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The Monte Carlo Simulation of Neutron Transmitted and Scattered by Disk Choppers of Various Compositions

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Abstract

We consider the transmission of neutrons through disk-type neutron choppers, considering both the uncollided neutron fraction ($\phi_u$) and scattered neutron fraction ($\phi_s$). We computed $\phi_u$, $\phi_s$, and the ratio $\phi_u/\phi_s$ through plates of five different absorber materials of various thicknesses to give information for selecting optimum materials and thicknesses. We also studied variance-reducing techniques for Monte Carlo calculation of chopper using MCNP4b, selecting those most effective for these calculations.

I. Introduction

A disk chopper rotating around an axis parallel to the beam is one of the standard ways to shape the pulsed neutron beam for time-of-flight (TOF) measurements. The disk chopper blocks the neutron beam for selected time intervals when it is desired to limit the range of wavelengths that reach the sample or to define a sharp pulse. In order to go from fully open to fully closed, a disk chopper must rotate neutron absorber through the effective beam-width W. This is the most simple mechanical construction giving the effect of a moving slit going past a stationary slit. The disk slit transmits a wide solid angle of neutrons [1]. The height of the slit and the speed with which the slit passes the neutron beam should be considered for optimum performance, but these factors are outside the purview of our present considerations.

The quantities that must be considered when designing choppers are (i) the neutrons transmitted ($\phi_u$) and (ii) the neutrons scattered (including resonance scattering) ($\phi_s$) through the material of the chopper when it is closed. An attenuation factor of about $10^{-6}$ is desired so that no effects of background from the source can be seen in an inelastic scattering experiment [2]. While the uncollided transmission factor is easy to compute, the scattered neutrons through the
material of chopper when a disk is closed must be considered when designing choppers. The purpose of this project is to study the fraction of transmitted neutrons and scattered neutrons through a chopper plate. We computed $\phi_0$, $\phi_s$, and the ratio of transmitted neutrons and scattered neutrons $\phi_s/\phi_0$. The computer code used in this investigation is MCNP4b [3] operating on a single-processor of Pentium III machine (running Linux) with neutron cross section libraries (ENDF60 and ENDL85) which include resonance scattering, important in this application, but treats all materials in the independent-atom free gas (300K) approximation.

II. Geometry

In this simulation, a pencil neutron beam source was placed at 1.5 cm from the center of disk plate. The thickness of disks varies from 0.5 mm to 8 mm. Disks were all of 25 cm radius. Two spheres with radii of 100 cm and 120 cm surround the disk chopper. The regions inside the inner sphere and between the inner sphere and the outer sphere were void but assigned neutron importance of 1. The region outside outer sphere is neglected. The inner sphere is modeled to include "surface tallies" which cover ranges in angle, say $0^\circ$-$0.1^\circ$, $1^\circ$-$10^\circ$, ..., $160^\circ$-$170^\circ$ with respect to the axis parallel to the beam (x-axis). The surface tally below $0.1^\circ$ detects the transmitted neutron fraction. Ring detectors were placed at $1^\circ$, $4^\circ$, $7^\circ$, $10^\circ$, $15^\circ$, $25^\circ$, $165^\circ$, and $175^\circ$ on the plane tangential to the points of intersection between the inner sphere and the beam axis, i.e., the intersection point behind beam source and diametrically opposite point to detect back scattered and forward scattered neutrons (see Figure 1).

![Diagram showing cell geometry used for detection of scattered and transmitted neutrons.](image)

Figure 1. Diagram showing cell geometry used for detection of scattered and transmitted neutrons.
II. Chopper Information used in this simulation

Single-disc choppers were investigated in this simulation, however, in some instances composed of several layers. The absorber materials are listed in Table 1.

