Monte Carlo Calculation of Neutrons Transmitted through Matter

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By

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Abstract

The neutron Monte Carlo code, CYGNUS, which is written in Fortran IV has been shown. This code can easily be used for several limitted geometries and requires considerably less computing time than O5R. In this paper, two methods of calculation are described: one by weight method and the other by collision density method, and the two techniques for determination of the anisotropic scattering angle in the center-of-mass system, i.e., Legendre expansion and Coveyou technique, and the method for determination of the excited level in the inelastic scattering are also described.

The results calculated with CYGNUS code are compared with the numerical solution by PALLAS code for the scaler flux in water and graphite spheres, and with experimental spectra for the angular neutron flux in water and iron shields. The agreement obtained between the CYGNUS calculations and numerical or experimental results is good.

1. Introduction

In the field of the neutron shielding, there is only one useful Monte Carlo code, O5R[1], in Japan. But the general purpose neutron transport code O5R is very complicated and time-consuming in practice because of a wide variety of neutron problems. So we hav made a neutron Monte Carlo code which can easily be used for particular problems. The construction of the code started from the Monte Carlo code by Dominic J. Raso[2], and some very important improvement was made: the introduction of a statistical weight, the use of expected values, the determination of the elastic scattering angle by Coveyou technique[1] and determination of the excited level in inelastic scattering, etc.

The two computer programs, one by weight method[1] and the other by collision density method[3),4] for a homogeneous medium are described in this paper. The

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calculation with these codes have been performed for several geometries and the obtained results are compared with other calculated and experimental ones.

2. Method of the Monte Carlo Calculation

The Monte Carlo calculation was used to estimate the energy-angular neutron flux on any position in a medium or on its boundary surface both by weight method and collision density method, and the flux at detector locations or field points by collision density method.

(1) Weight Method

Let $\Phi(E_l, \theta_m)$ denote the differential energy spectrum of neutrons that cross the spherical surface at $R=R'$ from both sides with energy in the l-th interval and direction in the m-th interval. This quantity is obtained by

$$\Phi(E_l, \theta_m) = \frac{1}{J}\sum_{j=1}^{J}\sum_{k=0}^{Lj} B_k(j) W_k(j) f_k^{lm}(j), \tag{1}$$

where j is the history number and k the scattering number. The factor $B_k\ (j)$ takes into account the boundary conditions, it is placed equal to unity when a neutron crosses the spherical surface at $R=R'$ from both sides and zero otherwise. The factor $W_k\ (j)$ is the probability that the neutron has not been absorbed in the j-th history prior to reaching the state immediately after its k-th scattering and given by

$$W_k(j) = \prod_{n=0}^{k-1} P_n(j), \qquad W_0(j) = 1, \tag{2}$$

where

$$P_n(j) = \frac{\sum_t\{E_n(j)\} - \sum_a\{E_n(j)\}}{\sum_t\{E_n(j)\}} . \tag{3}$$

$\sum_t$ and $\sum_a$ are macroscopic total and absorption cross sections, respectively and $E_n(j)$ is the energy of the neutron after its n-th scattering in the j-th history. $f_k^{lm}(j)$ is the energy-angle classification factor. It is equal to unity when $E_k\ (j)$ is in the l-th energy interval and cos $\theta_k(j)$ in the m-th angular interval, and zero otherwise.

The main program of this code (CYGNUS-W) is described in the form of a flow diagram shown in Fig. 1.

