High Energy Neutron Scattering Benchmark of Monte Carlo Computations

F.J. Saglime, Y. Danon, R.C. Block, M.J. Rapp, R.M. Bahran

Rensselaer Polytechnic Institute Department of Mechanical, Aerospace and Nuclear Engineering Troy, New York, 12180

D.P. Barry, G. Leinweber, N.J. Drindak (ret.), J.G. Hoole

Knolls Atomic Power Laboratory P.O. Box 1072, Schenectady, New York, 12301

ABSTRACT

Neutron scattering measurements are made using an array of proton recoil detectors surrounding a scattering sample, which is struck by a beam of neutrons. Detector signals are analyzed using a state of the art digital data acquisition system, and these measurements are compared with the expected detector response based on Monte Carlo simulation of the scattering experiment using existing nuclear data evaluations. In this way, high accuracy neutron scattering experimental benchmarks, combined with high accuracy Monte Carlo simulations, can be used to assess differences among nuclear data evaluations. Experiments were done with C, Be and Mo samples. There is excellent agreement for C, while Be and Mo show differences between the experiments and calculations using ENDF/B-VII.0

Key Words: scattering, neutron, benchmark, detection.

1. INTRODUCTION

Various evaluations and nuclear data sets are available which specify neutron scattering cross section information for the different elements and isotopes. These evaluations are based on a combination of theory and a limited number of experiments, and they do not always agree with each other. In such cases, additional high accuracy data and simulations can be used to help assess the differences and arbitrate among them. In the current work, a new scattering detection system and data processing methods were developed and validated using a benchmark. Two materials were measured which exhibit variation in scattering cross section information between the major data sets (molybdenum and beryllium) to demonstrate the effectiveness of the system and methods. A range of angles and energies were measured and the results were compared to theoretical predictions with existing data to provide a proof of principle confirmation of the new capability at the Rensselaer Polytechnic Institute (RPI) Linear Accelerator (LINAC).

2. METHOD

2.1. Current Method

The method enables discrimination between evaluations by measuring the scattered neutrons over a range of scattering angles and energies, and with proper experimental design, resolution of the issue was achieved in a single experiment instead of a long series of experiments [1,2]. Using a pulse of neutrons generated from a (γ ,n) reaction in tantalum, scattering information was acquired in the energy range from 0.5 MeV to 20 MeV simultaneously in an array of eight 5 in (dia) x 3 in EJ301 [3] detectors placed at specific angles around a scatterer (see Figure 1). The time-of-flight (TOF) method was employed to resolve incoming neutron energy, and pulse shape analysis was used to distinguish between gammas and neutrons [4,5,6]. The experiment was simulated with MCNP5 [7] using several neutron scattering cross section libraries. The calculations were compared to the experimental data revealing which cross section evaluation best fits the data [1,2].



Figure 1 – Scattering Experimental Setup (For illustration, only 4 of the 8 detectors are shown)

2.2. Comparison to other Benchmarks and Experiments

Other scattering experiments have been done using a pulsed neutron source with detectors placed at angles surrounding the sample. For example, the LLNL Pulsed Sphere Experiment [8] and the Fusion Neutronics Source (FNS) [9] which use a pulsed mono-energetic deuterium-tritium (D-T) source. In these experiments, the 14.2 MeV source neutrons lose energy through multiple scattering in thick samples. The energy distribution of the leakage flux was then measured using the TOF method at several angles. However, little differential scattering cross section information could be extracted for lower energies since the source neutrons collided numerous times in the sample. The results were highly dependent on the geometry and the total scattering cross section.

Scattering experiments done at ANL using mono-energetic neutrons were able to directly measure the differential scattering cross sections [1,2]. However, they were difficult and time consuming to perform since each energy required moving the experimental setup. In addition, there is the well known gap in energies (between 8 and 13 MeV) that can not be achieved using such methods [10]. At the other energies accurate angular distributions were obtained.

