

THERMAL NEUTRON SCATTERING SIMULATION USING FREE GAS MODEL AND SHORT COLLISION TIME APPROXIMATION

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ABSTRACT

The paper is concerned with the research effort to develop the idea underlying the technique which enables the information from Evaluated Nuclear Data Files in Monte Carlo calculations to be used directly without processing. The technique is realized in terms of BRAND code system. The algorithms of thermal neutron scattering simulation using free gas model and short collision time approximation are described. These algorithms are based on the substitution of variables proposed by Eriksson for free gas model. The algorithm proposed by Eriksson was modified. In the algorithm proposed by Eriksson it is suggested that the scattering cross sections and some subsidiary functions should be tabulated. But in BRAND's algorithm no tabulation is used. The algorithms described are compared with MCNP and MCU. The analytical formulas for the full scattering cross section calculation using free gas model and short collision time approximation are given. The examples of the calculation tasks on the spectrum of secondary neutrons scattered on the oxygen using free gas model and short collision time approximation are given. The results are in good agreement with numerically calculated spectrum results. The examples of the calculation tasks on energy spectrum calculation of the neutrons that penetrate the oxygen barrier and albedo neutron spectrum calculation are given. There are some disagreements between BRAND and MCNP results particularly in solving neutron penetration problem. It was assumed that these disagreements are possibly due to the fact that in BRAND code the calculations are made in strict accordance with standard algorithms ENDF-6, while NJOY and MCNP algorithms seem to be corrected for a better agreement with benchmarks.

Key Words: thermal neutrons, ENDF-6 format, free gas model, short collision time approximation

1 INTRODUCTION

The state-of-the-art of nuclear power engineering involves a number of urgent problems, such as: the improvement of safety, assurance of reliability, as well as the solution of ecological problems. The improved accuracy of calculations concerning neutronics characteristics of nuclear power plants is a most contributive factor to solving the problems concerned. Optimum solution of the problems due to ionizing radiation transport problem is impossible without detailed knowledge of differential properties characteristic of radiation fields caused by these radiations. The desired accuracy necessary for solving the transport equation is possible, as a rule, only when the real three-dimensional descriptive geometry of the object in question is

available, once the detailed information on the interaction between radiation and substance is taken account of; this is most accurately achieved through Monte Carlo approximation. The requirements to improve the accuracy of calculations performed make it necessary to use the most recent information, which, as a rule, is available in Evaluated Nuclear Data Files. Therefore the development of Monte Carlo programs adapted for using evaluated data libraries is urgent and currently of practical importance.

It is known that in the course of Monte Carlo calculations, the information taken from the Evaluated Nuclear Data Files is not used directly; it is used after preliminary processing. It is evident that the idea of processing itself has both advantages and disadvantages. The most evident disadvantage of data processing is that the processing itself involves an additional unevaluated error in the results calculated because it is impossible to distinguish between the error due to processing and that of the calculated results. The fact is that the data obtained in using processing programs do not contain additional inaccuracy; nevertheless, when such data are used, the methods to reduce the accuracy of calculations performed such as interpolation methods have to be applied. Therefore the full or partial integration of data processing into Monte Carlo program calculation process is of particular interest. The Monte Carlo code BRAND [1] has been under joint developed for more than twenty years in State Scientific Center of Russian Federation Institute of Physics and Power Engineering named after A.I. Leipunsky and Obninsk State Technical University of Nuclear Power Engineering. This code is designed for solving the problem of ionizing radiation transport as accurately as possible. The constant unit of BRAND code currently developed is a unique one with no analogs available in the world and in this sense is a real innovation in itself.

2 SCATTERING ON FREE GAS MODEL AND SHORT COLLISION TIME APPROXIMATION

Information on thermal neutron scattering is contained in file 7 of ENDF-6 format [2]. Incoherent inelastic scattering of thermal neutrons is represented as

$$\frac{d^2\sigma}{d\Omega dE'}(E \rightarrow E', \mu, T) = \sum_{n=0}^{NS} \frac{M_n \sigma_{bn}}{4\pi kT} \sqrt{\frac{E'}{E}} e^{-\beta/2} S_n(\alpha, \beta, T), \quad (1)$$

where β is energy transfer, $\beta = \frac{E'-E}{kT}$, α is momentum transfer, $\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{A_0 kT}$, the rest of

