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Neutronic studies of the coupled moderators for spallation neutron sources

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We investigate the neutronic performance of coupled moderators to be implemented in spallation neutron sources by Monte-Carlo simulation and give the slow neutron spectra for the cold and thermal moderators. CH_4 moderator can provide slow neutrons with highly desirable characteristics and will be used in low-power spallation neutron sources. The slow neutron intensity extracted from different angles has been calculated. The capability of moderation of liquid H_2 is lower than H_2O and liquid CH_4 due to lower atomic number density of hydrogen but we can compensate for this disadvantage by using a premoderator. The H_2O premoderator of 2cm thickness can reduce the heat deposition in the cold moderator by about 33% without spoiling the neutron pulse.

Keywords: neutronic studies, spallation neutron source, moderator
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1. Introduction

The function of a moderator is to convert high-energy neutron escaping from a target to slow neutrons with an energy spectrum and pulse characteristics suitable for experiments.[1,2] This slowing-down process is accomplished by inelastic and elastic collisions between fast neutrons and the nuclei of the hydrogenous moderator and ultimately the energies of the neutrons are reduced to the range from 10 meV to 0.01meV. These thermal neutrons can be used in the neutron scattering. In fact, only when the energy of fast neutrons is under 25MeV, it is possible for the moderator to produce the moderated thermal neutrons. Almost 90% of neutrons escaping from the target are within this range (see Fig.1).

Three kinds of moderators (liquid hydrogen, liquid methane and light water moderators) coupled with a beryllium or lead reflector are the primary candidates as high-resolution moderators in spallation neutron source, where liquid H_2 and CH_4 are used as cold moderator, H_2O as thermal moderator. The choice of the moderator is one of the most important steps in the design of every instrument. The coupled moderator is usually used for obtaining slow-neutron pulses with high integral intensity, but it is very difficult for the coupled moderator to obtain neutron pulses with a narrow pulse width and a fast decay.[3] Obviously, these are contradictory to each other. However, we can realize both high resolution and high intensity recently by using high-resolution time-of-flight powder diffractometer with supermirror neutron guide.

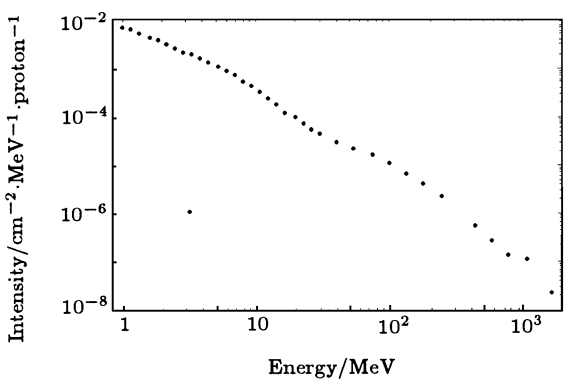


Fig.1. Energy spectrum of fast neutrons escaping from the target.

In principle, moderators have two basic configurations, the so-called wing and slab moderators, as shown in Fig.2. In the present investigation, we mainly concentrate on the wing moderator. It has been most widely used in the existing spallation neutron sources, since an instrument never views the target directly like a tangential beam hole in a reactor in

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which an instrument never views the reactor core. As a result of neutronic studies, the neutron energy spectra for the cold and thermal moderators have been calculated and we also compare the capabilities of moderating with the light water and liquid hydrogen. In spallation neutron source, slow neutrons are extracted not only from the normal direction but also at definite angles, thus we also consider the effect of extracting angles on slow-neutron intensity.

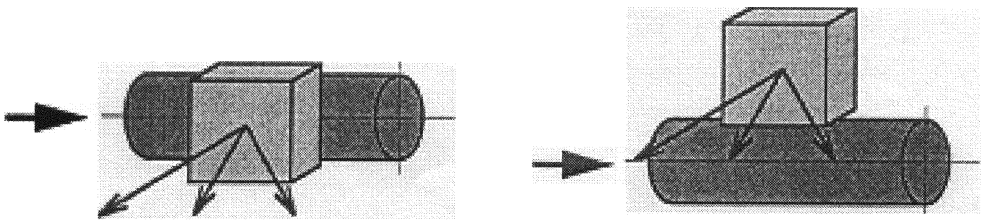


Fig.2. Illustration of two basic moderators.

