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

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1. INTRODUCTION

Efficient solving of many problems concerned with ionizing radiation transport problem is practicable only when based on the detailed knowledge of differential description of radiation fields caused by these radiations. The desired accuracy assurance necessary for solving the transport equation is possible, as a rule, when the real three-dimensional descriptional 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 (for example the libraries ENDF/B-6 (Rose, 1991), JENDL-3 (Nakajima, 1994), FENDL-2 (IAEA, 1999), BROND-2 (Manokin, 1989)). In the course of Monte Carlo calculations, the information taken from the Evaluated Nuclear Data Files, as is known, is not used directly, it is used after processing. Processing carried out by using special processing programs such as NJOY (MacFarlane, 1994). 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 of the calculations results, the latter is caused by the fact that the data prepared using processing programs do not contain the additional inaccuracy; nevertheless, when used, the methods to reduce the accuracy of calculations performed such as interpolation methods have to be applied. That is why the full or partial processing integration into Monte Carlo program calculation process is undoubtly of interest. The Monte Carlo code BRAND (Androsenko, 1991) 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 Institute of Nuclear Power Engineering. This code is designed to solve ionizing radiation transport problem as precisely as possible.

2. INCOHERENT INELASTIC SCATTERING

Incoherent inelastic scattering is represented in file 7 of ENDF-6 format (Rose, 1991) for a moderating molecule or a crystal by

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

where
E is the incident neutron energy,
E' is the secondary neutron energy,

β is the energy transfer,

$$\beta = \frac{E' - E}{kT},$$

α is the momentum transfer,

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{A_0 kT},$$

A_n is the mass of n^{th} type atom,
σ_{bn} is bound atom scattering cross section of the n^{th} type atom,
k is Boltzmann constant
μ is the cosine of the scattering angle (in the lab system).

The S(α,β,T) function may be represented in file 7 as a given tabulated function in some net junctions. Various interpolation laws between junctions are also determined in file 7. The S(α,β,T) function may be represented by analytical function as well using free gas model or short collision time approximation. For the short collision time approximation S(α,β,T) is equal to

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

and for free gas model to

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

3. ALGORITHMS OF INCOHERENT INELASTIC SCATTERING SIMULATION

Simulation algorithms in the case when S(α,β,T) in file 7 of ENDF-6 format is given as a table of values were presented in the paper (Androsenko, 2001). In the case when S(α,β,T) is presented by analytical function using free gas model or short

collision time approximation we use the substitute of variables proposed in paper (Eriksson, 1970) for free gas model. An equation for free gas model which was derived by Eriksson is given where new variables p and q were introduced. The following equation results

$$\sigma(p,q)=\sigma_{fr}[1+1/A_0]^2\pi^{-0.5}p\cdot\exp(-q^2),$$

where

$$p=\sqrt{\frac{\alpha A_0 kT}{E}},$$

$$q=\frac{\alpha+\beta}{2\sqrt{\alpha}}.$$

Simulation region transfers to

$$0\le p<\infty,$$

$$ap-b\le q\le ap+b,$$

where

$$b=\sqrt{\frac{A_0 E}{kT}},$$

$$a=b\frac{A_0+1}{A_0}.$$

For the short collision time approximation we use the same substitute of variables and obtain the following results:

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

where

$$A=\left(\frac{T}{T_{eff}(T)}-I\right)\frac{E}{A_0 kT},$$

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

$$C=\frac{T}{T_{eff}(T)},$$

$$I=\begin{cases}0 & if \quad p\le 2, q\le\dfrac{p}{2}\sqrt{\dfrac{E}{A_0 kT}}\\ 1 & else\end{cases}.$$

4. BRAND'S ALGORITHM OF SCATTERING SIMULATION USING FREE GAS MODEL

The density $f(p,q) = pe^{-q^2}$ has to be simulated in the region

$$0 \le p < \infty,$$
$$ap - b \le q \le ap + b.$$

First, simulate p with the density equal to

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

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

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

We simulate the random variable with the density f(p) using rejection technique. (We simulate the random variable with the density $\tilde{f}(p)$ using segmented line density simulation described in the paper (Androsenko, 1981).) Having simulated the value of p we simulate the random variable q at the interval $ap - b \le q \le ap + b$ with the density e^{-q^2} by the method of isotropic vector simulation described in (Frank-Kamenezki, 1978), rejecting the values of q if they are beyond the interval bounds. We calculate the momentum transfer and energy transfer according to the formulas