the terms used here are commonly used terms. Therefore they do not require a detailed description. The $S_n(\alpha, \beta, T)$ function may be presented in a table including various interpolation laws or analytically using free gas model or short collision time approximation. For example, in the case of H₂O the scattering law for hydrogen is presented in the table and the scattering law for oxygen is presented by the analytic function using free gas model, in the case of BeO the scattering law for beryllium is presented in the table and the scattering law for oxygen is presented by the analytic function using short collision time approximation. The algorithms for the tabulated case realized in BRAND and their verification were presented in [3]. In this paper the algorithms for free gas model and short collision time approximation are considered.

$S_n(\alpha, \beta, T)$ for free gas model is equal to

$$S(\alpha, \beta, T) = \frac{1}{\sqrt{4\pi\alpha}} e^{-\frac{\alpha^2 + \beta^2}{4\alpha}}. \quad (2)$$

This scattering law in paper [4] is presented in other terms:

$$\sigma(\mu, Z)d\mu dZ = \sigma_{fr} [1 + 1/A]^2 \pi^{-0.5} \chi^* \Phi(\mu, Z) \exp\{-[h(\mu, Z)\chi^*]^2\} d\mu dZ, \quad (3)$$

where $Z=v'/v$, v is the neutron velocity before scattering, v' is the neutron velocity after scattering, σ_{fr} is free atom scattering cross section, $\chi^*=v(A/(2kT))^{0.5}$, $\Phi(\mu, Z)=Z^2(1-2Z\mu+Z^2)^{-0.5}$, $\lambda=m/A$, m is a neutron mass,

$$h(\mu, Z) = \frac{Z^2(1+\lambda) - 2\lambda Z\mu - (1-\lambda)}{2(1-2Z\mu+Z^2)^{0.5}}. \quad (4)$$

Region $R(\mu, Z)$ of the possible values of (μ, Z) is:

$$-1 \leq \mu \leq 1, \quad 0 \leq Z < \infty. \quad (5)$$

For the short collision time approximation $S_n(\alpha, \beta, T)$ is equal to

$$S^{SCT}(\alpha, \beta, T) = \frac{e^{-\left(\frac{(\alpha-\beta)^2 T}{4\alpha T_{eff}(T)} + \frac{|\beta|}{2}\right)}}{\sqrt{4\pi\alpha \frac{T_{eff}(T)}{T}}}, \quad (6)$$

where $T_{eff}(T)$ is effective temperature.

3 SCATTERING DENSITY FACTORIZATION FOR THE GAS MODEL

The main idea of the paper [4] is the transfer to such new variables p and q

$$\sigma(\mu, Z)d\mu dZ = \sigma[\mu(p, q), Z(p, q)] \frac{\partial(\mu, Z)}{\partial(p, q)} dp dq, \quad (7)$$

that factorize the distribution density $\sigma(p, q)=P(p)Q(q)$ in two one-dimension densities $P(p)$ and $Q(q)$.

Using the substitution

$$p=(1-2Z\mu+Z^2)^{0.5}, \quad q = \chi^* \frac{\lambda(1-2Z\mu+Z^2)-1+Z^2}{2(1-2Z\mu+Z^2)^{0.5}}, \quad (8)$$

which gives the Jacobean

$$\frac{\partial(p, q)}{\partial(Z, \mu)} = \chi^* \frac{Z^2}{p^2} \quad (9)$$

in paper [4] the following equation is derived

$$\sigma(p, q) = \sigma_{fr} [1 + 1/A]^2 \pi^{-0.5} p \cdot \exp(-q^2). \quad (10)$$

The region $R(\mu, Z)$ unambiguously transfers to the region $R(p, q)$:

$$0 \leq p < \infty, \left(\frac{1 + \lambda}{2} p - 1 \right) \chi^* \leq q \leq \left(\frac{1 + \lambda}{2} p + 1 \right) \chi^*. \quad (11)$$

This substitution of variables underlies the algorithm proposed in paper [4] and MCU [5] and BRAND algorithms for scattering simulation using free gas model.

