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A. Maggiolo and G. Ricco: MONTE CARLO CALCULATIONS FOR A FAST NEUTRON COUNTER. -

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INTRODUCTION.

In this paper a Monte Carlo calculation will be described to estimate the density of thermal neutrons starting from a fast neutron source embedded in paraffin.

The practical purpose of this calculation is to obtain, if possible, a fast neutron counter with almost constant efficiency (flat counter) of the "Halpern -Mann" type. We shall calculate therefore, to satisfy our purpose, the best location of the thermal neutron counters in paraffin.

To simplify the calculations we have chosen a spherical symmetry instead of a cylindrical one with the source placed in the centre of a sphere with $R_1 = 54,5$ gr/cm² crossed by a cylindrical hole ($R_0 = 0,127$ gr/cm²) along the diameter. We have also chosen monoenergetic sources and the calculations have been performed for different values of E_0 ($E_0 = 8$ MeV, 14,1 MeV, 23 MeV, 35 MeV, 50 MeV).

Because of the long time employed by the computer we have used (IBM 1620) for a complete cycle from E_0 down to the thermal energy, the program has been broken in two parts. The first one is an ordinary Monte Carlo that stops every time a particle reaches an energy $E_f \leq 1,5$ MeV; the second one is an integral transformation that, starting from this final classification, gives the required density distribution as explained below.

PART I

Monte Carlo routine.

As it is well known this method consists in actually

following each one of a large number of particles from the source throughout its life history to its death in some of the terminal categories, if, of course, all relevant probabilities for the elementary events in the "life history" of such a particle are known.

Let us assume for the event x_j a probability p_j and let us produce a random number r in the interval $0 \le r < 1$. The fundamental principle of the M.C.M. says that

$$p_1 + \cdots + p_{j-1} \le r \le p_1 + \cdots + p_j$$

determines x;.

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In the continuous case we have a probability function p(x). So the event x is determined by

$$r = \int_0^x P(\xi) d\xi$$

Of course this way of dealing with problems of the kind we want to solve breaks up naturally into a well definite set of subroutines, which we shall briefly describe here, corresponding to different events in the random walk of the particle.

Source routine.

This routine describes the path of the neutron from the source to the first collision, taking care of the hole around the source.

Because of the spherical symmetry we need only two parameters: the radial distance R at the point of collision and the direction cosine α between the new direction and the vector OR. On starting we have $\alpha = 1$.

The free path is calculated by the usual probability function

$$p(1)d1 = e^{-N \epsilon_t l} N \epsilon_t d1$$

where

N = numerical density (target particles/cm³)
l free path
G_t = total collision cross section.

From this we obtain

$$l = -\lambda \ln r$$

where λ is the mean free path $\lambda = 1/N_{f_{+}}$.

The presence of the hole carriers a term (R_0/Q) where R_0 is the radious of the hole and Q is the since of the angle between the first path of the neutron and the direction of the hole. Q has been calculated in the usual way considering the source isotropical.

Collision routine.

By the first routine the neutron has been led to the point of collision. Now in CH₂ there are two different possibilities:

- α) a collision against a hydrogen nucleus with probability (2 $_{\rm H}\sigma_{\rm t}$)/($_{\rm c}\sigma_{\rm t}$ + 2 $_{\rm H}\sigma_{\rm t}$),
- β) a collision against a carbon nucleus with probability $1-[(2_H \sigma_t)/(c_t + 2_H \sigma_t)]$,

where $\boldsymbol{\sigma}_{t}$ is the total collision cross section interpolated among experimental data.

In the α) case the collision can only be an elastic scattering. If the energy of the neutron is about 14 MeV (ac tually we have chosen 14,1 MeV), the angular distribution is isotropical in the center of mass system, so we obtain directly

$$\mu = \cos \theta_{cm} = 2r - 1$$

and

$$a = \cos \theta_{lab} = \sqrt{(1+\mu)/2} = \sqrt{r}$$

If E > 14,1 MeV the angular distribution is no longer isotropical; we have fitted experimental plots by third degree polynomials (see Tab. I).

E	A _o (E)	A _l (E)	A ₂ (E)	A ₃ (E)
14,1 Me V	-4,297	-0,954	-0,097	52,631
17,9	-16,181	-19,886	-8,263	40,669
27,2	1,854	5,834	-2,848	26,051
28,4	55,637	-71,677	23,140	26,584
42,0	-5,446	2,633	0,833	14,349
90,0	-1,857	7,293	-0,428	3,696

TABLE I

For different energy values linear interpolation has been performed. The solution of the equation

$$r = P(\mu, E) = \frac{\int_{-1}^{\mu} \sum_{i=0}^{3} A_{i}(E) \mu^{i} d\mu}{\int_{-1}^{1} \sum_{i=0}^{3} A_{i}(E) \mu^{i} d\mu}$$

is not obtainable in closed analytic form. Using stored P(E) values, the problem can be solved by the discrete method.