2. Calculation model

A neutronics design is made by using the Monte Carlo N-Particle transport code system MCNP4A with the neutron cross sections based on the Evaluated Nuclear Data File ENDF/B-V, which has been developed at Los Alamos Laboratory. Proton and higher energy neutron behaviours were calculated with the NMTC/JAM code and these results were used in MCNP4A as basic source parameters including fast-neutron energy spectra and distribution along the moderator depth and height.[4]

In the present simulation, when a neutron collides with a nucleus of the moderator the following sequence ensues. The collision nuclide is identified; the velocity of the nucleus is sampled for low-energy neutrons; photons are optionally generated for later transport; neutron capture is modelled. As an example we consider the most important of the above processes, i.e. sampling the velocity of the nucleus of the moderator. A collision between a neutron and a nucleus of the moderator is affected by the thermal motion of the nucleus, and in most cases the collision is also affected by the presence of other nuclei nearby. A thermal treatment based on the free gas approximation is used to account for the thermal motion. The free gas thermal treatment assumes that the medium is a free gas in the appropriate ranges of atomic weight and neutron energy where thermal effects are significant. The most important step of the free thermal treatment consists of taking into account the velocity of the nucleus of the moderator when the kinematics of a collision is being calculated. If the energy of the neutron is greater than 400kT, where k is the Boltzmann constant, and the nucleus is not ^{1}H, the velocity of the nucleus is set to zero. Otherwise, the nucleus velocity is sampled. In the free gas thermal treatment, the probability distribution for a nucleus velocity V and cosine μ is

$$P(V,\mu)=\frac{\sigma_{\rm s}(v_{\rm rel})v_{\rm rel}P(V)}{2\sigma_{\rm s}^{\rm eff}(E)v_{\rm n}}. \tag{1}$$

Here, $v_{\rm rel}$ is the relative velocity between a neutron moving with a scalar velocity $v_{\rm n}$ and a nucleus of the moderator moving with a scalar velocity V, and μ is the cosine of the angle between the neutron and the nucleus. The equation for $v_{\rm rel}$ is

$$v_{\rm rel}=(v_{\rm n}^2+V^2-2v_{\rm n}V\mu)^{\frac{1}{2}}. \tag{2}$$

The scattering cross section at the relative velocity and the effective scattering cross section in the laboratory system for a neutron with kinetic energy E are denoted by $\sigma_{\rm s}(v_{\rm rel})$ and $\sigma_{\rm s}^{\rm eff}(E)$. $P(V)$ is the probability density function for the Maxwellian distribution of nuclei velocities

$$P(V)=\frac{4}{\pi^{\frac{1}{2}}}\beta^3V^2{\rm e}^{-\beta^2V^2}, \tag{3}$$

with β defined as

$$\beta=\left(\frac{AM_{\rm n}}{2kT}\right)^{\frac{1}{2}}, \tag{4}$$

where A is the mass of the nucleus in units of the neutron mass, $M_{\rm n}$ is the neutron mass in MeV·sh^2/cm^2, where sh is the unit of time and 1sh=10^{-8}s, and kT is the equilibrium temperature of the nuclei in MeV.

3. Neutronic design

The calculation model of the coupled moderator is shown in Fig.3. A rectangular tungsten target of dimensions 100mm×40mm×400mm is bombarded by

high-energy proton beam whose energy is 1.6GeV. Because the beryllium reflector can provide a pulse shape with a relatively shorter tail as compared with a lead one, we choose the cylindrical beryllium reflector with diameter 1000mm and height 1000mm surrounded by a cylindrical iron shield with diameter 2000mm and height 1000mm in our calculation model. The upstream moderator is placed on the location which has the highest fast-neutron flux by design. Then we consider the neutronic performance of the upstream moderator which can be a liquid hydrogen, liquid methane or light water moderator.