(2) Collision Density Method

a) Calculation of the Neutron Spectrum on the Surface of the Medium

The differential energy spectrum, $\Phi(E_l, \theta_m)$, is obtained by summations over the

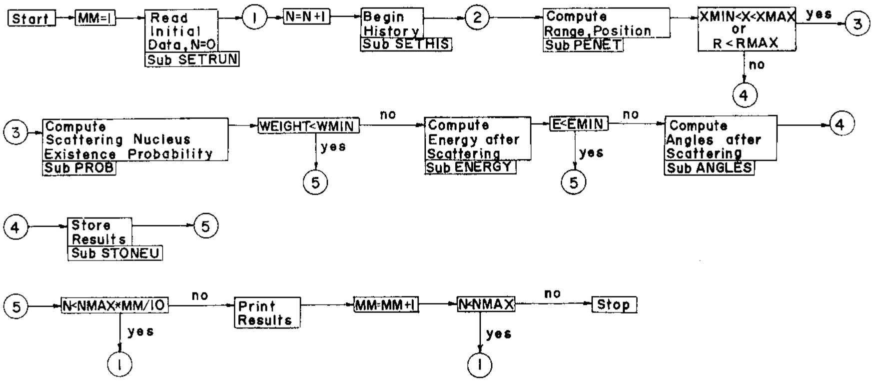

Fig. 1. Flow diagram of CYGNUS-W code.

sample collision density from each scattering point in the medium as follows;

$$\Phi(E_l, \theta_m) = \frac{1}{J}\sum_{j=1}^{J}\sum_{k=0}^{Lj} B_k'(j)P_k(j)Q_k(j)f_k^{lm}(j). \tag{4}$$

The factor denoting the boundary conditions, $B_k'(j)$, is unity when the neutron is in the medium and zero otherwise. The factor

$$P_k(j) = \prod_{n=0}^{k-1} \exp\left[-\Sigma_a\{E_n(j)\}\cdot l_{n+1}(j)\right], \tag{5}$$

is the probability that the neutron has not been absorbed in the j-th history prior to the state immediately after its k-th scattering, where $l_{n+1}(j)$ is the free path from the n-th scattering point to the $(n+1)$-th scattering point in the j-th history. The quantity $Q_k(j)$ denotes the probability that a neutron will reach the boundary surface without further collision from the k-th scattering point in the j-th history,

$$Q_k(j) = \exp\left[-\Sigma_t\{E_k(j)\}\cdot t_k(j)\right], \tag{6}$$

where $t_k(j)$ is the distance from the k-th scattering point to the boundary measured along the flight path after the k-th collision.

This calculation is performed to compare it with that by weight Monte Carlo method. For simplicity, the suffix, j, is omitted hereafter.

b) Calculation of the Neutron Spectrum at the Detector Position

The neutron spectra at the detector positions or field points, are calculated from summation of the product of the statistical weight of the neutron times its probability of reaching the detector from each collision point[3]. The differential energy spectrum,

$\Phi(E_l, \theta_m)$, is obtained from Eq. (4). But in this case the quantity Q_k is given by the following equations, not by Eq. (6). In the case of elastic scattering,

$$Q_k = \frac{1}{2\pi r_k^2} \sum_{l=0}^{L} \frac{2l+1}{2} f_l(E_{k-1}) P_l(\mu_k) \frac{(1+2A_i\mu_k+A_i^2)^{3/2}}{A_i^2(A_i+\mu_k)} \times \exp\{-\Sigma_t(\varepsilon_k)\cdot t_k\}, \tag{7}$$

and in the case of inelastic scattering,

$$Q_k = \frac{1}{4\pi r_k^2} \cdot \frac{(1+2A_i\mu_k+A_i^2)^{3/2}}{A_i^2(A_i+\mu_k)} \exp\{-\Sigma_t(\varepsilon_k)\cdot t_k\}, \tag{8}$$

where

r_k = the distance from the k-th collision site to the detector,

f_l = the Legendre expansion coefficient,

P_l = the Legendre polynomial,

A_i = the ratio of the mass of scatterer to the mass of the neutron,

μ_k = the cosine of the scattering angle in the center-of-mass system,

t_k = the path length in the medium from the k-th scattering point to the detector,

E_{k-1} = the neutron energy before the k-th collision,

ε_k = the neutron energy scattered toward the detector after the k-th collision, which is given by the following equation,

