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CALCULATION OF PULSE SHAPES FOR REENTRANT MODERATORS

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ABSTRACT

The calculation of neutron emission time distributions (pulse shapes) from reentrant moderators on pulsed spallation neutron sources is inherently difficult because of the need to combine the distributions for neutron emission from various surfaces to a common reference plane. Earlier calculations invoked approximations often made necessary by practical limitations on the amount of computational power available. The present work describes a more rigorous approach to pulse shape calculations that substantially improves the earlier results and extends pulse shape calculations to situations that could not be addressed with previous methods.

Key Words: spallation neutron source, neutron pulse shapes, reentrant moderators, Monte Carlo

1. INTRODUCTION

Spallation neutron sources have proven to be important tools in the development of new materials for a wide variety of applications. In these facilities, fast neutrons created by proton-induced spallation interactions in a heavy-metal target thermalize in nearby moderators to provide beams of slow neutrons ($E_n \leq 1$ eV) for experiments. The highest fluxes of low-energy neutrons are produced using moderators of cryogenic materials such as solid or liquid methane or liquid hydrogen. Moreover, reentrant (grooved) moderators provide higher fluxes than moderators with flat surfaces, at the sacrifice of somewhat broadened emission time distributions.

In a spallation facility, the proton beam typically has a pulse width on the order of 100 ns. During neutron thermalization, however, the resulting neutron pulses broaden in an energy-dependent manner to have widths on the order of tens of microseconds. The energy and time distributions of neutrons emerging from the moderators establish a fundamental limit on the experimental resolution achievable from the neutron beam, and thus directly impact the scientific applications. Accurate predictions of the energy and time distributions of neutrons leaving a moderator are of fundamental importance for predicting the performance of instruments located at a spallation source facility, and are thus required for the design of spallation source target/moderator/reflector systems.

In the present work, we examine some of the issues involved in estimating the time-dependent neutron emission from reentrant cryogenic moderators at spallation neutron sources. Further discussion of these calculations can be found elsewhere in the literature [1,2]. In particular, we compare the results from several different methods of calculating both the neutron energy spectrum and the energy-dependent time distributions of neutrons emerging from these moderators, and present an improved method for pulse-shape calculations.

2. CALCULATIONAL METHODS

We used the Monte Carlo radiation transport code MCNPX, version 2.4.0 [3] to calculate the neutron beam characteristics (moderator performance) of the moderators under study. MCNPX employs a combinatorial geometry that represents the physical system using generalized quadratic surfaces to define the boundaries of cells. The description of the system employed in the computer model is necessarily somewhat simpler than the design of the actual physical system. For example, our model omits coolant pipes for moderators and approximates the multiplicity of nested vessels surrounding the moderators as single homogenized volumes. However, the model does provide sufficient detail to obtain adequate estimates for quantities such as neutron beam characteristics of the moderators. MCNPX has the capability to calculate both the high-energy ($E > 20$ MeV) and the lower energy ($E < 20$ MeV) portions of the problem for all particles together. In all cases, MCNPX was used initially in a neutron-only calculation to generate weight window boundaries that improved the efficiency of the final calculations.

Because of practical constraints on computer processing resources, a Monte Carlo simulation can never yield information as detailed as can be obtained through measurements. For example, the energy and time resolutions of even modest instruments are much better than those practical for Monte Carlo calculations. We have generally used 20 bins per decade (power of ten) for characterizing both energy and time distributions, which gives a resolution ($\Delta E/E$ or $\Delta t/t$) of about 12.2%. In certain cases, we employ a higher energy resolution for comparison: either 50 bins/decade ($\Delta E/E$ = 4.7%) or 100 bins/decade ($\Delta E/E$ = 2.3%). For the calculations we describe, we used a cluster of four dual-processor AMD 2100+ computers running RedHat Linux 7.2 and the OSCAR cluster management software [4].

2.1. Description of Modeled Systems

2.1.1 IPNS C moderator

The Intense Pulsed Neutron Source (IPNS) at Argonne National Laboratory is a pulsed spallation source that generates neutrons by accelerating protons to 450 MeV and directing them onto a light-water-cooled depleted uranium target of diameter 10 cm and length 20 cm. The IPNS accelerator system produces a time-averaged current of 15 μA in 80-ns pulses at a rate of 30 Hz. The C moderator, located beneath and to the rear of the proton beam target, is a decoupled, unpoisoned solid methane moderator 10 cm x 10 cm x 8 cm thick, with vertical grooves approximately 4 cm deep and 1 cm wide in the viewed face. The grooves allow an instrument to focus onto a higher-source region at the base of one of the grooves. Instruments that view the entire surface also gain in intensity over a flat moderator of the same dimensions. Figure 1 shows a photograph of the C moderator, along with the MCNPX neutronics model.