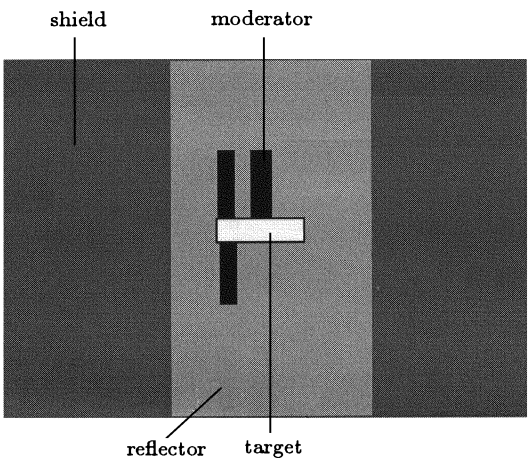


Fig.3. Sketch of the calculation model.

In the slowing-down region the spectrum is approximately proportional to $\frac{1}{E}$; more exactly, $(1/E)^{1-\alpha}$, where E is the neutron energy and α is a small number between 0.1–0.2 determined by the neutron leakage during the slowing-down. In the thermal equilibrium region the spectrum exhibits a Maxwellian distribution due to the detailed balance between neutrons and scattering atoms. For a room temperature moderator its spectrum, $\Phi(E)$, can be fitted by the following semi-empirical function[5]

$$E\Phi(E) = E\Phi_{\rm th}(E) + \Delta(E)E\Phi_{\rm epi}(E). \qquad (5)$$

Where $\Phi_{\rm th}(E)$ is the thermal equilibrium (Maxwellian) spectrum

$$E\Phi_{\rm th}(E) = J(E/E_{\rm T})^2\exp(-E/E_{\rm T}), \qquad (6)$$

J the normalization constant, $E_{\rm T} = kT_{\rm N}$, k the Boltzmann constant and $T_{\rm N}$ the Maxwellian characteristic temperature (neutron temperature). $\Phi_{\rm epi}(E)$ is the slowing-down spectrum,

$$E\Phi_{\rm epi} = \Phi_{\rm 1ev}(E/1{\rm eV})^{\alpha}. \qquad (7)$$

$\Delta(E)$ is the so-called joining function introduced to connect $\Phi_{\rm th}(E)$ and $\Phi_{\rm epi}(E)$ smoothly,

$$\Delta(E) = [1 + \exp(aE^{-1/2} - b)]^{-1}, \qquad (8)$$

where a and b are constants. There are several joining functions so far proposed and the above expression is a typical one. Figure 4 shows the spectrum of neutrons escaping from H_2O moderator, which fits the Eq.(1) very well. In a liquid H_2 moderator the equilibrium spectrum is not Maxwellian (see Fig.5). However, in the cold-neutron region, it can be fitted by a Maxwellian function as shown in Fig.6.

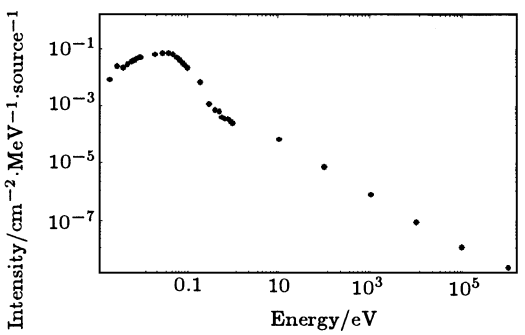


Fig.4. Slow-neutron energy spectrum from the light water moderator.

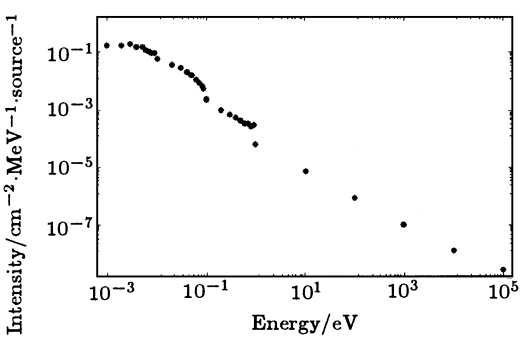


Fig.5. Slow-neutron energy spectrum from the liquid hydrogen moderator.