The full scattering cross section of the neutron with energy E is calculated by the formula

$$\sigma_s(E) = \frac{\sigma_{fr}}{\chi^{*2}} \left[\left(\chi^{*2} + \frac{1}{2} \right) \text{erf } \chi^* + \frac{1}{\sqrt{\pi}} \chi^* \exp(-\chi^{*2}) \right]. \quad (12)$$

In paper [4] it is suggested that the scattering cross sections and some subsidiary functions should be tabulated to accelerate (p, q) values simulation. But in MCU and BRAND's algorithm no tabulation is used.

4 BRAND ALGORITHM FOR SCATTERING SIMULATION USING FREE GAS MODEL

Let

$$a = \frac{1 + \lambda}{2} \chi^*, \quad b = \chi^*. \quad (13)$$

The two-dimensional random variable with the density $f(p, q) = p e^{-q^2}$ has to be simulated in the region

$$0 \leq p < \infty, \quad ap - b \leq q \leq ap + b. \quad (14)$$

First, simulate p with the density

$$f(p) = \int_{ap-b}^{ap+b} f(p, q) dq = p[\operatorname{erf}(ap+b) - \operatorname{erf}(ap-b)]. \quad (15)$$

It is evident that $f(p) \leq 2p$ (since $\operatorname{erf} x \leq 1$ for any x). It is known that at $x \geq 5$ the values of $\operatorname{erf} x$ are very close to 1, consequently at $p \geq \frac{b+5}{a}$ the values of $f(p)$ will be very close to zero. Neglecting the values of $f(p)$ at $p \geq \frac{b+5}{a}$ we obtain the following majoring density:

$$\tilde{f}(p) = \begin{cases} 2p & \text{if } p \leq \frac{b+5}{a} \\ 0 & \text{if } p > \frac{b+5}{a} \end{cases}. \quad (16)$$

We simulate the random variable with the density $f(p)$ using rejection technique. Having simulated the value of p we simulate the random variable q in the interval $ap-b \leq q \leq ap+b$ with the density e^{-q^2} , simulating the random variable with normal distribution and rejecting the values of q , if they are beyond the interval bounds. Having simulated p and q we calculate the new neutron energy and the cosine of the angle of scattering.

5 MODIFIED MCU ALGORITHM FOR SCATTERING SIMULATION USING FREE GAS MODEL

Using the p and q definitions and the inequalities that determine the limits of possible values of p and q the following expressions are derived

$$-\chi^* \leq q < \infty, \left(\frac{q}{\chi^*} - 1\right) \frac{2}{1+\lambda} \leq p \leq \left(\frac{q}{\chi^*} + 1\right) \frac{2}{1+\lambda}. \quad (17)$$

Since $0 \leq p$, then $p_{\min} \leq p \leq p_{\max}$, where

$$p_{\min} = \begin{cases} 2(q/\chi^* - 1)/(1+\lambda) & \text{if } q > \chi^* \\ 0 & \text{if } q \leq \chi^* \end{cases}, \quad p_{\max} = \left(\frac{c}{\chi^*} + 1\right) \frac{2}{1+\lambda}. \quad (18)$$

First, simulate q with the distribution

$$f(q) = \int_{p_{\min}}^{p_{\max}} p e^{-q^2} dp = \frac{1}{2} (p_{\max}^2 - p_{\min}^2) e^{-q^2} = \begin{cases} f_1(q) & \text{if } q > \chi^* \\ f_2(q) & \text{if } q \leq \chi^* \end{cases}, \quad (19)$$

where

$$f_1(q) = \frac{8qe^{-q^2}}{\chi^*(1+\lambda)^2}, \quad f_2(q) = 2\left(\frac{q}{\chi^*} + 1\right)^2 \frac{e^{-q^2}}{(1+\lambda)^2}. \quad (20)$$