$$\alpha = \frac{Ep^2}{AkT},$$
$$\beta = 2q\sqrt{\alpha} - \alpha\,.$$

Then we calculate the new neutron energy and the cosine of the angle of scattering

$$E' = E + \beta kT,$$

$$\mu = \frac{E' + E - \alpha AkT}{2\sqrt{EE'}}.$$

Integrated scattering cross section for free gas model is calculated according to the formula

$$\sigma_s(E) = \frac{\sigma_{fr}}{b^2}\left[\left(b^2 + \frac{1}{2}\right) erf\, b + \frac{1}{\sqrt{\pi}} b \exp\left(-b^2\right)\right].$$

5. BRAND'S ALGORITHM OF SCATTERING SIMULATION USING SHORT COLLISION TIME APPROXIMATION

The two-dimensional random variable with the distribution density proportional to

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

has to be simulated in the region

$$0 \le p < \infty,$$
$$ap - b \le q \le ap + b.$$

Let

$$c = \frac{1}{2}\sqrt{\frac{E}{A_0 kT}}\,.$$

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

First subregion:

$$0 \le p \le 2\,,$$
$$ap - b \le q \le cp\,.$$

Second subregion:

$$0 \le p \le 2\,,$$
$$cp < q \le ap + b\,.$$

Third subregion:

$$2 < p < \infty\,,$$
$$ap - b \le q \le ap + b\,.$$

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 upon simulating p and q.

In the first subregion the density for p-simulation is proportional to

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

We simulate p with this density in a similar way to p-simulation for free gas model.

In the second subregion the density for p-simulation is proportional to

$$f_2(p)=\int_{cp}^{ap+b} f(p,q)dq=\frac{1}{2}\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2}\left(erf\left(\left(\frac{B}{2\sqrt{C}}+\sqrt{C}a\right)p+\sqrt{C}b\right)-erf\left(\left(\frac{B}{2\sqrt{C}}+\sqrt{C}c\right)p\right)\right)$$

.

It is evident that $f_2(p)\le\frac{1}{2}\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2}$ (since $0\le erf\,x\le 1$ for any $x\ge 0$). It is known that at $x\ge 5$ the values of erf x are very close to 1. Consequently at $p>\frac{5}{\frac{B}{2\sqrt{C}}+\sqrt{C}c}$ the values of $f_2(p)$ will be very close to zero. Neglecting the values of $f_2(p)$ at $p>\frac{5}{\frac{B}{2\sqrt{C}}+\sqrt{C}c}$ we obtain the following majoring density:

$$\tilde{f}_2(p)=\begin{cases}\frac{1}{2}\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2} & if \quad p\le\frac{5}{\frac{B}{2\sqrt{C}}+\sqrt{C}c}\\ 0 & if \quad p>\frac{5}{\frac{B}{2\sqrt{C}}+\sqrt{C}c}\end{cases}.$$

We simulate the random variable with the density $f_2(p)$ using rejection technique (We simulate random variable with the density $\tilde{f}_2(p)$ using inverse functions method).

In the third subregion the density for p-simulation is proportional to

$$f_3(p)=\int_2^{\infty} f(p,q)dq=\frac{1}{2}\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2}\left(erf\left(\left(\frac{B}{2\sqrt{C}}+\sqrt{C}a\right)p+\sqrt{C}b\right)-erf\left(\left(\frac{B}{2\sqrt{C}}+\sqrt{C}a\right)p-\sqrt{C}b\right)\right)$$

.

Similarly to the previous case, as $erf\,x\le 1$ for any x, then $f_3(p)\le\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2}$. As at $x\ge 5$ the values of erf x are very close to 1, then at $p>\frac{\sqrt{C}b+5}{\frac{B}{2\sqrt{C}}+\sqrt{C}a}$ the values of $f_3(p)$ will be very close to zero. Neglecting the values of $f_3(p)$ at $p>\frac{\sqrt{C}b+5}{\frac{B}{2\sqrt{C}}+\sqrt{C}a}$ we obtain the next majoring density:

$$\widetilde{f}_3(p)=\begin{cases}\sqrt{\frac{\pi}{C}}pe^{\left(\frac{B^2}{4C}-A\right)p^2} & if \quad p\le\frac{\sqrt{C}b+5}{\frac{B}{2\sqrt{C}}+\sqrt{C}a}\\ 0 & if \quad p>\frac{\sqrt{C}b+5}{\frac{B}{2\sqrt{C}}+\sqrt{C}a}\end{cases}.$$

The random variable with such density is simulated by the inverse functions method. The random variable with the density $f_3(p)$ is simulated using rejection technique.