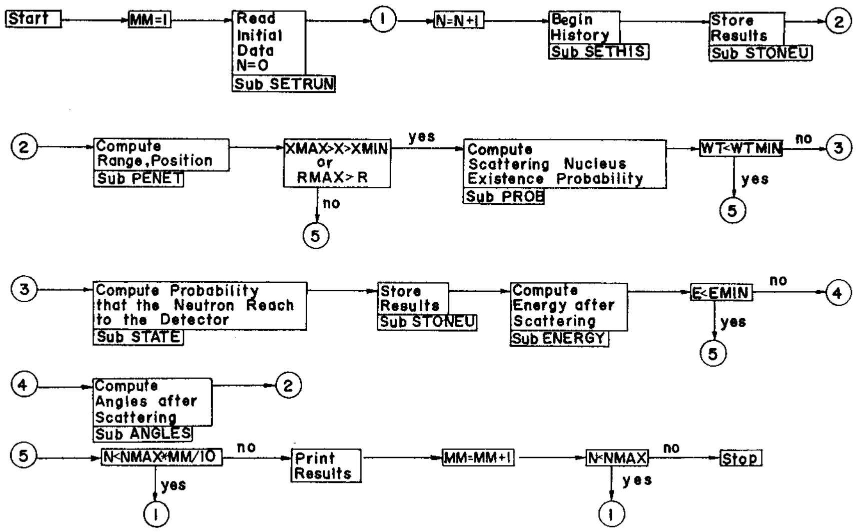

Fig. 2. Flow diagram of CYGNUS-C code.

$$\varepsilon_k = E_{k-1}\cdot\left\{1-\frac{2A_i}{(A_i+1)^2}\cdot(1-\mu_k)\right\}. \tag{9}$$

The main program of the collision density Monte Carlo code (CYGNUS-C) is described in the form of a flow diagram shown in Fig. 2.

(3) Methods for Selecting Neutron Scattering Angles from Anisotropic Distribution

The angular distributions of elastically scattered neutrons become anisotropic in the center-of-mass system at neutron energies at slightly above 100 KeV, the degree of anisotropy increasing with neutron energy. For many problems in neutron transport at such energies a satisfactory solution is obtained by considering only an approximate anisotropy.

When the Monte Carlo method is used to solve neutron transport problems, angular distributions can be included to as high a degree of accuracy as desired; however, in general the higher the degree of accuracy demanded the more costly the solution, since the selection of a scattering angles becomes an elaborate procedure and requires a large amount of computer time.

In the present work, two methods were adopted for selecting neutron scattering angles: one is the Legendre expansion method and the other the Coveyou technique. The Coveyou technique gives the same accuracy as that obtained by the Legendre expansion but requires considerably less computer time.

a) The Legendre Expansion Method[2)]

In this method, the microscopic differential elastic scattering cross section, $\sigma_{el}^{i}(E_k, \mu)$, can be expanded to the Legendre series, in the terms of the cosine of the scattering angle in the center-of-mass system, μ.

$$\sigma_{el}^{i}(E_k, \mu) = \sum_{l=0}^{n}\frac{2l+1}{2}f_l(E_k)\cdot P_l(\mu), \tag{10}$$

where

$$f_l(E_k) = \int_{-1}^{1}\sigma_{el}^{i}(E_k, \mu)P_l(\mu)d\mu. \tag{11}$$

For selecting μ, we should have a formula for the function

$$\sigma_{el}^{*}(E_k, \mu) = \sigma_{el}^{i}(E_k, \mu)/\{\max\ \sigma_{el}^{i}(E_k, \mu)\ \text{on}\ -1\leq\mu\leq 1\}, \tag{12}$$

and use the routine which is familiar as a von Neumann device.

b) The Coveyou Technique[1)]

Consider a distribution function $C(\mu)$ given by

$$C(\mu)=\sum_{k=0}^{n}\phi_k\delta(\mu-\theta_k). \tag{13}$$

Expanding the δ-function gives

$$C(\mu)=\sum_{k=0}^{n}\phi_k\left\{\sum_{l=0}^{\infty}\frac{2l+1}{2}P_l(\theta_k)P_l(\mu)\right\}$$

$$=\sum_{l=0}^{n}\frac{2l+1}{2}\left\{\sum_{k=0}^{n}\phi_k P_l(\theta_k)\right\}\cdot P_l(\mu)+\sum_{l=n+1}^{\infty}\frac{2l+1}{2}\left\{\sum_{k=0}^{n}\phi_k\cdot P_l(\theta_k)\right\}\cdot P_l(\mu). \tag{14}$$

Now if one sets

$$f_l=\sum_{k=0}^{n}\phi_k P_l(\theta_k), \tag{15}$$

Eq. (14) and Eq. (10) are identical; hence they are useful to the same degree as when Eq. (14) is truncated at n.