To do this, we calculate first the probability of $q > \chi^*$ by the formula

$$x = \frac{\int_{\chi^*}^{\infty} f(q) dq}{\int_{-\chi^*}^{\infty} f(q) dq} = \frac{4e^{-\chi^{*2}}}{2e^{-\chi^{*2}} + \left(2\chi^* + \frac{1}{\chi^*}\right)\sqrt{\pi} \operatorname{erf} \chi^*}, \quad (21)$$

then if $\gamma < x$, we simulate q with the density $f_1(q)$ in the interval $\chi^* < q < \infty$, otherwise we simulate q with the density $f_2(q)$ in the interval $-\chi^* \leq q \leq \chi^*$. (γ is a random variable uniformly distributed in the interval $(0,1)$). The density $f_1(q)$ is simulated using the inverse functions method according to the formula of simulation

$$p = \sqrt{\chi^{*2} - \ln \gamma}. \quad (22)$$

The density $f_2(q)$ is simulated using rejection technique from the normal distribution. From the inequality $-\chi^* \leq q \leq \chi^*$ is derived $\left(\frac{q}{\chi^*} + 1\right)^2 \leq 4$ and $f_2(q) \leq \frac{8e^{-q^2}}{(1+\lambda)^2}$.

Having simulated the value of q we calculate p_{\max} , p_{\min} and simulate the value of p using the inverse functions method: $p = \sqrt{\gamma(p_{\max}^2 - p_{\min}^2) + p_{\min}^2}$.

6 MCNP ALGORITHM OF SCATTERING SIMULATION USING FREE GAS MODEL

The algorithm realized in MCNP [6] consists of the following steps. First, the velocity of the nucleus on which the scattering occurred is simulated. Then the elastic scattering is simulated within the frame of reference in which the nucleus is motionless and the velocity of the neutron is recalculated and transferred to the lab system. MCNP uses a set of equiprobable cosines of the angles of scattering for elastic scattering simulation that is prepared beforehand by the processing program (usually NJOY) and is stored in the library. That is MCNP uses processing for free gas scattering simulation.

7 SUBSTITUTION OF VARIABLES FOR THE SHORT COLLISION TIME APPROXIMATION

Substitution of variables proposed by the author of paper [4] gives the following result for the short collision time approximation:

$$f(p, q) = pe^{-(Ap^2 + Bpq + Cq^2)}, \quad (23)$$

where

$$A = \left(\frac{T}{T_{eff}(T)} - I \right) \frac{E}{A_0 kT}, \quad B = 2 \left(I - \frac{T}{T_{eff}(T)} \right) \sqrt{\frac{E}{A_0 kT}}, \quad C = \frac{T}{T_{eff}(T)}, \quad (24)$$

$$I = \begin{cases} 0 & \text{if } p \leq 2, q \leq \frac{p}{2} \sqrt{\frac{E}{A_0 kT}} \\ 1 & \text{else} \end{cases} \quad (25)$$

8 BRAND ALGORITHM FOR SCATTERING SIMULATION USING SHORT COLLISION TIME APPROXIMATION

The two-dimensional random variable with distribution density

$$f(p, q) = pe^{-(Ap^2 + Bpq + Cq^2)} \quad (26)$$

has to be simulated in the region

$$0 \leq p < \infty, \quad ap - b \leq q \leq ap + b. \quad (27)$$

Let

$$c = \frac{1}{2} \sqrt{\frac{E}{A_0 kT}}. \quad (28)$$

Let us decompose the region of p and q simulation into three subregions.

The first subregion:

$$0 \leq p \leq 2, \quad ap - b \leq q \leq cp. \quad (29)$$

The second subregion:

$$0 \leq p \leq 2, \quad cp < q \leq ap + b. \quad (30)$$

The third subregion:

$$2 < p < \infty, \quad ap - b \leq q \leq ap + b. \quad (31)$$

In every subregion the values of A, B and C do not depend on p and q.

The scattering simulation algorithm involves the following steps:

1. Simulation of the subregion for p and q simulation according to the probabilities of hitting in every subregion.
2. Simulation of p in the simulated subregion.
3. Calculation of the interval bounds for the q-simulation, given the value of p for the subregion involved.
4. Simulation of the q with normal distribution in the interval obtained.
5. Calculation of the secondary neutron energy and the cosine of the angle of scattering according to the simulated p and q.