After p-simulation the value of q with normal distribution is simulated:

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

The probabilities of hitting in every subregion are calculated in the following way. Let

$$r=\frac{B}{2\sqrt{C}}+\sqrt{C}c,$$

$$s=\frac{B}{2\sqrt{C}}+\sqrt{C}a,$$

$$t=\frac{B^2}{4C}-A,$$

$$p_1 = \int_0^2 f_1(p)dp = \frac{1}{2}\sqrt{\frac{\pi}{C}}\left(\frac{8r^2-1}{4r^2} erf(2r) - \frac{e^{-4r^2}}{r\sqrt{\pi}} - \frac{8s^2-2C-1}{4s^2} erf\left(2s-\sqrt{C}b\right) - \right.$$

$$\left. - \frac{4s+\sqrt{C}b}{2s^2\sqrt{\pi}} e^{-\left(2s-\sqrt{C}b\right)^2} - \frac{(2C+1)erf\left(\sqrt{C}b\right)}{4s^2} + \frac{\sqrt{C}be^{-Cb^2}}{2s^2\sqrt{\pi}} \right),$$

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

$$\left. - \frac{s}{\sqrt{s^2-t}} e^{\frac{tCb^2}{s^2-t}} \left(erf\left(2\sqrt{s^2-t} + \frac{s\sqrt{C}b}{\sqrt{s^2-t}} \right) - erf\frac{s\sqrt{C}b}{\sqrt{s^2-t}} \right) + \frac{r}{\sqrt{r^2-t}} erf\left(2\sqrt{r^2-t}\right) \right),$$

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

$$\left. + \frac{s}{\sqrt{s^2-t}} e^{\frac{tCb^2}{s^2-t}} \left(erf\left(2\sqrt{s^2-t} + \frac{s\sqrt{C}b}{\sqrt{s^2-t}} \right) - erf\left(2\sqrt{s^2-t} - \frac{s\sqrt{C}b}{\sqrt{s^2-t}} \right) \right) \right).$$

Then the probability of hitting in the ith subregion will be equal to

$$\frac{p_i}{p_1 + p_2 + p_3}.$$

The integrated scattering cross section for the short collision time approximation will be equal to

$$\sigma(E,T)=\sigma_b(p_1+p_2+p_3)/4.$$

6. 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. The results obtained are compared with numerically calculated spectrum (we numerically calculate the integral $\int_{-1}^{1} f(E',\mu)d\mu$). There is a very good agreement between the numerically calculated spectra and the spectra calculated using BRAND code for all energies. That is why we present on Fig. 1 the secondary neutron spectrum only for initial energy 1 eV. We calculate the energy spectrum of the secondary neutrons scattered by the oxygen in BeO using BRAND's algorithm of scattering simulation for short collision time approximation and analytically 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. The results

are compared with analytically calculated spectra. As in previous case there is a very good agreement between spectra calculated using BRAND and analytically calculated spectra. The results for initial energy 10^{-1} eV are presented in Fig. 2.

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 H_2O and albedo neutron spectrum are calculated. Calculations have been performed using BRAND and MCNP (Breismeister, 1996) for initial neutron energies 1, 10^{-1}, 10^{-2}, 10^{-3}, and 10^{-4} eV at the temperatures of the moderator of 1° K and 300° K. There are some disagreements between BRAND and MCNP especially for penetration. These disagreements may be explained by the fact that data processing is used for scattering simulation in MCNP while BRAND code does not use it. The spectra of neutrons which penetrate the barrier at the initial energy of 1 eV at the temperature of the moderator of 300° K are presented in Fig. 3, the albedo neutron spectra are presented in Fig. 4.