**Table 1.** Chopper information used in this simulation.

<table>
<thead>
<tr>
<th>Chopper Name</th>
<th>Absorber</th>
<th>Thickness (mm)</th>
<th>Transmission for 0.0316 eV at maximum thickness</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gd/Al</td>
<td>Gadolinum-aluminum alloy (17.2 % Gadolinium by weight)</td>
<td>0.5, 1, 2, and 3</td>
<td>9.4368E-12</td>
</tr>
<tr>
<td>Al/Cd/Al</td>
<td>Cadmium with aluminum layers at front and back</td>
<td>aluminum : 2.5</td>
<td>2.3367E-10</td>
</tr>
<tr>
<td></td>
<td></td>
<td>cadmium : 0.5, 1, and 2</td>
<td></td>
</tr>
<tr>
<td>Al/B₄C+epoxy/Al</td>
<td>B₄C-epoxy mixture with aluminum layers at front and back (80% B₄C by</td>
<td>aluminum : 2.5</td>
<td>1.7459E-19</td>
</tr>
<tr>
<td></td>
<td>volume)</td>
<td>B₄C-epoxy : 2, 5, and 8</td>
<td></td>
</tr>
<tr>
<td>Daimler</td>
<td>¹⁰⁷B(99% purity)/epoxy layers on front and back (about 55% ¹⁰⁷B by volume)</td>
<td>boron/epoxy : 0.145, 0.29, and 0.507 fibre/epoxy : 0.335</td>
<td>9.1260E-12</td>
</tr>
<tr>
<td></td>
<td>and fibre/epoxy layer at center</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Gd₂O₃+epoxy/Al</td>
<td>Gd₂O₃/epoxy mixture (20% Gd₂O₃ by volume) and aluminum at the other side</td>
<td>Gd₂O₃/epoxy: 1, 2, and 4</td>
<td>4.6413E-12</td>
</tr>
<tr>
<td></td>
<td></td>
<td>aluminum : 2.5</td>
<td></td>
</tr>
</tbody>
</table>

III. Results

We computed the fraction of scattered neutrons per unit solid angle as a function of emerging angle (ϕₑ), the fraction of transmitted neutrons (ϕₒ), and the ratio between these fractions (ϕₒ/ϕₑ). The thicknesses of the chopper layers are adjusted to minimize the leakage when the chopper is closed [2]. The chopper material and its thickness are selected to give optimum strength, machineability, rigidity, and large absorption cross-section for neutrons. The maximum thicknesses estimated in this simulation are varied depending on absorber materials. The maximum thicknesses are 3mm for Gd/Al, 7mm for Al/Cd/Al (2.5mm aluminum at each side), 13mm for Al/B₄C+epoxy/Al, 1.335mm for Daimler, and 6.5mm for Gd₂O₃+epoxy/Al.

The fractions of transmitted neutrons which were calculated by Monte Carlo simulation agreed with analytical calculations. Figure 2 shows that the attenuation factors for neutrons of energies less than 0.05eV are $> 10^{-6}$ for all simulated absorber materials (throughout epoxy is modeled as CH₂ with density 1.115 g/cm³) and maximum thicknesses. Figure 2 indicates that the Al/B₄C+epoxy/Al is the best option when only low “closed” transmission is considered. However, the Daimler is most effective, because the transmitted neutron factor is least next to Al/B₄C+epoxy/Al and the thickness is least among simulated materials. The cadmium sheet is
very effective to block neutrons of energies of about 0.08eV through 0.2eV (Figure 2) because its macroscopic cross section is high in that region (Figures 3).

Figure 2. The comparison of transmitted neutron fractions at the maximum thicknesses for several absorber materials.

Figure 3. The comparison of total neutron cross sections for disk absorbing materials.
The fraction of neutrons scattered at angle $\Theta$ is calculated as follows:

$$
\phi_s \left( \frac{\text{scat - n}}{\text{steradian} \cdot \text{s - n}} \right) = \frac{\phi \left( \frac{\text{scat - n}}{\text{s - n}} \right)}{\Delta \Omega} \quad \text{or} \\
\phi_s \left( \frac{\text{scat - n}}{\text{steradian} \cdot \text{s - n}} \right) = \rho(\theta)^2 \varphi \left( \frac{\text{scat - n}}{\text{s - n}} \right)
$$

(1)

where

$$
\Delta \Omega = \frac{\Delta A}{\rho(\theta)^2},
$$

$\Delta \Omega$ = solid angle,

$\Delta A$ = unit area = 1 cm$^2$,

scat-n = scattered neutron,

s-n = source neutron,

$\rho(\theta)$ = the distance to ring detector from the point at which the uncollided neutron beam exits through chopper

$$
= r^2(1+\tan^2\theta) = r^2 \quad (\text{for} \quad \theta = 1^\circ),
$$

$r$ = radius of ring detector = 100 cm, and

$\varphi$ = ring detector tally (n/cm$^2$/s-n).