The density for p-simulation is proportional to:

in the first subregion:

$$f_1(p) = \int_{ap-b}^{cp} f(p, q) dq = \frac{1}{2} \sqrt{\frac{\pi}{C}} p \left(\operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}c \right) p \right) - \operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}a \right) p - \sqrt{C}b \right) \right), \quad (32)$$

in the second subregion:

$$\begin{aligned} f_2(p) &= \int_{cp}^{ap+b} f(p, q) dq = \\ &= \frac{1}{2} \sqrt{\frac{\pi}{C}} p e^{\left(\frac{B^2}{4C} - A \right) p^2} \left(\operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}a \right) p + \sqrt{C}b \right) - \operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}c \right) p \right) \right), \end{aligned} \quad (33)$$

in the third subregion:

$$\begin{aligned} f_3(p) &= \int_2^{\infty} f(p, q) dq = \\ &= \frac{1}{2} \sqrt{\frac{\pi}{C}} p e^{\left(\frac{B^2}{4C} - A \right) p^2} \left(\operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}a \right) p + \sqrt{C}b \right) - \operatorname{erf} \left(\left(\frac{B}{2\sqrt{C}} + \sqrt{C}a \right) p - \sqrt{C}b \right) \right). \end{aligned} \quad (34)$$

In every subregion we construct the majoring density similar to the majoring density construction for free gas model.

In the subregion concerned we simulate p using rejection technique. Having simulated p, we simulate q with normal distribution:

$$f(p, q) = p e^{-(Ap^2 + Bpq + Cq^2)} = p e^{\left(\frac{B^2}{4C} - A \right) p^2} e^{-\frac{\left(q + \frac{Bp}{2C} \right)^2}{2 \left(\frac{1}{\sqrt{2C}} \right)^2}}. \quad (35)$$

The probabilities of hitting in every subregion are calculated in the following way. Let $r = \frac{B}{2\sqrt{C}} + \sqrt{C}c$, $s = \frac{B}{2\sqrt{C}} + \sqrt{C}a$, $t = \frac{B^2}{4C} - A$,

$$p_1 = \int_0^2 f_1(p) dp = \frac{1}{2} \sqrt{\frac{\pi}{C}} \left(\frac{8r^2 - 1}{4r^2} \operatorname{erf}(2r) - \frac{e^{-4r^2}}{r\sqrt{\pi}} - \frac{8s^2 - 2C - 1}{4s^2} \operatorname{erf}(2s - \sqrt{C}b) - \frac{4s + \sqrt{C}b}{2s^2\sqrt{\pi}} e^{-(2s - \sqrt{C}b)^2} - \frac{(2C + 1)\operatorname{erf}(\sqrt{C}b)}{4s^2} + \frac{\sqrt{C}be^{-Cb^2}}{2s^2\sqrt{\pi}} \right), \quad (36)$$

$$p_2 = \int_0^2 f_2(p) dp = \frac{1}{4t} \sqrt{\frac{\pi}{C}} \left(e^{4t} (\operatorname{erf}(2s + \sqrt{C}b) - \operatorname{erf}(2r) - \operatorname{erf}(\sqrt{C}b)) - \frac{s}{\sqrt{s^2 - t}} e^{\frac{tCb^2}{s^2 - t}} \left(\operatorname{erf}\left(2\sqrt{s^2 - t} + \frac{s\sqrt{C}b}{\sqrt{s^2 - t}}\right) - \operatorname{erf}\frac{s\sqrt{C}b}{\sqrt{s^2 - t}} \right) + \frac{r}{\sqrt{r^2 - t}} \operatorname{erf}\left(2\sqrt{r^2 - t}\right) \right), \quad (37)$$

$$p_3 = \int_2^\infty f_3(p) dp = \frac{1}{4t} \sqrt{\frac{\pi}{C}} \left(e^{4t} (\operatorname{erf}(2s - \sqrt{C}b) - \operatorname{erf}(2s + \sqrt{C}b)) + \frac{s}{\sqrt{s^2 - t}} e^{\frac{tCb^2}{s^2 - t}} \left(\operatorname{erf}\left(2\sqrt{s^2 - t} + \frac{s\sqrt{C}b}{\sqrt{s^2 - t}}\right) - \operatorname{erf}\left(2\sqrt{s^2 - t} - \frac{s\sqrt{C}b}{\sqrt{s^2 - t}}\right) \right) \right). \quad (38)$$

Then, the probability of hitting in the i^{th} subregion will be equal to $\frac{p_i}{p_1 + p_2 + p_3}$. Full scattering cross section for the short collision time approximation is calculated by the formula $\sigma(E, T) = \sigma_b(p_1 + p_2 + p_3)/4$.