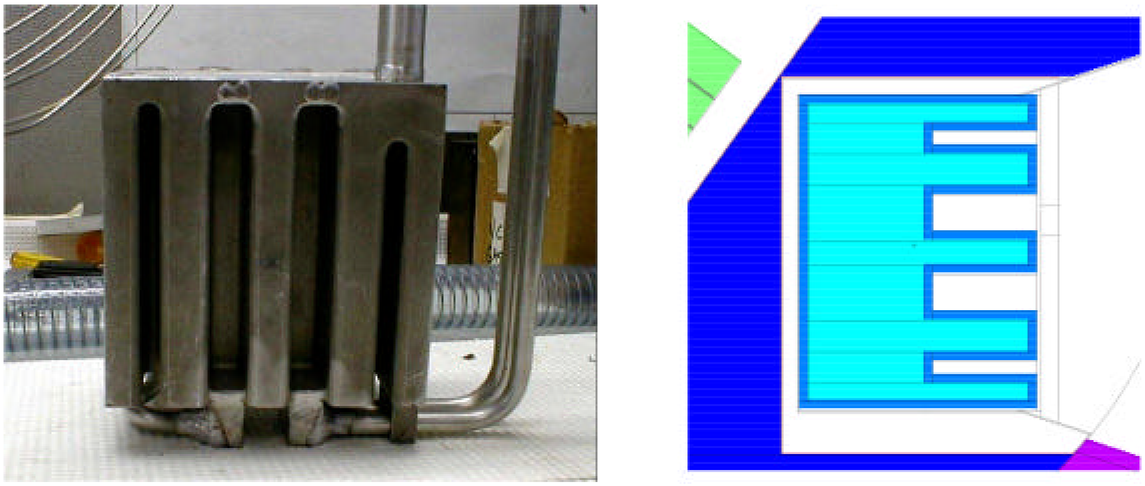

Figure 1. (left) Photograph of the IPNS C moderator, looking at the viewed face. (right) MCNPX neutronics model of the C moderator (plan view).

2.1.2 SNS Long Wavelength Target Station

The proposed Long Wavelength Target Station (LWTS) [5] at the Spallation Neutron Source (SNS) being constructed at Oak Ridge National Laboratory is designed to operate at 10 Hz, allowing a broad wavelength band of neutrons to be used while simultaneously permitting the use of cold, efficient moderators for producing long-wavelength neutrons. The LWTS reference concept includes a 1 GeV proton beam producing neutrons from a vertically extended target of clad tungsten metal plates cooled with D_2O. The plates measure 7 cm wide × 20 cm high and have variable thickness, with a total length of 40 cm. The reference LWTS model (Figure 2) contains three moderators adjacent to the neutron-producing target. The High-Intensity Cold Moderator is the moderator to the left of the target when viewed from the perspective of the incident proton beam. It is unpoisoned and fully coupled to the reflector. The viewed surface of the moderator has horizontal V-shaped grooves with an opening angle of 30°. In the calculations we will discuss here, the moderating material is liquid hydrogen at 20 K.

2.2. Quantities Calculated

The quantities used here to determine the performance of spallation-source moderators are the angle-dependent energy spectrum of neutrons emerging from the viewed moderator face (also called the spectral intensity) and the energy- and angle-dependent emission time distributions. From these data one can generate pulse-shape metrics such as average emission time and pulse width, or obtain the thermal neutron intensity.

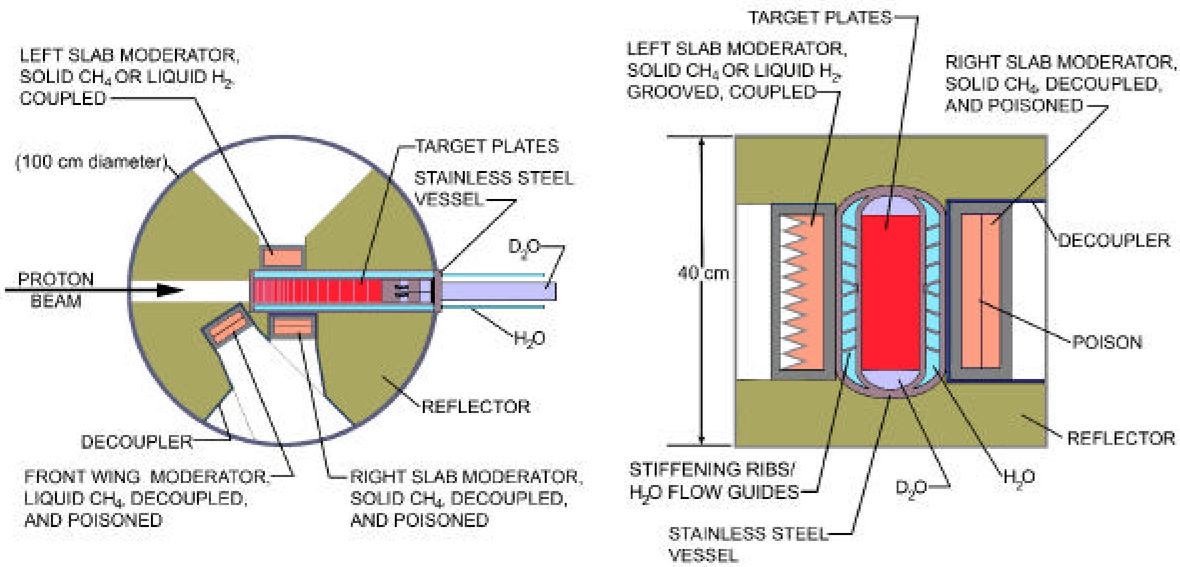

Figure 2. (left) Plan view of the proposed Long Wavelength Target Station at SNS. (right) Cross sectional view of the LWTS target station showing the grooved coupled moderator to the left of the target.