7. CONCLUSIONS

The algorithms of direct simulation of incoherent inelastic neutron scattering using free gas model and short collision time approximation are realized in terms of BRAND code system. The comparison of the results calculated using BRAND and MCNP is given. There are some negligible disagreements between BRAND and MCNP. The cause of these disagreements requires the detail comparison of BRAND's algorithms and NJOY+MCNP ones.

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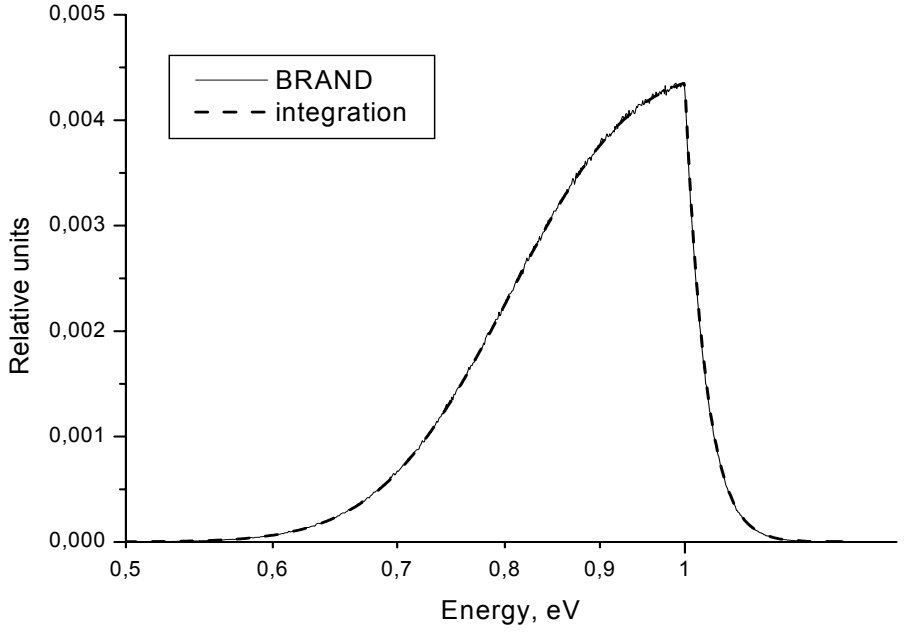

Fig. 1 *Secondary neutron spectrum for oxygen for 1 eV initial energy for free gas model*

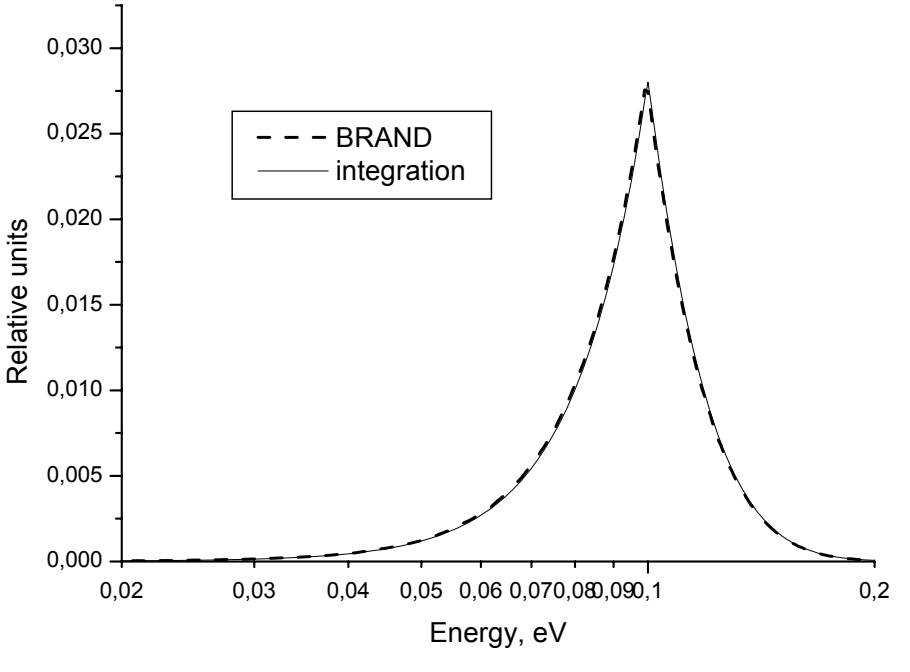

Fig. 2 *Secondary neutron spectrum for oxygen for 0.1 eV initial energy for short collision time approximation*