9 CALCULATION RESULTS

The energy spectrum of the secondary neutrons scattered by oxygen for initial energies 5, 3, 2, 1, 10^{-1} , 10^{-2} , 10^{-3} , and 10^{-4} eV at the temperature of the moderator of 300 K has been calculated using BRAND's algorithm for free gas model, modified MCU algorithm and analytically (we calculate the integral $\int_{-1}^1 f(E', \mu) d\mu$ numerically). There is a very good agreement between the numerically calculated spectra and the spectra calculated using BRAND algorithm and modified MCU algorithm for all energies. Therefore in Fig. 1 we present the secondary neutron spectrum only for initial energy 0.1 eV. The energy spectrum of the secondary neutrons scattered on oxygen in beryllium oxygen using short collision time approximation is also calculated. The agreement with numerically calculated spectra is also very good.

The energy spectrum of neutrons which penetrate the infinite flat oxygen plate 25 cm thick with nuclear density equal to the density of O in H₂O and albedo neutron spectrum are calculated. Calculations have been performed using BRAND with BRAND algorithm, BRAND

with modified MCU algorithm and MCNP for initial neutron energies 1, 10^{-1} , 10^{-2} , 10^{-3} , and 10^{-4} eV at moderator temperatures of 1 K and 300 K. The spectrum of neutrons which penetrate the barrier at the initial energy of 1 eV at a moderator temperature of 1 K is presented in Fig. 2. The spectrum of neutrons which penetrate the barrier at initial energy of 1 eV at a moderator temperature of 300 K is presented in Fig. 3, the albedo neutron spectrum is presented in Fig. 4. There are some disagreements between BRAND and MCNP especially for the case of penetration. To account for the cause of such disagreements requires the detailed comparison of BRAND's algorithms and NJOY+MCNP ones. Apparently, such disagreements are possibly due to the fact that BRAND carries out calculations according to the algorithms recommended by ENDF-6 standard whereas NJOY and MCNP algorithms were corrected for better coincidence with experimental benchmarks.

Comparison of the calculation time in using BRAND algorithm with the modified MCU algorithm shows that at neutron energies greater than 1 eV the simulation time in using BRAND algorithm is 1.5 – 2 times less than the simulation time in using MCU one but at initial energies less than 1 eV the modified MCU algorithm is preferable.

10 CONCLUSIONS

The algorithms of direct scattering simulation using free gas model and short collision time approximation are realized in terms of BRAND code system. The calculation results using BRAND, MCU and MCNP are given in the paper. There are some disagreements between BRAND results and MCNP ones. To account for the cause of such disagreements requires the detailed comparison of BRAND's algorithms and NJOY+MCNP ones.

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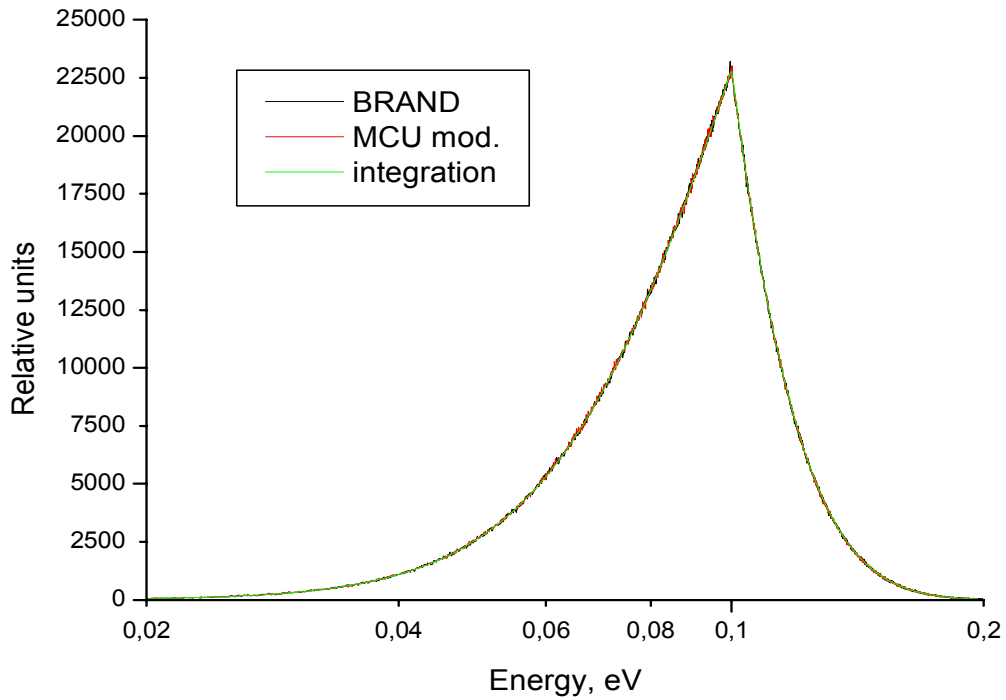