After subdividing the (-1 l) μ interval in twenty parts and storing the P_{λ} (E) values of P(E) in the λ th subin terval, the λ value is chosen so that

 $r - P_{\lambda}(E) < 0$

and

$$\mu = \mu - \frac{P_{\lambda} (E) - r}{P_{\lambda} (E) - P_{\lambda - 1}(E)} (\mu_{\lambda} - \mu_{\lambda - 1})$$

The corresponding final E' value is given by the well known formula

$$E^{*} = \frac{1}{2} (1 + \mu) E$$

In the /3) case we may have different possibilities to choose according to the relative cross sections: elastic scattering, anelastic scattering, neutron capture (np, n α , etc.) and, at last, (n2n) reactions.

The elastic scattering case is quite similar to the preceding one for hydrogen. Now the differential cross section is fitted by 4th degree polynomials (see Tab. II).

TABLE II

E	A _o (E)	A _l (E)	$A_2(E)$	A ₃ (E)	A ₄ (E)
2,7 MeV	-0,001617	0,013343	0,185252	0,007061	0,063653
2,9	-0,209439	0,018976	0,620151	-0,000051	0,055464
3,08	0,223674	-0,010341	0,079080	0,002285	0,044661
4,1	0,571758	0,012545	0,030750	-0,088435	0,071290
5,6	0,146753	0,094525	0,039530	-0,070347	0,053255
7,0	0,068707	0,062369	-0,020586	0,010463	0,040522
14,0	0,655096	0,327870	-0,305728	-0,087674	0,037752
17,0	0,658317	0,583652	-0,269552	-0,200163	0,029079
95,0	216,791029	-731,011545	922,583130	-516,435920	108,174163

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and $E^{*} = E (0,857 + 0,142 \mu)$.

The anelastic scattering is more complicated because experimental data are not available in all cases.

To simplify the calculation discrete energy values have been considered only as far as they are experimentally known (< 23 MeV); after continuous level density has been taken.

In both cases isotropical angular distributions have been assumed, and energy distributions have been calculated according to the statistical model.

In the discrete case, the energy levels have been stored and the scattering level ε_j has been chosen using the probability function $\mathcal{G}(E_j^*)$ for the energy of the scattered neutrons.

The E^{*}_j value has been obtained by the cinematic formula E^{*}_i = E $\left[0,857 - (12/13) (\epsilon_i/E) + 0,142 \mu \sqrt{1-(13/12) (\epsilon_i/E)}\right]$

and $G(E_1^2)$ by the well known statistical formula:

(1)
$$\overline{\sigma(e'_{j})} = \frac{E'_{j} \delta_{c}(e'_{j}) e^{2\sqrt{a(e-e_{j})}}}{\sum_{j=1}^{T_{max}} E'_{j} \delta_{c}(e'_{j}) e^{2\sqrt{a(e-e_{j})}}}$$

has been used with experimental & values (total cross section for all the anelastic processes); a has been calculated by extrapolation from the experimental level density above 23 MeV in C¹², E_{max} is the energy corresponding to the highest level we can excite by the given neutron energy.

In the continuous case Maxwellian distribution has been found to be more convenient

$$P(X) = (X/X_{max}) \exp\left[1 - (X/X_{max})\right];$$
 where $X = E^{*} - \beta$

It can be shown indeed that the $\sigma(E)$ value obtained from (1) using the σ_c expression given by the continuum theory (ref. n° 2)

$$\sigma_{c} = \pi R^{2} \alpha (1 + (\beta/E))$$
 where $\alpha = 0,76 + 0,22A^{-1/3}$

is only slightly different from our Maxwell distribution provided that the right theoretical \mathbf{x}_{\max} value is taken

$$X_{max} = a^{-1} \left\{ \left[a(E+\beta) + 0, 25 \right]^{\frac{1}{2}} - 0, 5 \right\}$$

The values X < 11 X_{max} have been rejected as less than 10^{-4} of the total particles are emitted in this energy range.

Quite similar is the calculation in (n 2n) case taking care of the right Q value of this reaction (23 MeV).

So the energy will be $(E-23 + \beta)$ for the first emitted neutron, $(E-23-E_1 + \beta)$ for the second one.

The multiplicity of the neutrons has been stored making use of a weight L, which is never changed except in this routine where L becomes 2L. The pair of outgoing neutrons is considered as a unique neutron, with mean energy (E₁+E₂)/2, counted twice.

Geometrical routine.

After every collision the neutron must be led to the next point of collision. Taking into account the spherical symmetry only two parameters are needed to describe the geometrical path: the distance R from the source and the cosine α of the angle between OR and the new direction.

Knowing the previous a and R values we have

 $R' = R^2 + l^2 + 2Rl\alpha$ where $\alpha = \cos \gamma$ and

 $l = -\lambda \ln r$ is the free path (the mean free path λ is stored as function of the energy). Then

$$\alpha' = \frac{R'^2 + 1^2 - R^2}{2 R' 1}$$

is the α value.