Figures 4(a) through (e) show the fractions of neutrons scattered through $1^\circ$ at several energies as a function of absorber thickness. At the maximum thickness of each chopper absorber $\text{B}_4\text{C}$/epoxy mixture shows the least fraction of scattered neutrons. However, when compared at the same absorber thickness of 1 mm, the fractions of scattered neutrons are least for Daimler chopper and are highest for the $\text{B}_4\text{C}$/epoxy mixture with aluminum layers at each side (20% epoxy by volume and 21.7% carbon by weight) and $\text{Gd}_2\text{O}_3$/epoxy mixture with aluminum layer at one side (80% epoxy by volume) because both chopper materials include a high volume fraction of epoxy or carbon. Figure 5 shows that the scattered neutron fraction as function of angle ($\phi_s(\theta)$) is approximately constant with $\theta$ between $0^\circ$ to $5^\circ$. 

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Figure 4. Scattered neutron fraction at 1°. (a) Gd/Al; (b) Al-Cd-Al; (c) Al/B₄C+epoxy/Al; (d) Daimler; (e) Gd₂O₃+epoxy/Al.
Figure 5. Scattered neutron fraction normalized to value at 0° as a function of scattered angle for 0.5 mm Gd/Al case.

Figure 6 shows the fractions of neutrons scattered at 1° as a function of energy for each of the chopper materials at the maximum simulated thicknesses. The fractions of scattered neutrons of Gd$_2$O$_3$+epoxy/Al are greatest among the studied materials at each energy. At the energies between 0.08 and 0.3eV the fractions of scattered neutrons of Al/Cd/Al are lowest. The fractions of scattered neutrons of Gd/Al alloy decrease rapidly below the energy of around 0.3eV and are lowest below 0.05eV. For Al/B$_4$C+epoxy/Al the fractions of scattered neutrons are low over the entire energy range.

Figure 6. The comparison of scattered neutron fractions at the maximum thicknesses for several absorber materials.
The next important characteristic to be studied is the ratio of scattered neutrons to uncollided neutron. The true number of neutrons transmitted through a chopper and accepted by a guide is not $\phi_u$ as usually thought, but rather can be expressed as:

\[
T_{\text{eff}} = \phi_u + \phi_s(\theta) \cdot \Omega \quad \text{or} \\
T_{\text{eff}} = \phi_u \left( 1 + \frac{\phi_s(\theta)}{\phi_u} \cdot \Omega \right)
\]

where

- $T_{\text{eff}}$ = true number of neutrons transmitted through the absorber material and accepted by the guide,
- $\phi_s(\theta)$ = scattered neutron through absorber material at $\theta$, angle less than the critical angle of guide, and
- $\Omega$ = solid angle acceptance of guide.

It is shown in figure 5 that the scattered neutron fractions are constant for the range of scattered angles of $0^\circ$ through $5^\circ$. The critical angle of guide is expressed as:

\[
\theta_c = m \lambda \gamma_s^{\text{Ni}}
\]

where

- $\theta_c$ = critical angle of guide,
- $\lambda$ = wavelength,
- $m$ = multiplication factor, and
- $\gamma_s^{\text{Ni}} = 0.0017 \text{rad/Å}.$

Thus, the critical angle for supermirror of $m=3$ and $\lambda_c=1$Å and for the energy of 1Å (81.787meV) is 5.1e-3 rad (0.3°). The solid angle $\Omega$ can be expressed as $\theta_c^2$ because $\theta_c$ is small.