Fig. 1 Secondary neutron spectrum for oxygen for 0.1 eV initial energy

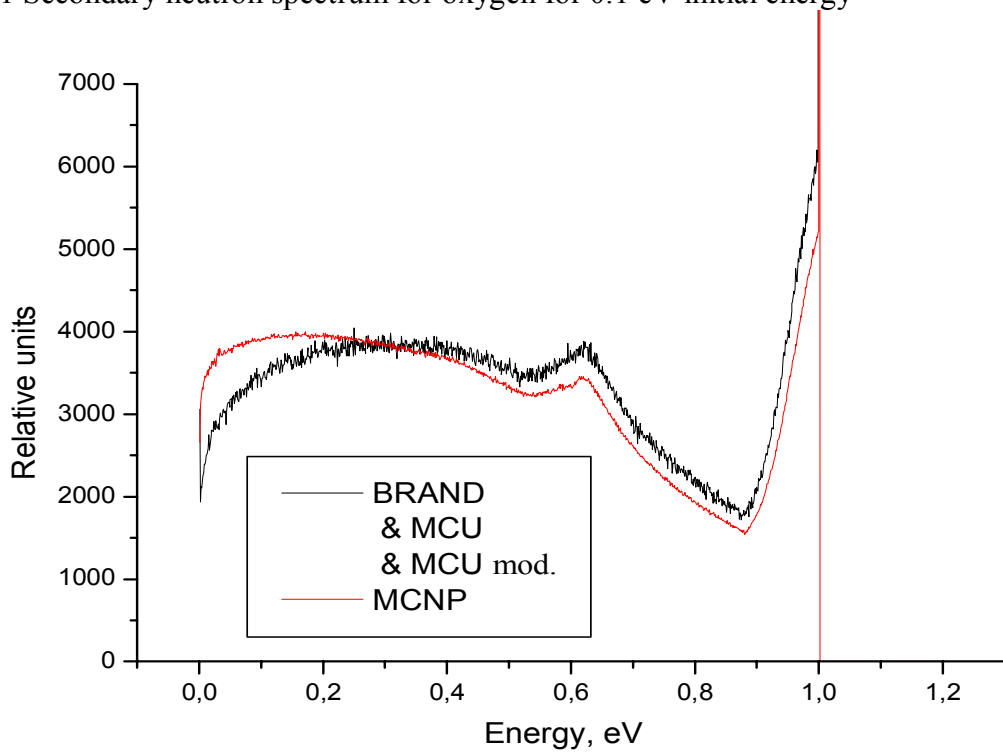


Fig. 2 Spectrum of neutrons that penetrate the barrier at a moderator temperature of 1 K