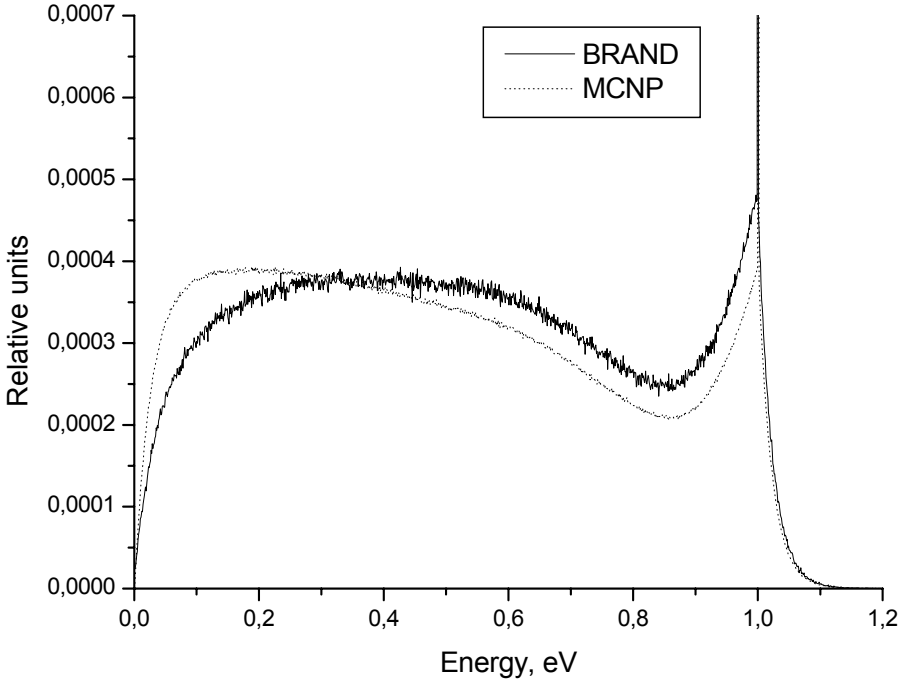

Fig. 3 *Spectrum of neutrons that penetrate the barrier at the initial energy of 1 eV*

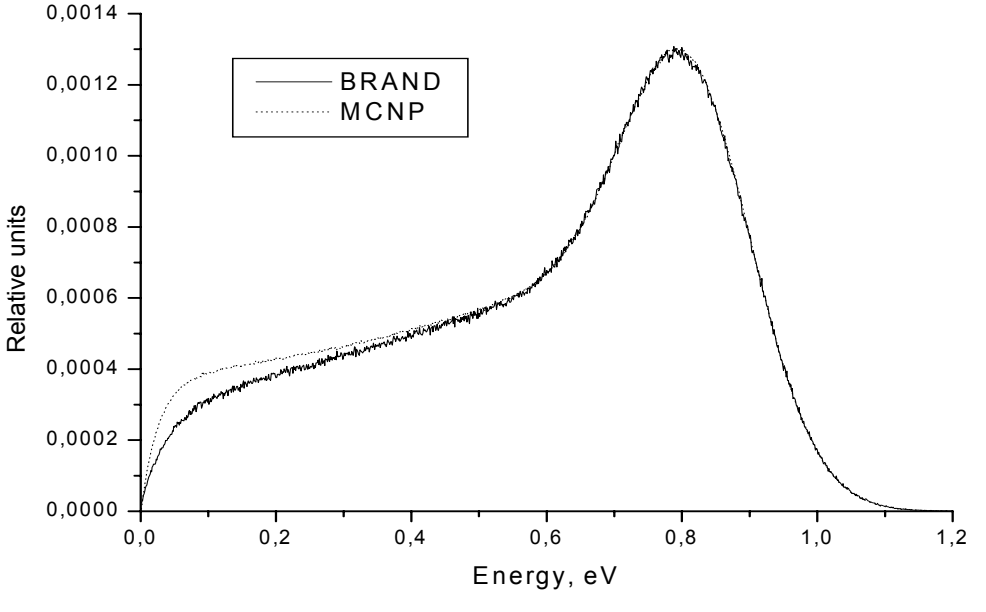

Fig. 4 *Albedo neutron spectrum at 1 eV initial energy*