Let the $n+1$ values of θ_k be the roots of $P_{n+1}(\mu)$; i.e.,

$$P_{n+1}(\theta_k)=0\ . \tag{16}$$

So ϕ_j is given by

$$\phi_j=\frac{\sum_{l=0}^{n}\frac{2l+1}{2}f_l P_l(\theta_j)}{\sum_{l=0}^{n}\frac{2l+1}{2}[P_l(\theta_j)]^2}. \tag{17}$$

Note that if $C(\mu)$ is normalized, then

$$\int_{-1}^{1}C(\mu)d\mu=1=\sum_{k=0}^{n}\phi_k. \tag{18}$$

A value of μ is selected from one of the θ_j's by choosing a random number, r, and letting $\mu=\theta_j$ if

$$\sum_{k=0}^{j-1}\phi_k<r\leq\sum_{k=0}^{j}\phi_k. \tag{19}$$

The results calculated with the Legendre expansion and the Coveyou technique

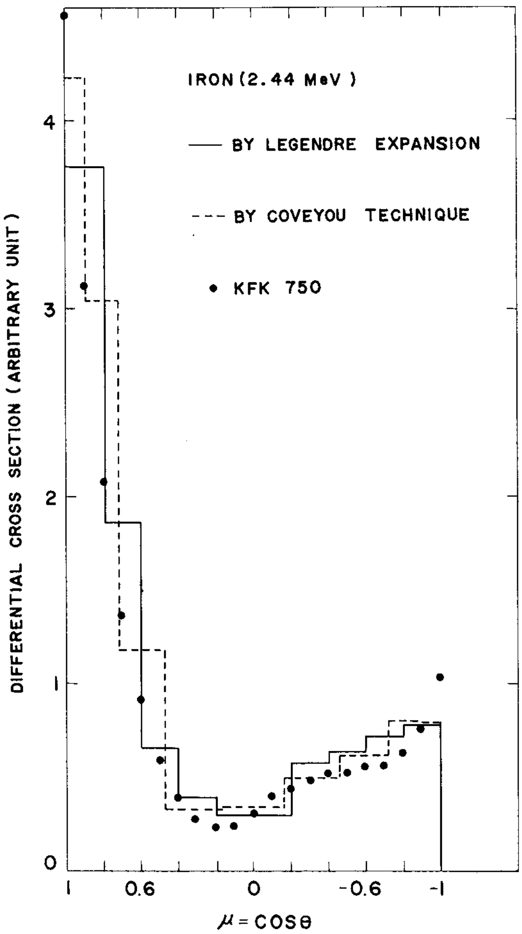

Fig. 3. Angular distribution of elastic scattering. The solid line is the result calculated by the Legendre expansion and the calculation of 1000 histories required 8.5 seconds. The dotted line is that by the Coveyou technique and the calculation of 1000 histories required 3.9 seconds. The points show the differential cross section data from KFK 750[5].

are compared with the reference data[5] of angular distribution of elastic scattering in Fig. 3. From Fig. 3, it is recognized that both results are in good agreement with the reference data and that the Coveyou technique requires considerably less computing time than the Legendre expansion method.