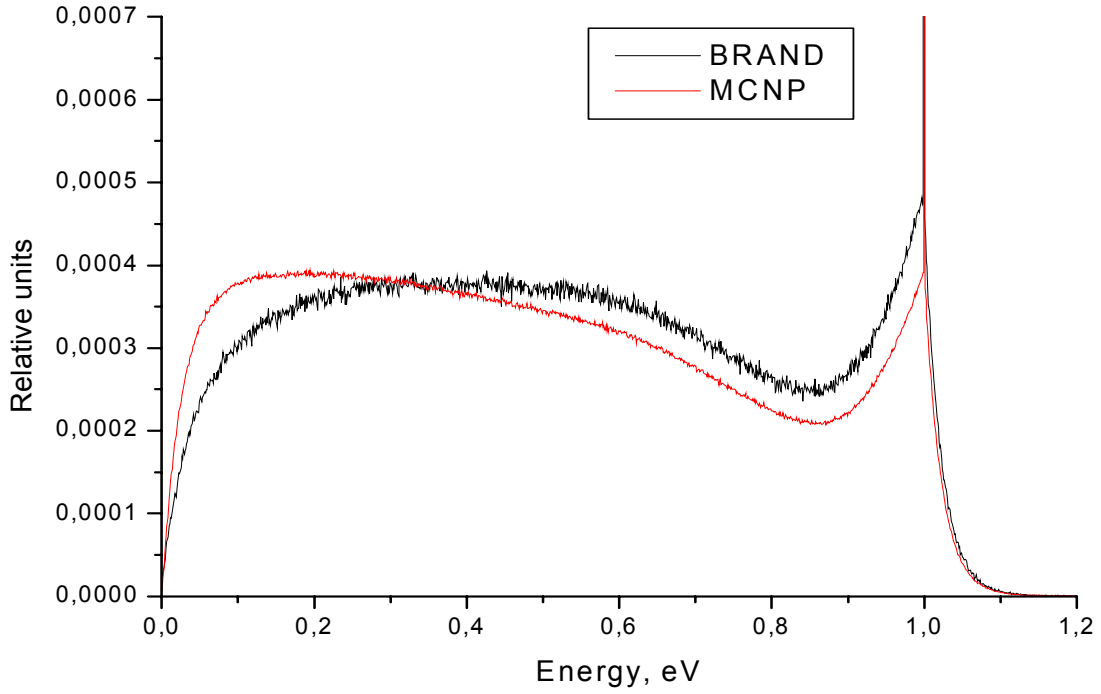


Fig. 3 Spectrum of neutrons that penetrate the barrier at a moderator temperature of 300 K

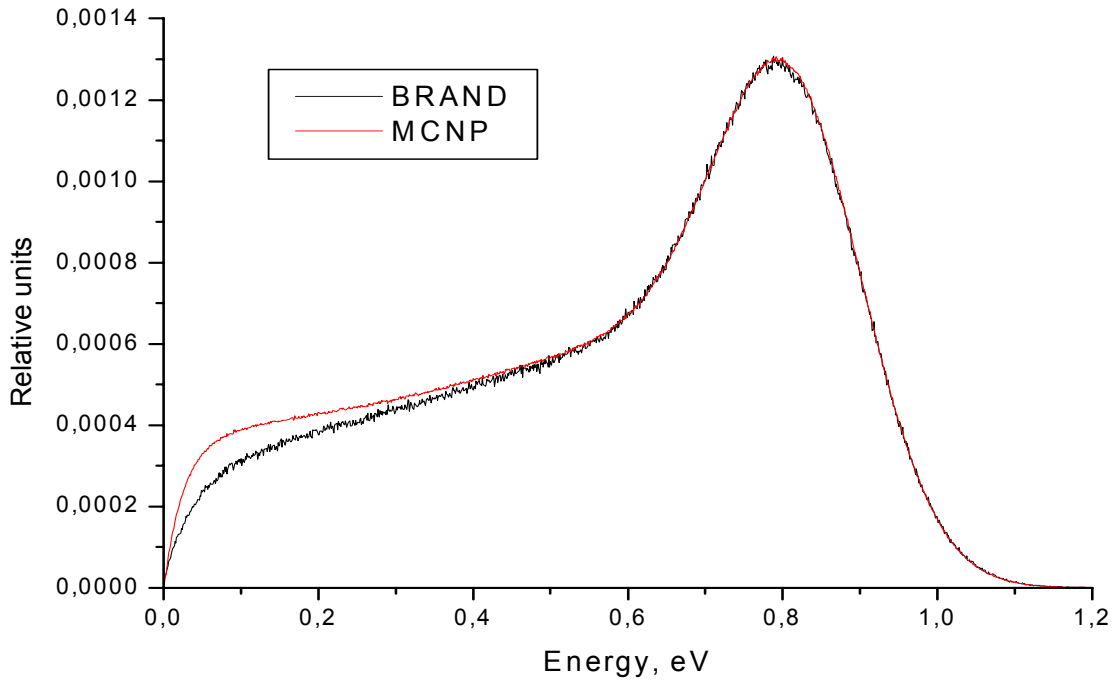


Fig. 4 Albedo neutron spectrum at a moderator temperature of 300 K