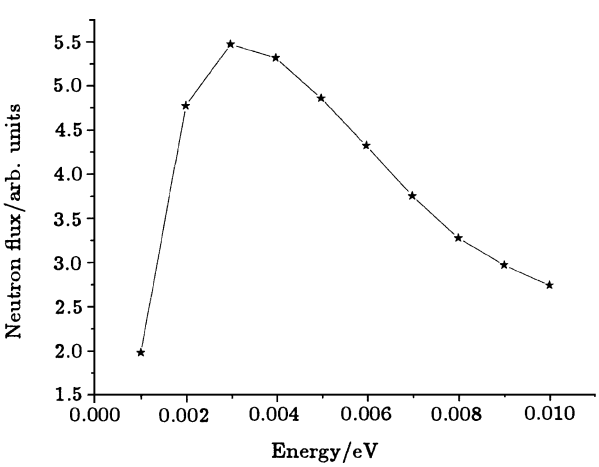


Fig.6. Cold-neutron energy spectrum from the liquid hydrogen moderator.

It is well known that conventional methane moderator cannot be used with high-power spallation neutron sources. In the liquid state (around 100K) methane suffers from severe polymerization induced by radiation, to such a level that the high-power spallation sources significantly limit the lifetime of the liquid methane moderator vessels. As an example, the methane moderator of ISIS with its average nuclear power 160 kW is typically changed on the order of every 2000 hours and this rapid replacement schedule is regarded by ISIS operations and instrument personnel as a rather significant drawback.[6] However, CH_4 has a rotational level of about 1meV that is very effective at thermalizing the neutrons to low temperature and it can provide slow neutrons with highly desirable performance characteristics (e.g. similar wavelengths to inter-atomic distances in condensed matter, see Fig.7). As a result, we still choose CH_4 as a high-efficiency cold moderator for kW-level spallation neutron sources. Furthermore, since it seems to be very difficult to repair the moderators under the high-radiation level and possible hazards due to chemical poisoning of beryllium reflector, the moderator vessel for methane moderator in spallation neutron source can be made as a part of the "inner plug" assembly, which also includes some portion of the reflector and has a longer life-span. Reducing the repairing cost would be a very significant factor for decision-making a practice engineering.

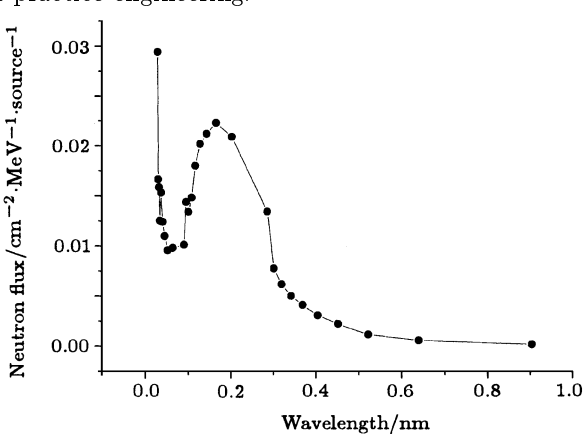


Fig.7. Wavelength-dependent neutron spectrum from the liquid methane moderator.

In most spallation sources, slow neutrons are extracted from a moderator not only in the normal direction but also in the direction that makes a certain angle with the normal direction. Then we consider the effect of emitting angle θ on the time-integrated neutron intensity. Figure 8 shows that slow neutrons reduce when θ increases, which can be expressed as

$$I(\theta) = I(\theta = 0)\cos\theta. \tag{9}$$

In addition the beam cross section is proportional to $\{a/\cos\theta\}$, where a is the area of the viewed surface, the intensity is approximately proportional to $\cos^2\theta$. Thus for a large-angle neutron beam extractor the loss in neutron intensity must also be taken into account. Moreover, neutron pulse characteristics deteriorate with θ increasing. This effect is more important than the reduction of intensity.

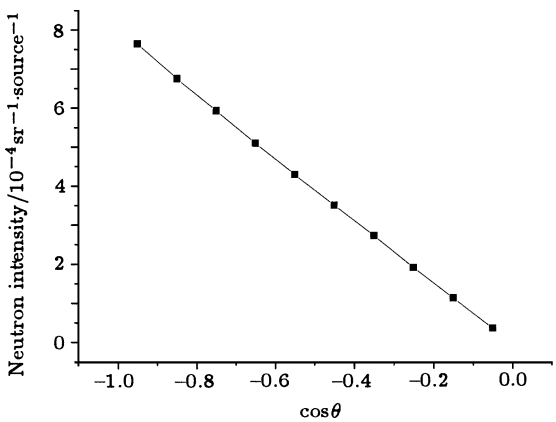


Fig.8. Slow-neutron intensity from the light water moderator as a function of beam-extraction angle θ.