The spectral intensity *i(E)* of a moderator is the number of neutrons leaving the entire viewed face of the moderator at a particular energy E and is related to the differential flux $f(E)$ at a point some large distance L from the moderator by a "$1/r^2$" relationship, that is,

$$i(E) = L^2 \; f(E)\big|_L \; , \tag{1}$$

where by convention the flight path is normal to the viewed moderator face. This intensity characterizes the moderator independently of the flight path length from which it is viewed. If the flight path is not normal to the moderator face, the observed intensity is approximately proportional to the cosine of the angle between the flight path and the normal to the moderator surface (Lambert's Law).

The spectral intensities are calculated both by "point detector" tallies, which give rapid convergence, absolute scaling, and directional sensitivity, and by "emission current" tallies, which have slower convergence but also provide intensities for high-energy neutrons. [The way that the point detector tally works in MCNPX does not permit determining the contributions from high-energy neutrons.] The two tallies should agree when they are calculating the same physical quantity and are properly normalized. Emission current tallies have the advantage of representing exactly the neutrons crossing the viewed surface of a moderator. With point detector tallies, one can speed convergence by restricting contributions to the regions of the problem that contribute to the quantity being tallied, but to get accurate results all the important regions must be included explicitly. As an alternative, a zero-importance mask can be used to define the viewed surface of the moderator for the point detector tally.

The emission time distribution *i(E,t)* of the moderator for a given neutron energy, also called the pulse shape function, is the intensity distribution as a function of the time at which neutrons of given energy cross the moderator surface. It is related to the spectral intensity by

$$i(E) = \int_0^\infty i(E,t)\,dt. \tag{2}$$

The emission time distribution of the neutrons leaving the moderator is usually assumed to depend on the viewing angle only in the scaling of the overall intensity. However, we demonstrate that this is not a good assumption in the case of reentrant moderators. Emission time distributions will be given as differential values averaged over the MCNPX energy and time bins, and also averaged over the viewed moderator surface. In certain instances, we normalize the time distributions by point detector tallies for spectral intensity.

3. PULSE SHAPE CALCULATIONS FOR THE IPNS C MODERATOR

3.1. Pulse Shape Calculations

Calculation of pulse shapes from reentrant moderators is inherently difficult because the emission takes place from more than one surface. Ideally the calculated quantities should all be referred to a single surface or point in space (i.e., to correspond to what is called a "physical observable" in Quantum Mechanics). This can be done in one of several ways, and our intention in this paper is to compare and contrast the different methods.

For a flat-surface moderator, the typical approach is to calculate *i(E,t)* using an emission current tally over the full 2π solid angle in the outward direction from the surface. The same time distribution is then assumed to pertain to all angles from the surface normal, which is usually a good assumption for thermal energies but is not, we find, as good in the slowing-down region. This approach does not work well for the case of the reentrant IPNS C moderator, as shown for 10 meV neutrons in Figure 3. Experimentally, we observe that the time distribution has two components, corresponding to emission from the tips of the fins and from the bottoms of the grooves.[1] These two components are not seen separately in an emission current tally into the outward 2π solid angle at the moderator surface. However, they can be recovered by tallying neutron emission separately from the fin tips and from the grooves. The two components are then added together after time-shifting the contribution from the grooves by $t = L/v$, where L is the distance between the two emission surfaces and v is the velocity that corresponds to the nominal energy of an energy bin (usually taken here as the logarithmic mean energy) in the MCNPX calculation.

This shift-and-add method has several drawbacks. First, it represents a large amount of post-processing of the data after the MCNPX run has finished. Second, there is the possibility of double-counting neutrons that cross both surfaces. Also, it is difficult, if not impossible, to generalize this result to the case of a larger number of emitting surfaces or to the case of a continuous emission surface such as the LWTS grooved moderator. Finally, the most important

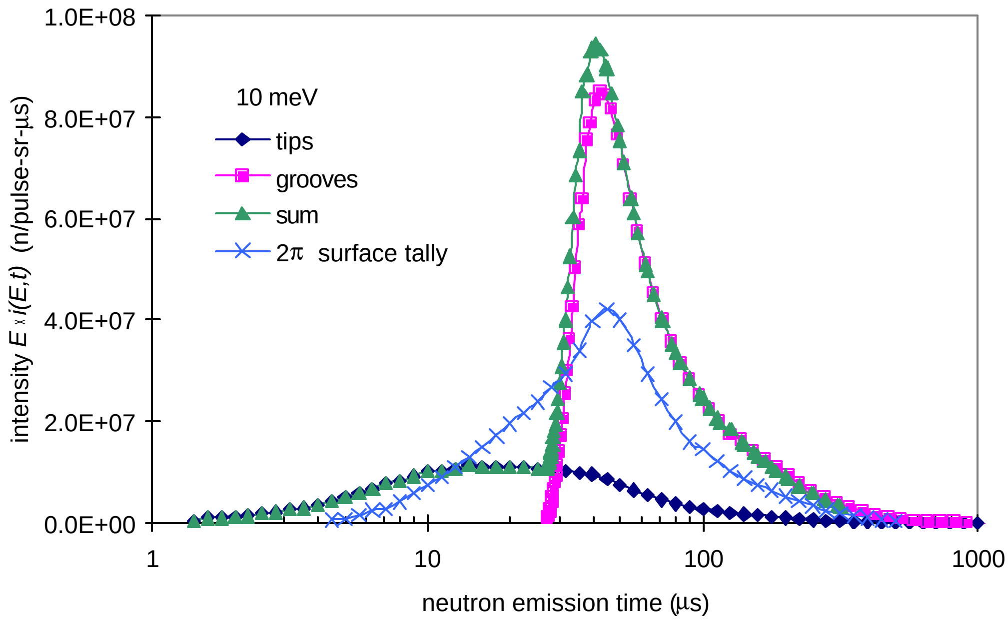

Figure 3. Neutron pulse shapes for 10 meV neutrons from the IPNS C moderator.

defect of this method is that it describes the neutron emission at all angles to the surface normal by time distributions of the same shape.