(4) Determination of the Excited Level in Inelastic Scattering

The excited level of the i-th nuclide after inelastic scattering with neutron, e, is determined from the probability density function for inelastic scattering at the k-th scattering, $P_{inel}{}^{i}(E_{k-1}, E_e)$, given by

$$P_{inel}{}^{i}(E_{k-1},\ E_e) = \frac{\sigma_{inel}{}^{i}(E_{k-1},\ E_e)}{\sum_{e=1}^{n} \sigma_{inel}{}^{i}(E_{k-1},\ E_e)}, \tag{20}$$

where

n = the total number of excited level for the neutron of energy E_{k-1},
E_{k-1} = the energy of the neutron immediately after the $(k-1)$-th scattering,
E_e = the e-th excitation energy for the i-th nuclide,
$\sigma_{inel}{}^{i}(E_{k-1},\ E_e)$ = the microscopic inelastic scattering cross section exciting the i-th nuclide into the e-th excited level.

If the following inequality

$$\sum_{m=1}^{e-1} P_{inel}{}^{i}(E_{k-1},\ E_m) < r \leq \sum_{m=1}^{e} P_{inel}{}^{i}(E_{k-1},\ E_m), \tag{21}$$

is satisfied, where r is the random number, then the excitation energy is equal to E_e.

3. Results and Discussion

In order to examine the accuracy of CYGNUS described in the previous section, several calculations have been performed and compared with other results.

(1) Comparison between CYGNUS-W and CYGNUS-C Calculation

The neutron flux transmitted through the boundary face was calculated with Eq. (1) or with Eq. (4), according as weight or collision density method to compare these two methods. For this purpose, the case was selected where a 2.9-MeV point isotropic source was placed 32.2 cm away from the surface of the infinite plane wall of 4.5-cm-thick iron. The angular spectrum of the neutrons transmitted through iron was calculated by two methods and the results obtained are shown in Fig. 4.

This figure shows that the agreement between the results obtained by two methods is very good for all cases. Therefore the calculation of the neutron flux on any spherical surface in the medium or on the boundary was mainly carried out by use of CYGNUS-W.

(2) Comparison with Other Calculations

The Monte Carlo results were compared with those obtained by PALLAS code[6] which is the numerical integration code of the transport equation, in the following two cases.

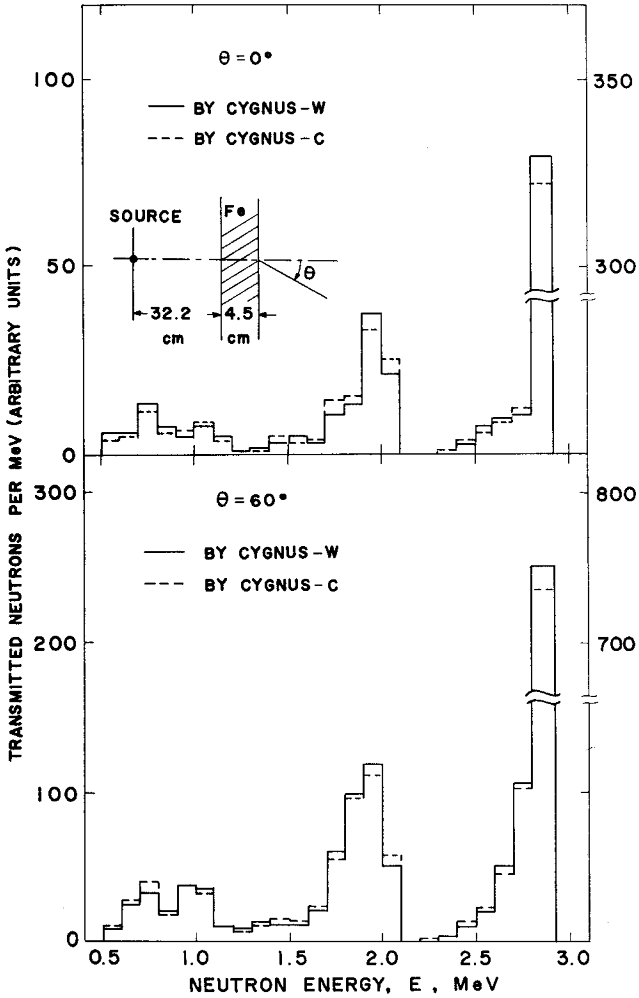

Fig. 4. Comparison between CYGNUS-W- and CUGNUS-C-calculated spectra transmitted through iron slab.

a) The neutron spectra on several spherical surfaces in a water sphere (radius of 35 cm) are shown in Fig. 5 with those by PALLAS code. The 6-MeV point isotropic source is placed at the center of the sphere. The values of cross sections of oxygen and hydrogen are adopted from KFK 750[5] and ENDF/B[7] for CYGNUS-W and PALLAS codes, respectively.