As mentioned above, spallation sources use liquid H_2 and CH_4 as cold moderators. Compared with CH_4, liquid H_2 is more stable against radiant damage. It is the most promising candidate as a cold moderator for high-power spallation neutron sources. But it lacks effective low energy levels to thermalize neutrons and has lower atomic number density of hydrogen (i.e. the lower macroscopic scattering cross section), which also makes its moderating capability lower than the other two moderators. As an example, Fig.9 gives the difference of moderating capability between H_2 and H_2O. In order to compensate for this disadvantage the use of a premoderator has been proposed. Premoderator consisting of hydrogenous material at room temperature is attached just outside the cold moderator except for the viewed surfaces. There are two materials that can be used as premoderators, namely water and polyethylene. Note that although a polyethylene premoderator may give better performance due to higher atomic number density than H_2O premoderator, it cannot be used with high-power spallation source due to the serious radiant damage. We use H_2O premoderator of 2cm thickness to increase the moderating efficiency, as shown in Fig.10. This premoderator gives a larger

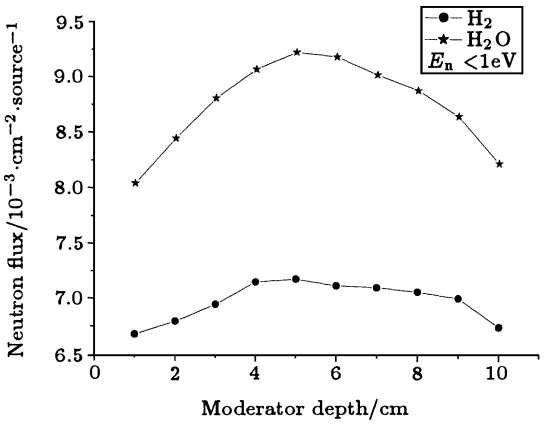


Fig.9. The difference of moderating capability between the liquid hydrogen and the light water moderators.

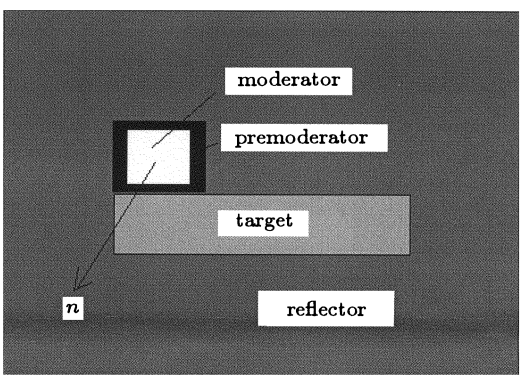


Fig.10. Coupled reflector-premoderator-moderator system.

separation between the cold moderators and the target, which lets the fast neutrons lose their energy quickly and does not spoil the neutron pulse shape. Another more important advantage for the use of premoderator is to decrease the energy deposition in cold moderators. It is clear from Table 1 that the presence of H_2O premoderator reduces the heat deposition in H_2 and CH_4 by about 33%, which increases the efficiency of the cold moderator and decreases the requirements for the moderator cooling power and the running cost.

Table 1. The heat deposition in moderators.

H_2O (300K)	255W	
H_2 (25K)	148W	105W (2cm premoderator)
CH_3 (100K)	247W	176W (2cm premoderator)

4. Conclusion

In summary, we have given the slow neutron spectra for the coupled moderators. The calculation shows good agreement with the semi-empirical thermal-neutron spectrum. Liquid CH_4 moderator can provide slow neutrons with highly desirable performance characteristics and can be used in kW-level spallation sources. Neutrons are usually extracted from a moderator not only from the normal direction but also at definite angles. The slow neutron intensity extracted from different angles has been calculated. The capability of moderating for liquid H_2 is lower than H_2O and liquid CH_4 due to lower atomic number density of hydrogen, but we can compensate for this disadvantage by using a premoderator. The H_2O premoderator of 2cm thickness can reduce the heat deposition in the cold moderator by about 33% without spoiling the neutron pulse.

For all simulations, the relative error does not exceed 2%.

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