Some investigators had proposed that the contributions to the time distribution from the grooves and tips were not separately visible in the 2π surface tally in Figure 3 because the velocity dispersion within an energy band would wash out these details. That is, the difference in velocity between neutrons at the top and bottom of an energy bin would cause neutrons from the bottoms of the grooves to cross the outer surface at much different times. For example, assume that two neutrons with energies corresponding to the top and bottom of an energy bin 12.2% wide (20 bins per decade) with nominal energy 10 meV are emitted from the base of the groove at the same time. Their velocity difference would cause them to cross the outer viewed moderator surface (which is 4 cm away) 1.67 microseconds apart. As a test of this hypothesis, the emission current crossing the outer viewed surface was tallied using energy bin sizes of 20, 50, and 100 bins per decade. The results of these calculations, shown in Figure 4, reveal that there is in fact little dependence of the pulse shapes calculated into the 2π solid angle on the size of the energy bins used, at least for the range of energy resolutions considered here.

There is, on the other hand, a considerable difference in the pulse shape calculated as a function of the solid angle used for the tally. Figure 5 shows the results of emission current tallies into cones with axes normal to the moderator viewed surface and having the half-opening angle indicated. As the tally is made into an increasingly narrow cone about the beamline direction, the time distribution becomes more sharply defined. [In Figures 5-8, the curves have been normalized to the same integral value to allow better comparison of the pulse shapes.] Below a half-opening angle of 10 degrees there is no further change in the pulse shape. This cone angle was used in all subsequent calculations.

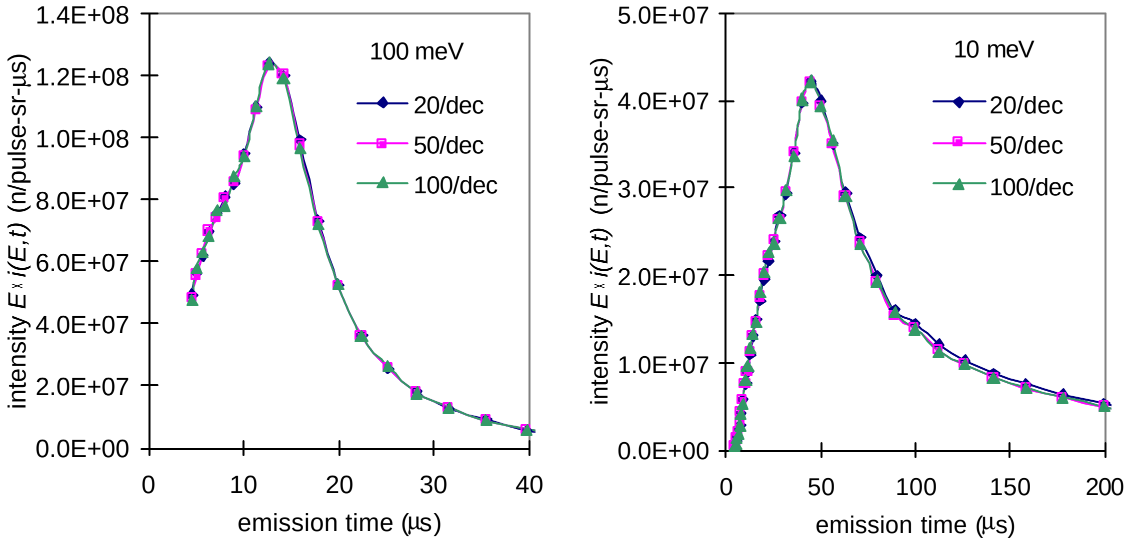

Figure 4. Calculated neutron pulse shapes from the IPNS C moderator as a function of energy bin width (bins per decade).