These figures show that the agreement between the two codes is valid for all cases. It is considered that the difference at about 5 MeV is due to the overestimate in PALLAS calculation[8] and the small difference in other energy region, to the differences between

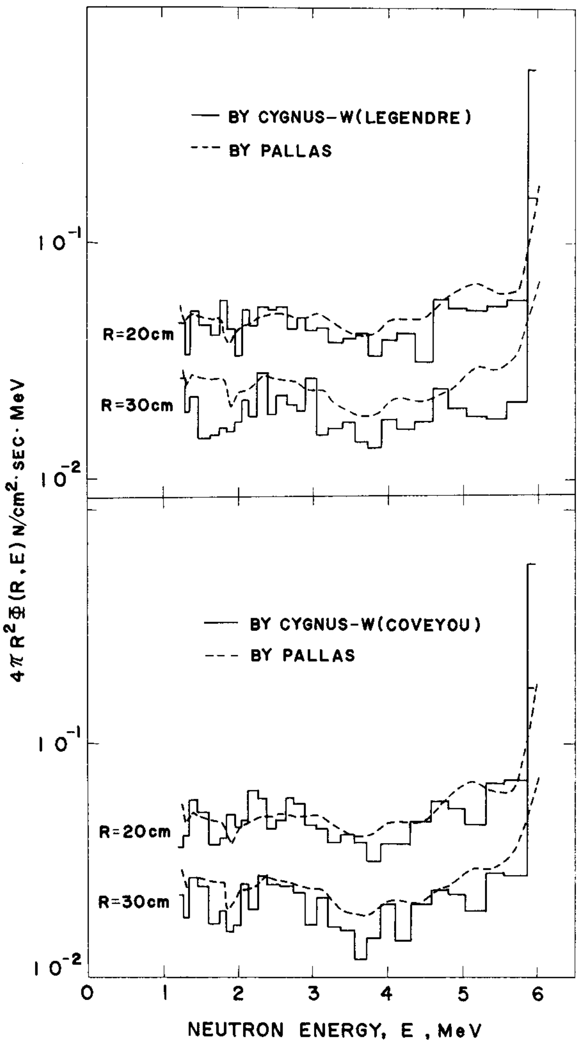

Fig. 5. Comparison between CYGNUS-W- and PALLAS-calculated spectra in water sphere. The spectra have been normalized for one incident neutron.

the cross sections adopted. The times required for CYGNUS-W calculation with Legendre expansion and with Coveyou technique were 106 seconds and 85 seconds for 10000 histories, respectively.

b) The neutron spectra on several spherical surfaces in a graphite sphere (radius of 50 cm) are shown in Fig. 6 with those by PALLAS code. The point isotropic fission source is placed at the center of the sphere. The values of cross sections of