A test is carried out to see if the line of flight cuts the outer boundary of the sphere. If this happens the neutron is classified as escaped.

The second part of this routine is obvious and is concerned with the final direction parameter α of the particle after scattering at an angle of cosine α in the laboratory system.

Final classification.

All the neutrons which do not follow the events considered in the collision routine are classified as captured.

The output data have been given, by a particular routine, in form of a matrix (m n) which catalogues the density $4 \pi R^2 g_1$ of the neutrons that have reached the limit energy E_f in the shell [(R/m)(R/(m+1))] having their own energy contained

between (E/n) and (E/(n+1)). Escaped and captured neutrons are also counted separately (see Tab. III).

E	no	tot.neutrons progr.	escaped neutrons	captured neutrons
8	MeV	665	32	8
14,1	MeV	1251	76	5 O
23	MeV	1314	158	6 3
35	MeV	1829	439	352
50	MeV	2451	750	321

TABLE III

The random number generator program, taken by ref. $n^{\circ}5$, has been checked by generating 10000 random numbers and plotting their frequency for every subinterval in (0 1). This test has been found quite satisfactory. Also the real periodicity of these quasi random numbers has been tested to avoid periodical repetitions.

PART II.

Numerical integration.

The final classification gives the neutrons with a uniform energy spectrum from 0 to E_f . We can now consider every shell as a continuous distribution of point sources with a rectangular energy spectrum. If $\mathcal{G}_2(E)$ is the neutron density due to a monocromatic source of energy between E and E+dE, we can write for small energy intervals

 $9_2(E)dE = (a + bE)dE$

The g_2 value given by our sources is then

$$g_{2}(E_{f}) = \int_{0}^{E_{f}} g_{2}(E)n(E)dE = c \int_{0}^{E_{f}} g_{2}(E)dE$$

By normalizing we have also

$$\int_{0}^{E_{f}} n(E)dE = cE_{f} = 1 \qquad c = 1/E_{f}$$

$$g_{2}(E_{f}) = a + b(E_{f}/2)$$

that is exactly the neutron density due to a monocromatic source of energy

$$E_{f}/2 \simeq 0,75 \text{ MeV}$$
 ($E_{f} = 1,5 \text{ MeV}$).

A source of this kind is $N_a-\gamma$ -Be; its experimental g_2 values for epithermal neutrons have been taken from ref. n°3.

For every E_0 value, the source distribution $4\pi R^2 g_1(R,E_0) = \int (R,E_0)$ is given as output of part. II.

We must now only perform an integral transformation over χ . The final density of the neutrons slowed from E down to the epithermal energy at the distance R' from the source is

$$\mathcal{G}(\mathbf{R}',\mathbf{E}_{0}) = -\frac{1}{2} \int_{0}^{\mathbf{R}_{1}} \chi(\mathbf{R},\mathbf{E}_{0}) d\mathbf{R} \int_{-1}^{1} \mathcal{G}_{2}\left(\sqrt{\mathbf{R}^{2} + \mathbf{R'}^{2} - 2\mathbf{R}\mathbf{R'}\cos\theta}\right) d(\cos\theta)$$

This integration is very difficult to perform with small error because the χ and R₂ functions are given in form of hystograms with few intervals.

We have chosen the Newton's method of four points by an I.B.M. standard program of numerical integration on a computer I.B.M. 650.

The hystograms obtained have been normalized so that their area is equal to the ratio of the number of the neutrons slowed down to 1,5 MeV in paraffin to the total number of neutrons outgoing from the source. The units of length used are (gr/cm^2) (1/M), where M is the molecular weight of the paraffin.

The integration gives a widening of χ (R,E_o) owing to the slowing of the neutrons down to the epithermal energy, so that we find a density of neutrons \neq 0 also at distances larger than the radius of the paraffin sphere (dashed line in the hystogram).

We have compared our theoretical distribution at 14,1 MeV with an experimental one in H_2O (ref. n°4), using the same normalization.

The best location of the BF₃ counters in the sphere is obtainable by setting a counter at the distance R == 0,80 (gr/cm²) (1/M) and eleven others at R = 2,94 (gr/cm²) (1/M).

We can estimate the efficiency of this structure subdividing every counter in ten parts, calculating for each part the contribution to the total efficiency and adding up all of them.

The curve in figure gives the relative variation of the efficiency with E_0 in arbitrary units. No account has been taken of albedo. The calculation has been performed for BF₃

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counters (ϕ 5 cm; h 4 o cm).

The crossed points show the efficiency of our counters at E \simeq 0,9 MeV (N_a- γ -Be) and E = 6 MeV (Ra- α -Be) calculated from the experimental curves normalized at 1, assuming that at these energies there are neither escaped nor captured neutrons. The absolute value of efficiency is about (1/100) of the one in figure.

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