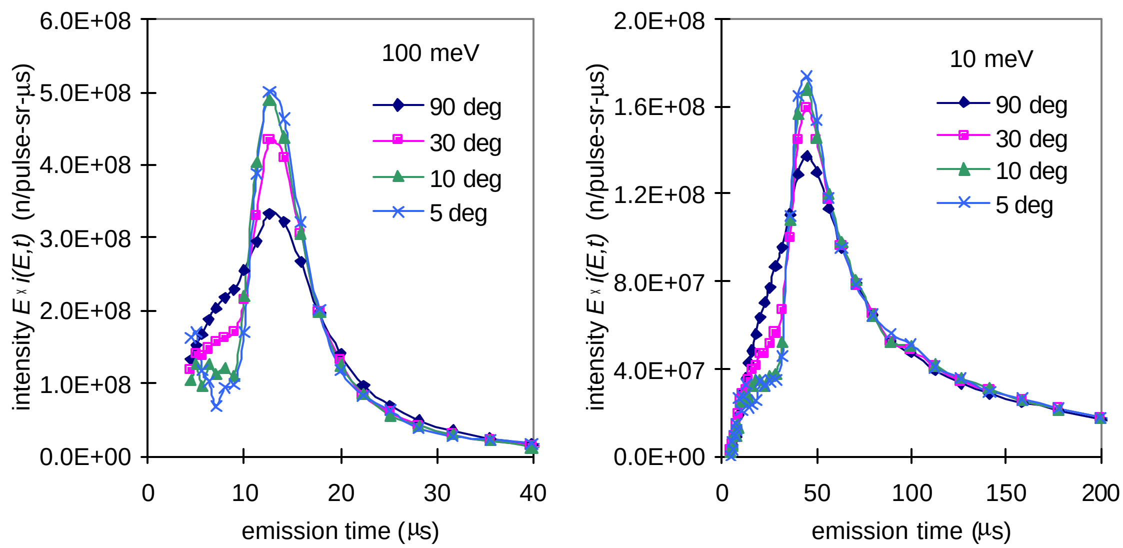

Figure 5. Calculated neutron pulse shapes from the IPNS C moderator as a function of solid angle about the surface normal (20 energy bins per decade).

We can then compare the results of pulse shape calculations using the emission current into a 10-degree cone at the moderator surface with those obtained by the shift-and-add method. These results are shown in Figure 6. The shift-and-add method underestimates the leading part of the pulse and overestimates the large peak because the currents are tallied at the interface between the moderator material and the aluminum jacket. This has the effect of underestimating the contribution from the fin tips and overestimating that from the bases of the grooves. Standard pulse shape metrics (time of maximum emission, average emission time, FWHM) for the two methods appear to have nearly the same values, except for energies below 1 meV. This is a confirmation of the usual warning to instrument designers to use the detailed pulse shapes in instrument performance calculations rather than simply relying on metrics obtained from a reduction of the data.

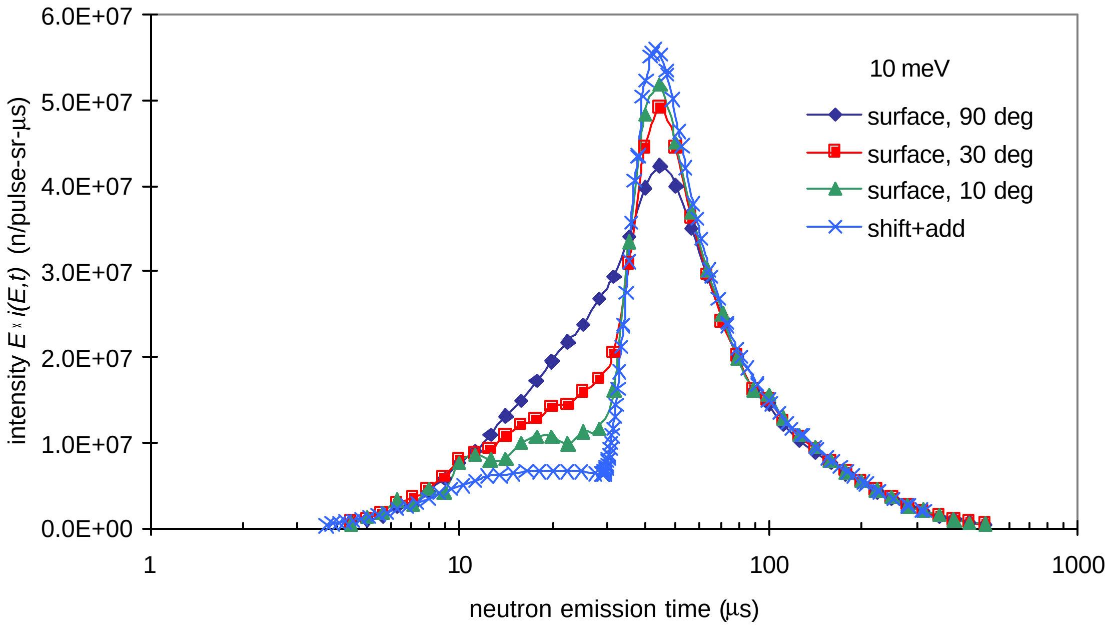

Figure 6. Neutron pulse shapes for the IPNS C moderator.

The shift-and-add method treats all angles as having the same relative time distribution, which is clearly not true. Figure 7 shows the calculated pulse shapes at the viewed surface of the vertically grooved C moderator for the beamline normal to the moderator face (designated C2) and for beamlines located ±18° from the normal in the horizontal plane (designated C1 and C3). For each case, the time distributions were calculated by an emission current tally into a cone of half-angle 10° around the beamline direction. The sharp inflection point between the neutron emission from the tips and the grooves visible for the C2 beamline is not seen in the C1 and C3 beamlines because (a) these beamlines do not directly view the bottoms of the grooves, and (b) they view a continuum emission surface along the tips and sides of the grooves. Standard pulse shape metrics such as FWHM also have different values for each beamline.