The advantages of the present experiment were that a pulsed white source was located far enough away from the scatterer that the TOF method could be used to measure the initial energy of the scattered neutrons, and by controlling the thickness of the sample the amount of multiple scattering contribution can also be controlled. Unlike the FNS [9] and the LLNL Pulsed Sphere Experiments [8] scattering continuations to all energies have a single scattering component. The main advantage of the integral measurements at FNS and the LLNL Pulsed Sphere Experiments was their cross section sensitivity. And the main advantage of the ANL mono-energetic measurements was the ability to extract differential scattering cross sectional information directly. The experiment described here offered the ability to do a quasi-integral benchmark experiment which gave results that were still sensitive to the differential scattering cross sections.

3. RESULTS

3.1. System Validation

To validate the system, measurements were done with Carbon for which the total cross section is predominantly scattering. In the desired energy range carbon has a total cross section which has been extensively measured and for which all evaluations agree. Recent high precision measurements of total cross section provided additional verification of the ENDF/B total cross section for this material[11]. The geometry, neutron flux energy distribution and detector efficiency information were input to a Monte Carlo (MCNP5) analysis to simulate the entire experiment. Several effects were simulated in the MCNP model including the transmission and scattering in air, detector efficiency and size, but the detectors themselves were not modeled, so scattering from the detectors was not included since the effect was so small. Validation is accomplished by comparing the calculated results to the experimental results

The detector efficiency was found by using SCINFUL, a Monte Carlo code for determining efficiency of proton recoil detectors [12], and validated experimentally with an independent inbeam flux measurement using a Li-6 glass detector. Pulses that over ranged the analog to digital converter (ADC) were rejected which leads to a lower efficiency than would otherwise be observed.

The LINAC target produces an energy spectrum that is closely approximated by an evaporation spectrum with a 0.5 MeV temperature. The LINAC also produces an intense gamma flash. Therefore, a 1 in. thick piece of depleted uranium was used as a gamma shield. This changed the flux shape at the scattering sample, but was easily accounted for in the MCNP model. The flux was found using an average between the EJ301 flux measurement and the Li-6 glass measurement weighted by the confidence level in the energy region for each detector.

3.2. Results for Carbon Benchmark

The cross section of carbon has structure in the 2 to 10 MeV range resulting in complicated differential scattering distributions. Therefore, the results from the transport model were sensitive to the characterization of the differential scattering distribution. This unique fingerprint

in the detector response provided a way to test the timing and resolution of the data collection system. In order to optimize the scattering yield in the detectors, a 7cm thick slab of carbon was used. Figure 2 shows the experimental and simulation results together; the results are in excellent agreement. The structure in the detector response below 2 MeV comes from interaction of the neutrons with the air, which the neutrons pass through before striking the carbon, and must be accounted for in the simulation. Below 1 MeV, the efficiency of the detector falls off rapidly and has a cutoff at about 0.5 MeV. As a result, the detector response goes to zero even though neutrons as low as 0.1 MeV are actually present. The structure above 2 MeV comes from the carbon [1].



Figure 2 – Carbon (7cm thick) Scattering Results – EJ301 Detector Response at 52 deg. (left) and 90 deg. (right)

3.3. Proof of Principle Results

Using the same system and methods, the carbon scatterer was replaced with a material of interest. In the same manner as above, measurements and MCNP5 simulations were performed using various existing data sets. Observed differences between experiment and simulation indicate potential errors in the evaluation. Figure 3 shows the result of such an experiment with 8 cm of molybdenum at a scattering angle of 90 degrees. Unlike carbon, there is no significant structure in this energy range. The only visible structure is due to neutron attenuation in air. The MCNP simulations used to compare to the experimental results in both Figures 3 and 4 include air effects. Simulations with ENDF/B-VI.8 and ENDF/B-VII.0 yield significantly different results, and this method gives a reliable way of selecting which evaluation agrees better with experiment (ENDF/B-VII.0 and JEFF 3.1). Figure 4 shows the result of another experiment with beryllium. The ENDF/B-VI.8, ENDF/B-VII.0, and JEFF 3.1 libraries are all in very close agreement. Only one resonance stands out. The thin sample scattering results agree with the Monte Carlo calculation more closely than the thick sample scattering results. In the thick sample case, there is almost twice as much multiple scattering taking place as in the thin sample. This suggests that small errors in the scattering cross section evaluation used in the simulation are accumulating resulting in a noticeable error for the thick sample. In general, selection of

sample thicknesses can be done to optimize for scattering yield or control the amount of multiple scattering.



