21   0283   0060
410     60   0251   0412
412     31   0003   0415
415     10   0284   0420
420     21   0284   0425
425     60   0252   0428
428     31   0003   0430
430     10   0285   0435
435     21   0285   0440
440     60   0286   0445
```

445	10	0255	0450
450	21	0286	0455
455	60	0287	0460
460	10	0256	0465
465	21	0287	0470
470	60	0288	0475
475	10	0257	0480
480	21	0288	0485
485	60	0289	0490
490	10	0258	0495
495	21	0289	0060
80	60	0258	0083
83	35	0005	0085
85	30	0005	0087
87	21	0050	0088
88	44	0410	0090
490	10	0050	0495
495	21	0289	0500
500	60	0253	0505
160	21	0283	0360
360	60	0253	0500
505	21	0290	0060
505	30	0003	0510
510	10	0290	0515
515	21	0290	0060

ABSTRACT

We have undertaken to develop a method for determining the resonance escape probability of homogeneous reactors containing acqeous solutions of a resonance absorber. $TH(NO_3)_4$ was selected as a salt since it is readily dissolvable in water. Even at the highest concentration, the atomic densities of thorium and nitrogen are small compared to hydrogen and oxygen. Only the latter two contribute significantly to the slowing down in the high energy range; therefore, a water Monte Carlo serves adequately as the neutron supply to the resonance region of thorium.

In order to find an escape probability we determine the ratio of the number of neutrons that attain energies below the resonance region to the number that appear in the resonance region for the first time. The difference between the two numbers in the ratio occurs due to absorption by the resonance absorber, in this case thorium, and due to leakage.

The initial source of neutrons comes from $H^2(d,n)He^3$ reaction where the deuteron beam strikes the deuterium target at the center of one face of the containing parallelepiped.

Once the water Monte Carlo is run one has a set of data cards which can be used as the input data to a second Monte Carlo designed to calculate the resonance escape probability. Our prime concern is this second Monte Carlo.

The resonance escape Monte Carlo is a direct analog type using known physical distributions and laws. The decisions about what events occur in the history of a neutron are based on these distributions and laws. The detailed effect of the thorium resonances on the number of neutrons absorbed is described by the cross section as a function of energy. A Breit-Wigner Doppler broadened single level formulation gives the scattering and absorption parts of the cross section as a function of energy. Given a neutron-thorium interaction, the neutron is either absorbed or scattered with probabilities $\frac{\sigma_{ab}}{\sigma_{ab} + \sigma_{sc}}$ and $\frac{\sigma_{sc}}{\sigma_{ab} + \sigma_{sc}}$. A new statistical weight is assigned the neutron by taking the latter fraction of the old weight. A new neutron is picked from the source supply only after the previous neutron has delivered a weight to low energy or to the exterior of the pile.

The heart of the Monte Carlo method lies in the determination of a random variable, distributed according to some known probability function. This requires a source of

random numbers which in our case is provided by the IBM-650 computer.

The resonance escape probability as a function of thorium number density fits very closely to a straight line with small negative slope throughout the whole range of stable concentrations. The Monte Carlo statistics provides probable errors of less than 0.3% for all five points calculated. Each of the five points lies close enough to the straight line of least squares fit to give an error less than 0.3%.

A theoretical determination of the resonance escape probability based on resonance integral theory for the eight peaks used in the Monte Carlo calculation gives good enough agreement to make both methods plausible.

Although other resonance escape calculations have been done by the Monte Carlo method, they have been for radically different systems. In all such cases the system was heterogeneous with "lumped" uranium for the absorber. Therefore comparisons between existing Monte Carlo calculations is impossible. We hope to be able to provide experimental verification for the applicability of the Monte Carlo model.