Calculation of the emission current into a narrow cone at the viewed surface also has the advantage of allowing estimates of the spectral intensities and pulse shapes for a somewhat different system without fully modeling it in the geometry. For example, we can estimate the pulse shapes from a coupled horizontally-grooved C moderator at IPNS, using the same MCNPX model as in the calculations above, by calculating the neutron emission within a small cone about the direction vectors that point vertically ±18° from the direction of the C2 beamline. Note that

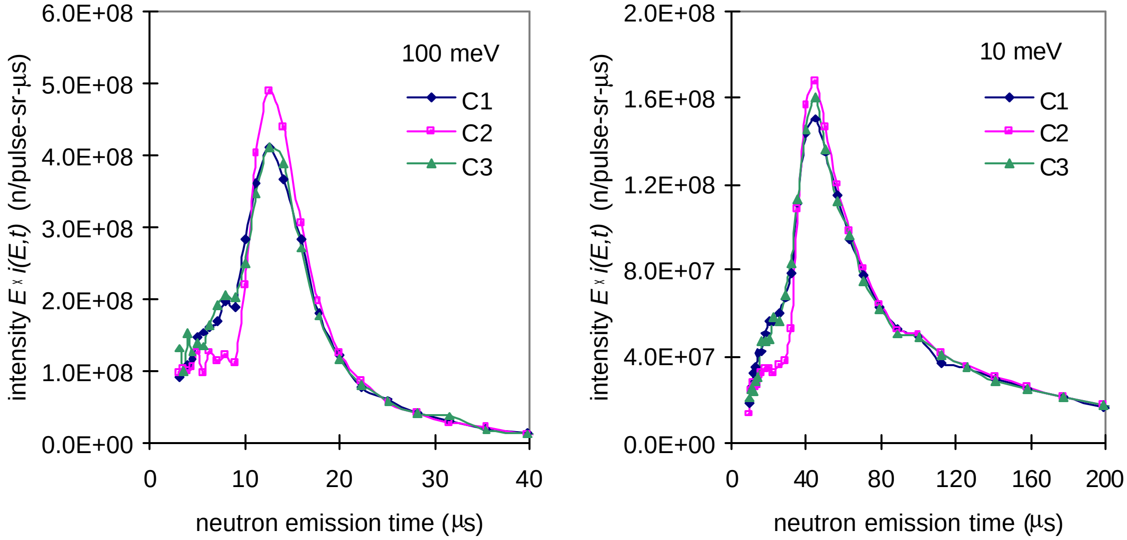

Figure 7. Neutron pulse shapes for beamlines on the IPNS C moderator.

we could not calculate these pulse shapes using the standard technique because (i) the technique yields the same pulse shapes for all angles and (ii) one cannot put a point detector in the appropriate location for the spectral intensity tally, as that point detector would no longer be aligned with the neutron beamline opening. Figure 8 shows the results from such a calculation. Here we see that the pulse shapes are nearly the same for the three beamlines because they are all looking at both the tips and grooves of the moderator face. Also, the sharp inflection in the pulse shape is preserved because the beamlines do not see as much of the sides of the grooves. Thus the shift-and-add method appears to give better results for the case of a horizontally-grooved C moderator than for a vertically-grooved moderator.

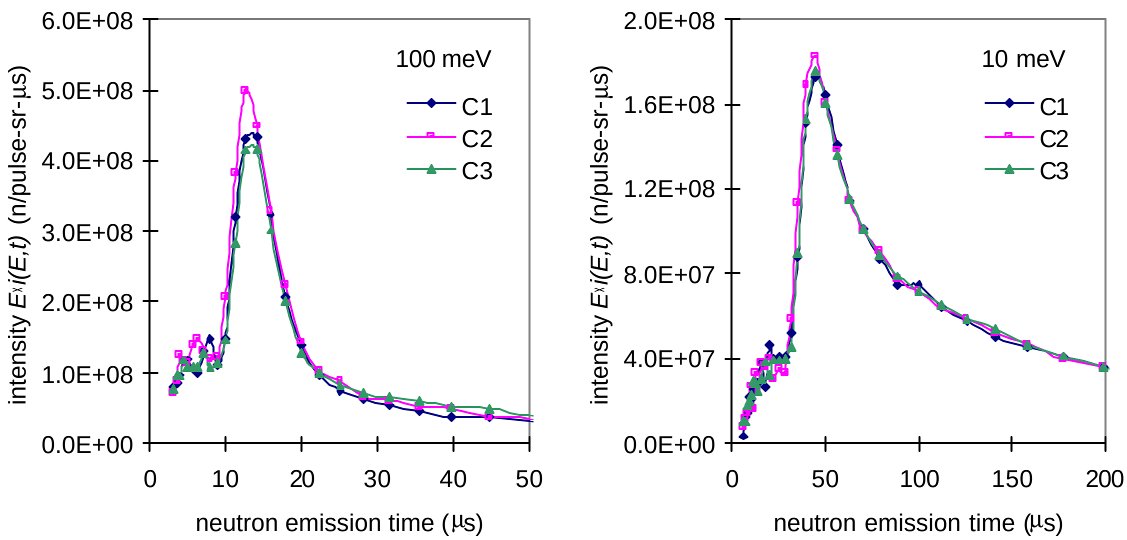

Figure 8. Neutron pulse shapes for beamlines on a horizontally-grooved IPNS C moderator.