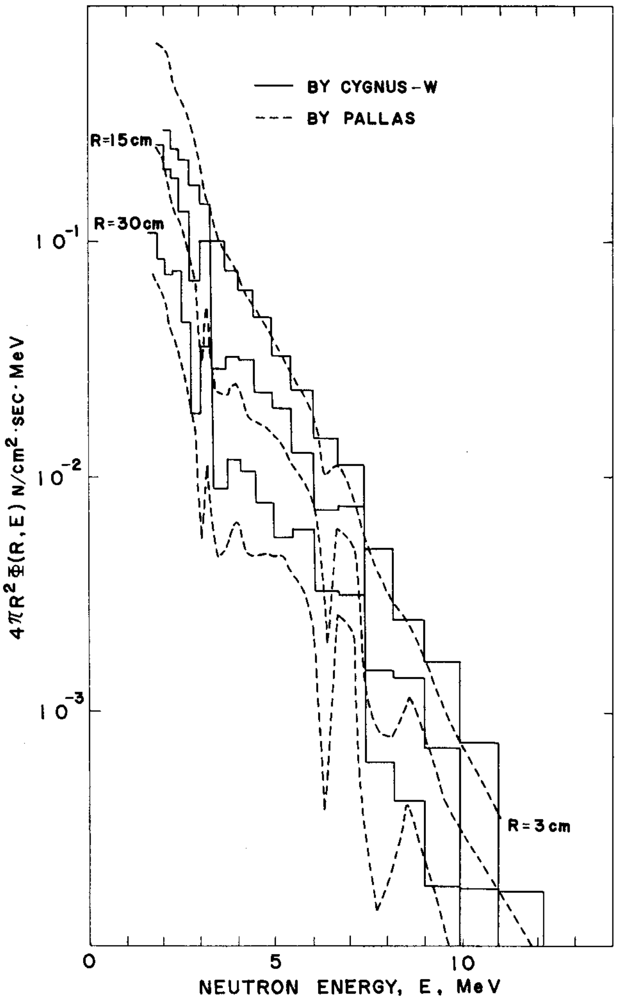

Fig. 6. Comparison between CYGNUS-W- and PALLAS-calculated spectra in graphite sphere. The spectra have been normalized for incident neutron.

graphite were adopted from KFK 750 and ENDF/B for CYGNUS-W and PALLAS codes, respectively.

From these figures it is shown that the agreement between the two codes is very good for the neutron spectrum at 3 cm in radius except for the energy region below 3 MeV. At other radii, the results by CYGNUS-W are a little larger than those by PALLAS for the high energy region, but the shapes of these spectra resemble each other. These differences are considered to be due to the difference between two cross sections and the insufficiency of histories in CYGNUS-W calculation. The time required for CYGNUS-W calculation was about 4 min. for 10000 histories.

(3) Comparison with Experiment

a) The neutron angular spectra transmitted through the plane wall of water (20 and 40 cm in thickness) are shown in Fig. 7 with the experimental results by V. V. Verbinski et al.[9] The experiment was carried out by the use of a small lead target