Figure 3 – Molybdenum Scattering Results at 90 degrees



Figure 4 – Beryllium Scattering Results: 4 cm thick sample (left) and 8 cm thick sample (right)

3.4 Sample Thickness Effects

The validation with carbon was done using a single sample thickness since the carbon cross section was assumed to be reliable. However, for testing a cross section library, multiple thicknesses should be used in the experiment. A thick sample will have more multiple scattering. This weakens the link between the angular data collected by the detectors and the differential scattering cross section. In spite of this, the increased number of interactions in the

sample makes for a better benchmark. Unless the data library is perfect, increased thickness will result in worse agreement between simulation and experiment. The discrepancies tend to appear in the forward and backward angles as sample thickness is increased. A thin sample will have less multiple scattering, and is therefore more correlated to the differential scattering cross sections. In this case, the angular data collected by the detectors can be used to produce the energy dependent angular distributions. But, a thin sample will also have a much lower scattering yield, so it would require more time (cost) to achieve the same statistical accuracy under the same beam conditions. To discriminate between nuclear data libraries, it is best to use a sample thickness which optimizes the scattering yield as one of the samples.

4. CONCLUSIONS

The method proposed here uses a combination of Monte Carlo calculation and experiment to assess differences in the scattering cross section evaluations. The Monte Carlo code is required to accurately model the experimental setup including the neutron source, detector efficiency and the time dependent neutron transport in the sample and the rest of the system. As was shown, a combination of MCNP and SCINFUL provided results that were in excellent agreement with carbon data and validate the system and methods. Preliminary results on two materials (molybdenum and beryllium) show this benchmarking method can be useful to discriminate between nuclear data evaluations at energies where there are differences in the angular distributions for the differential scattering cross sections. In addition to elemental samples, heterogeneous and composite materials can easily be accommodated as well. Ongoing work at the LINAC to improve the source strength will allow thinner samples to be used. This will reduce the amount of multiple scattering, opening up the possibility for direct differential scattering measurement over a wide range of energies in one experiment.

REFERENCES

- 1. A. Smith and P. Guenther, Argonne National Laboratory Report, ANL/NDM-43 (1978).
- 2. A. Smith and P. Guenther, Argonne National Laboratory Report, ANL/NDM-76 (1982).
- 3. Eljen Technology, "EJ-301 Liquid Scintillator", http://www.eljentechnology.com/datasheets/EJ301%20data%20sheet.pdf
- 4. S. Marrone, et al, "Pulse shape analysis of liquid scintillators for neutron studies", *Nuclear Instrumentation and Methods in Physics Research A*, 490, pp. 299-307 (2002).
- 5. J. H. Lee, and C. S. Lee, "Response function of NE213 for 0.5 6MeV neutrons measured by an improved pulse shape discrimination", *Nuclear Instrumentation and Methods in Physics Research A*, **402**, pp. 147-154 (1998)
- 6. G. F. Knoll, Radiation Detection and Measurement, Wiley, New York & USA (1989).
- 7. MCNP, A General Monte Carlo Code for Neutron and Photon Transport, Version 5, LA-UR-05-8617 (2005).
- 8. C. Wong, et al, Livermore Pulsed Sphere program: Program Summary through July 1971, UCRL-51144, Rev. 1, 1972.

- 9. Y. Oyama, S. Yamaguchi, and H. Maekawa, "Measurements and analyses of angular neutron flux spectra on graphite and lithium-oxide slabs irradiated with 14.8 MeV neutrons", J. *Nucl. Sci. Techn.* **25** pp 419-428, 1988.
- 10. R. C. Haight, J. M. O'Donnell, L. Zanini, M. Devlin, and D. Rochman, Los Alamos National Laboratory Report, LA-UR-02-5486 (2002).
- M. Rapp, et al, "High Energy Neutron Time of Flight Measurements of Carbon and Beryllium Samples at the RPI LINAC", International Conference on Mathematics, Computational Methods & Reactor Physics (M&C 2009)
- 12. Scintillator Full Response to Neutron Detection (SCINFUL), PSR-0267, Oak Ridge National Laboratory, 1988.
- 13. The n_TOF Collaboration, Proposal for a neutron time-of-flight facility, CERN/SPSC 99-8, SPSC/P 310 (1999).