3.2. Pulse Shape Normalization

In earlier work, the pulse shapes as calculated by the emission current tally were normalized at each energy to the results of a point detector tally to get the absolute neutron emission. For reasons of efficiency, the point detector calculations usually included contributions from scattering events only within the moderator material (i.e., neglecting the effects of the moderator jacket) and within the reflector region immediately behind the moderator. However, the proper thermal neutron intensity cannot be calculated unless one includes scattering events in the structural material of the jacket. Figure 9 shows a comparison of the neutron spectral intensity from both an emission current tally into a 10-degree cone and from a point-detector tally where contributions are made from various regions in and around the moderator. The thermal neutron intensity calculated using a point detector is less than that calculated by the emission current tally unless contributions from the moderator jacket are included. In the slowing-down region, even when we include contributions from the part of the reflector that lies directly behind the moderator, the point detector tally still underpredicts the epithermal neutron intensity. This indicates that some epithermal neutrons come from adjacent regions of the reflector. Of course, including contributions from a larger volume in the point detector calculation reduces its efficiency relative to the emission current tally.

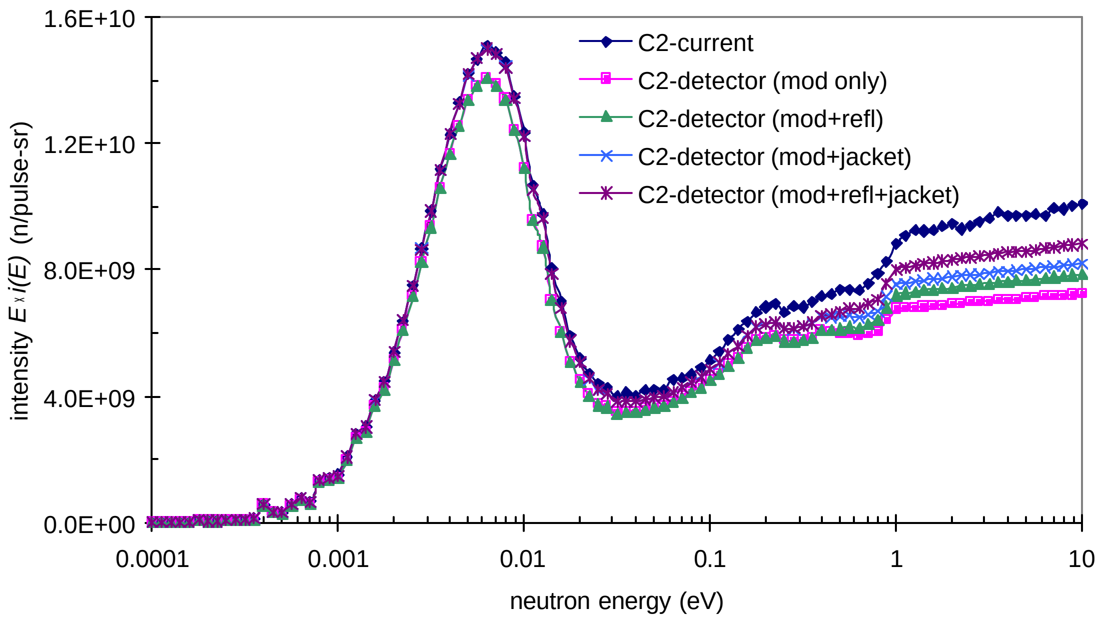

Figure 9. Comparison of neutron spectral intensity for the IPNS C moderator calculated by current and point detector tallies.

3.3. Time-of-Flight Point Detector Tally

We have generated some preliminary results using a time-of-flight point detector routine [6] written for MCNPX version 2.1.5. This tally operates by assigning each detector tally contribution to the time at which a neutron crossed a specified surface on the way to the point detector rather than the time at which it reaches the point detector location. The name derives from the fact that the neutron time-of-flight is used to adjust the time recorded in the tally. Figure 10 shows a comparison of the neutron emission time distributions at 100 meV and 10 meV as calculated using both the time-of-flight point detector and the neutron emission current tally into a cone with an opening half-angle of 10° (as in Section 3.1). There is excellent agreement between the two calculations. What is particularly impressive is that the time-of-flight point detector tally reaches a 5% fractional standard deviation at the peak of the 10 meV emission distribution in only 22 minutes of computer time, compared with about 4460 minutes for the emission current tally. [For comparison, the shift-and-add technique for pulse shape calculation takes about 370 minutes to reach the same level of statistics.] While the time-of-flight point detector is not yet sufficiently developed to be used for routine calculations, these results show that it has exceptional promise.