Then we can rewrite equation (2) as:

\[
\phi_s(\theta) = \phi_s \quad \text{for} \quad \theta < \theta_c
\]

\[
T_{\text{eff}} = \phi_u \left( 1 + \frac{\phi_s}{\phi_u} \cdot \Omega \right) 
\]

Figures 7(a) through (e) show the curves of the ratio of $\phi_s/\phi_u$ as functions of absorber thickness. For the Gd/Al we find that the curves of the ratio of $\phi_s/\phi_u$ are similar like one line in all simulated energies while for the other materials the curves diverge strongly in the low energy region between 0.01 and 0.1eV. For Gd/Al the values of the ratio of $\phi_s/\phi_u$ change with thickness very gradually for the energy range between 0.01 and 1eV and the slope of curve is decreasing. For other materials, the values of the ratio of $\phi_s/\phi_u$ with thickness converge with one line for the energies between 0.1 and 1eV (excepting cadmium) and the slope of the curve is decreasing. For cadmium the values of the ratio of $\phi_s/\phi_u$ with distance diverge for the energies of 0.1eV, 0.178eV, and 0.316eV while converge to one line for the energies of 0.0178eV, 0.0316eV, 0.0562eV, and 0.562eV. At the maximum thickness of each chopper the absorber B$_4$C/epoxy mixture shows the greatest value of the ratio of $\phi_s/\phi_u$ with thickness. However, when compared
at the same absorber thickness of 1 mm, the Daimler chopper shows the greatest value of the ratio of $\phi_s/\phi_a$ with thickness.

Figure 7. Scattered neutron fraction at $1^\circ$ per transmitted neutron. (a) Gd/Al  (b) Al/Cd/Al  (c) Al/B$_4$C+epoxy/Al  (d) Daimler  (e) Gd$_2$O$_3$+epoxy/Al. The ratio $\phi_s/\phi_a$ of Cd at the energy 0.178 eV has not been calculated because it is too thick optically to do Monte Carlo simulation at that energy.
Figure 8 shows $\phi_0/\phi_a$ at the maximum thicknesses for five absorber materials. Above about 0.1 eV the ratio $\phi_0/\phi_a$ is constant (Figure 8). However, at the energies below 0.1 eV the ratio $\phi_0/\phi_a$ is rapidly increasing inversely with energy (Figure 8) in other simulated absorbers excepting Gd/Al alloy and Cd (highest at 0.178 eV). For the Gd/Al alloy the ratio $\phi_0/\phi_a$ is constant in the entire simulated energy range and is lowest of all the materials.

![Graph showing scattered neutron fractions at 1° vs. transmitted neutron fractions at the maximum thicknesses for several absorber materials.](image)

Figure 8. The comparison of scattered neutron fractions at 1° vs. transmitted neutron fractions at the maximum thicknesses for several absorber materials.

Table 2 shows the comparison of the true number of neutrons for GdAl, Al/B$_4$C+epoxy/Al (for m=3, $\lambda = 1$ Å, and E=81.787 meV) and Gd$_2$O$_3$+epoxy/Al (for m=3, $\lambda = 2.14$ Å, and E=17.8 meV) at their maximum thicknesses. For Gd/Al the ratio $\phi_0/\phi_a$ is insignificant. However, for Al/B$_4$C+epoxy/Al the true number of neutrons $T_{eff}$ is 1500 times as high as $\phi_a$. For Gd$_2$O$_3$+epoxy/Al the true number of neutrons $T_{eff}$ is 1E+05 times as high as $\phi_a$.

Table 2. The comparison of the true number of neutrons passed into guide through absorber materials at maximum thicknesses (m=3, $\lambda = 1$ Å, and E=81.787 meV). For Gd$_2$O$_3$+epoxy/Al E = 17.8 meV (2.14 Å).

<table>
<thead>
<tr>
<th>Chopper</th>
<th>$\phi_a$ (transmitted neutron/source neutron)</th>
<th>$T_{eff}$ (eqn. (5)) (transmitted neutron/source neutron)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gd/Al</td>
<td>2.83x10$^5$</td>
<td>2.83x10$^5$</td>
</tr>
<tr>
<td>Al/B$_4$C+epoxy/Al</td>
<td>1.28x10$^{12}$</td>
<td>2.00x10$^9$</td>
</tr>
<tr>
<td>Gd$_2$O$_3$+epoxy/Al at 17.8 meV</td>
<td>8.15x10$^{16}$</td>
<td>8.81x10$^{11}$</td>
</tr>
</tbody>
</table>
VI. Summary

We have calculated the true neutron transmission of various chopper material configurations. Our calculations show that the neutrons transmitted through disk chopper materials after scattering in the disk can be more significant than the uncollided fraction.

References