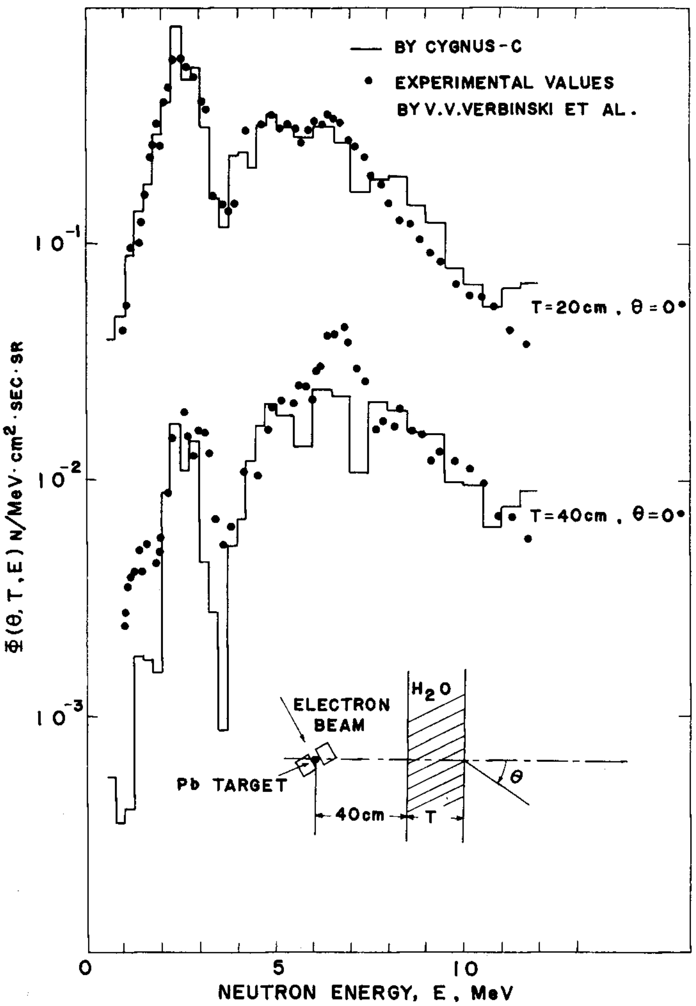

Fig. 7. Comparison between CYGNUS-C-calculated and measured spectra[9] transmitted through water slab. The CYGNUS-C-calculated spectra have been normalized to a single point at 5 MeV on the measured 20 cm spectrum.

(5 cm diam. by 2 cm thick) irradiated with short bursts of electrons from the linear accelerator, and the neutron spectrum was measured with a 5-in.-diam by 5-in.-long encapsulated NE-213 liquid scintillation detector after passing down a 50 cm flight path.

The CYGNUS-C calculation was carried out with Eqs. (4) and (6) under the assumption that a narrow photoneutron beam is incident normally to the water wall. The agreement between the experimental and calculated results is very good for the 20-cm-thick wall. It is considered that a small difference in 40-cm-thick wall is due to the insufficiency of histories in CYGNUS-C calculation. The time required for the calculation with Legendre expansion method was about 5 min. for 20000 histories.

b) The neutron spectrum transmitted through the plane wall of iron (10 cm in thickness) is shown in Fig. 8 with the experimental results by G. During et al.[10] The experiment was carried out by the use of a target situated 20 cm away from the surface

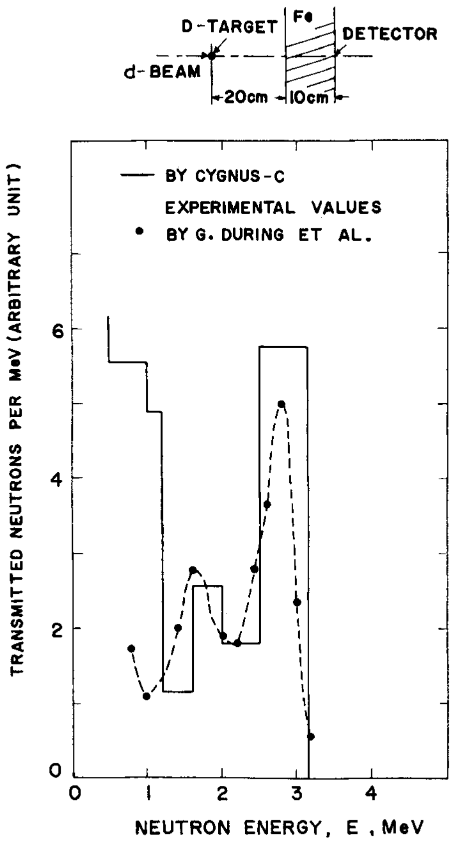

Fig. 8. Comparison between CYGNUS-C- calculated and measured spectrum[10] transmitted through iron slab. The spectrum has not been normalized.

of the wall (size of 70×70 cm), irradiated with a beam of 230-KeV deuterons, and the neutron spectrum was measured with the stilben and BEB detectors situated behind the wall on the beam axis.

CYGNUS-C calculation was carried out with Eqs. (4) and (7) or (8) under the assumption that a 3-MeV point isotropic source is placed 20 cm away from the surface of the infinite wall and the detector is situated at the same position as in their experiment. This figure reveals that the agreement between the two is very good for neutron energy above 1 MeV. The time required for the calculation was about 5 min. for 9000 histories.

4. Summary

It is concluded that CYGNUS-W and CYGNUS-C have high accuracy for the calculation of neutron transmission from the various comparisons described above. They may be used for various geometries by a little change on boundary conditions and have the advantage that they can more easily be treated with and require considerably less calculating time than O5R does.

Acknowledgments

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