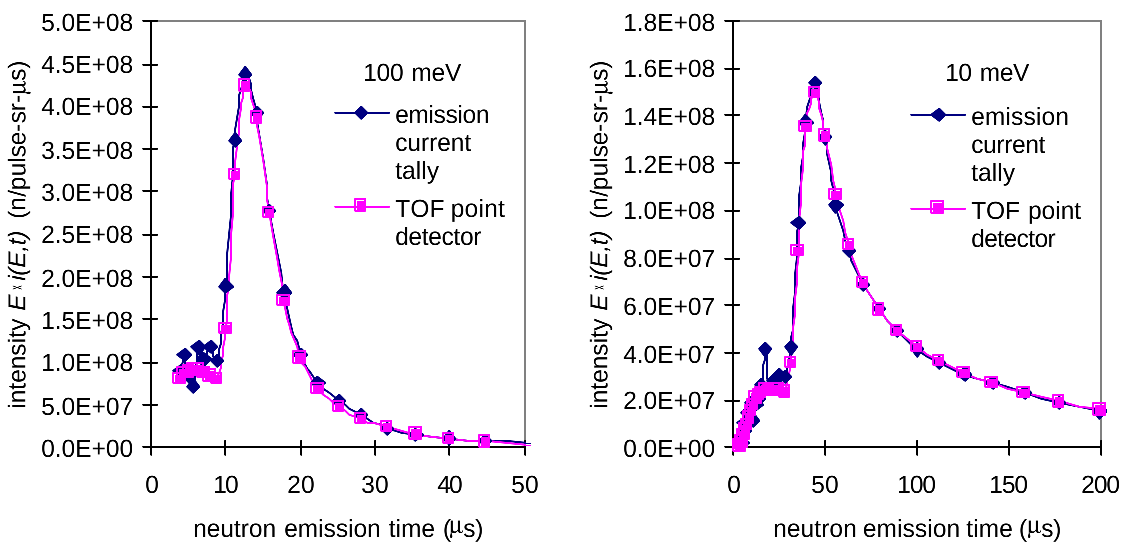

Figure 10. Comparison of pulse shapes calculated by neutron emission current tally and by time-of-flight point detector tally.

4. PULSE SHAPE CALCULATIONS FOR THE LWTS GROOVED MODERATOR

The reference design for the coupled, horizontally-grooved moderator at the LWTS specifies nine beamlines spaced 11.25° apart in the horizontal plane, with the central beamline in the direction normal to the moderator surface. Energy-dependent pulse shapes were calculated for these beamline directions, numbered P1 through P9 (where P1 was inclined toward the upstream end of the target and P5 is normal to the viewed moderator surface). Figure 11 shows these results for neutron energies of 100 meV and 10 meV. In these graphs, the results have been normalized so that the peak height of all the curves is the same, permitting the differences in pulse shapes for individual beamlines to be more readily visible. At increasing angles from the normal, we see that there is a much longer tail to the time distribution. The larger peak and average emission times are caused by the fact that the path length to the tally surface is longer for neutron beams at a larger angle to the normal, rather than a real physical effect. Not shown in these figures is the fact that the peak of the distribution is lower at the larger angles, and that neutrons with a temperature characteristic of the reflector begin showing up at larger angles [7].

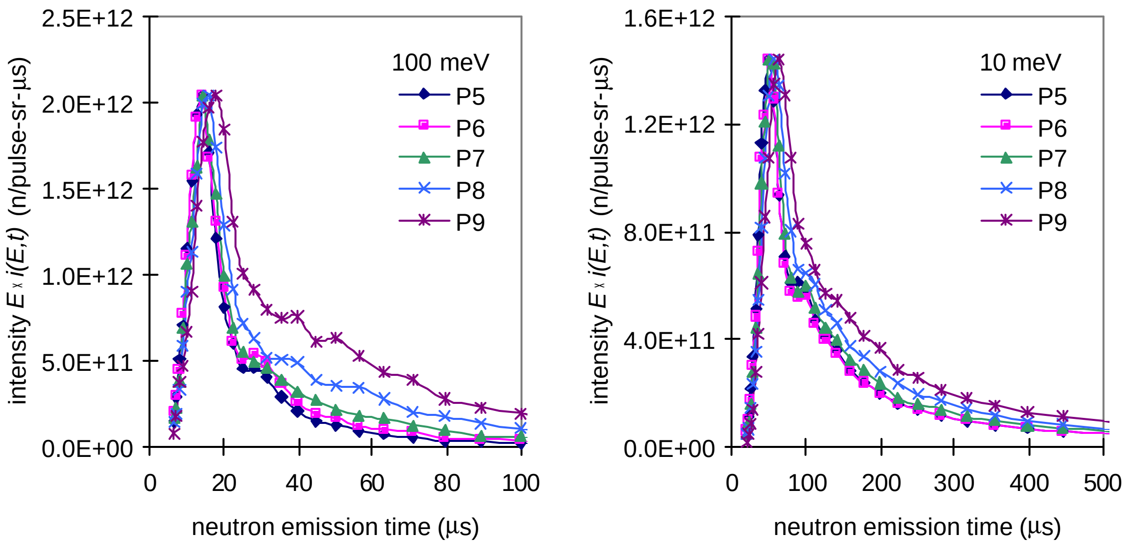

Figure 11. Neutron emission time distributions for beamlines on the LWTS coupled grooved moderator.

5. CONCLUSIONS

Previous methods for calculating pulse shapes from reentrant moderators used the same technique that has been applied to flat moderators: determining the pulse shapes by calculating neutron emission time distributions into the outward 2π solid angle through the viewed face, and normalizing the results at each energy to the result of a point detector tally for spectral intensity. Such calculations served as an approximation to the true result, often made necessary by practical limitations on the amount of computational power that could be brought to bear on the problem. The present work describes a more rigorous approach to pulse shape calculations that substantially improves the earlier results and extends pulse shape calculations to situations that could not be addressed with previous methods. With the ready availability of inexpensive computer hardware and software to build clustered systems, the ability to perform such calculations is now well within the reach of even modest research budgets. A time-of-flight adjusted point detector tally could calculate the pulse shapes more rapidly and to the same accuracy as an emission current tally into a small cone, assuming that the time distribution at each energy does not depend on the geometric regions included in the tally.

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