STATUS OF DEUTERIUM NUCLEAR DATA FOR THE SIMULATION OF HEAVY WATER REACTORS

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Abstract

An overview is presented of the status of the deuterium nuclear data used in reactor physics simulations of heavy water (D_2O) reactors and of ongoing activities to improve their accuracy. The main subjects having noticeable reactivity impact for critical systems involving D_2O are the degree of backscatter in D(n,n)D elastic scattering at neutron energies <3.2 MeV, the value of the elastic scattering cross section at thermal neutron energies and the adequacy of their numerical representation in evaluated nuclear data libraries. The scope includes fundamental nuclear-data measurements; three-body nuclear-theory calculations; and MCNP5 simulations of experiments involving D_2O or deuterated targets.

1. Introduction

Although great strides have been made in the accurate representation of reactors using Monte Carlo particle transport codes, such as MCNP5 (Monte Carlo N-Particle) [1], the reliability of the results of such simulations is limited by the completeness and accuracy of the description of the fundamental physical processes involving the creation, transport and removal of neutrons as represented in associated input nuclear data files. MCNP5 uses data files that are prepared using a data processing code, such as NJOY [2, 3], from evaluated nuclear data libraries and converted from ENDF (Evaluated Nuclear Data File) format [4] into ACE (A Compact ENDF) format.

In typical MCNP simulations of Heavy Water (D_2O) Reactors (HWRs), the deuterium (D = ^2H) nuclear data play a key role since about 190 collisions typically occur per source neutron (i.e., produced from fission), of which about 65% involve deuterium (about 29% involve ^{16}O). A reasonably complete description of the deuterium nuclear data for HWR simulations requires three separate ACE files:

- A 'fast' D data file, containing descriptions of the following nuclear reaction channels, and combinations thereof
    - D(n,n)D elastic scattering, the differential cross section of which is given by

$$\sigma_s(E,\mu) = \frac{\sigma_s(E)}{2\pi} P(E,\mu) \tag{1}$$

in b/sr where μ is the cosine of the scattering angle in the centre-of-mass (CM) reference frame, E is the incident neutron energy, $\sigma_s(E)$ is the elastic scattering cross section and $P(E,\mu)$ is the energy-angle (cosine) probability distribution. $\sigma_s(E)$ and $P(E,\mu)$ are the main subjects of this paper, as the values used in various evaluated nuclear data libraries have noticeable impact on the physics of HWRs, such as the calculated neutron multiplication constant, k-effective (k_{eff}), up to a level of about 1% (10 mk = 1000 pcm). Increasing $\sigma_s(E)$ increases k_{eff} as does increasing the relative amount of backscatter in $P(E,\mu)$, in part, since both effects reduce neutron leakage.

- $D(n,\gamma)^3H$ neutron capture. Recent work [5] suggests that the thermal (0.0253 eV) capture cross section should be increased by about 8.1% to 549 ± 10 mb. However, the reactivity impact of this change is small (~1 mk or less [6]) because few captures occur in D (only ~1% of the particle weight [1] lost to captures in an HWR occurs in D).

- $D(n,2n)^1H$ deuterium breakup. Noticeable differences are observed [7] between the (n,2n) cross section values for D in different evaluated data libraries and from values derived from nuclear theory. However, the particle weight gain from (n,2n) reactions in D is only about 0.6% of that gained from fission in a typical HWR simulation, so that the reactivity impact of such differences is small [7].

- A 'thermal' data file for D-in-D_2O. The thermal data file is produced from an ENDF file for D using the LEAPR module of NJOY and Thermal Scattering Law (TSL; $S(\alpha,\beta)$) data for D_2O. While the TSL data for D_2O have been re-evaluated [8] and improvements made concerning the numerical treatment of the thermal data [9], such changes were not found to have significant reactivity impact for HWR applications. However, a small discrepancy exists between experimental data and the new evaluation [8] and its possible impact on HWR simulations warrants further investigation.

- A photonuclear data file for the $D(\gamma,n)^1H$ deuterium breakup reaction for photon energies above the 2.2246 MeV threshold. Although usually neglected in MCNP5 HWR simulations, explicit treatment of the D photonuclear reaction was found to increase k_{eff} by about 0.4 to 0.7 mk in the simulation of several critical experiments [6]. Recent work [10] suggests that the photonuclear cross section for D should be increased at incident energies <7 MeV. While MCNP5 simulations of critical experiments showed an increase of about 12% in the production of photoneutrons from D using data based on Reference [10], the impact of this change on k_{eff} was very small (<0.2 mk) [6].

2. Reactivity sensitivity to $P(E,\mu)$

During post-release testing of the final version of ENDF/B-VI (ENDF/B-VI.8), it was discovered [11] by R.D. Mosteller of Los Alamos National Laboratory (LANL) that calculated eigenvalues for a set of D_2O solution benchmarks had decreased substantially (by about 10 mk) relative to an earlier version, ENDF/B-VI.4. The cause was traced to modifications made to the deuterium cross sections in ENDF/B-VI.5 and retained through ENDF/B-VII.0 [12]. In the ENDF/B-VI.5 evaluation, $\sigma_s(E)$ and $P(E,\mu)$ below 4 MeV were compared to results of a coupled-channels R-matrix analysis [13]. The $\sigma_s(E)$ from ENDF/B-VI.4 was found to be consistent with this R-matrix analysis and was retained. However, the $P(E,\mu)$ data below 3.2 MeV were replaced with new tabulated distributions from the R-matrix analysis [13].

The experiments displaying high sensitivity to the $P(E,\mu)$ encompass two sets performed at LANL in the early 1950s using homogeneous solutions of High-Enriched Uranium (HEU; 93.7 atom % ^{235}U) fluoride in D_2O – one with D_2O-reflected spheres, HEU-SOL-THERM-004 (HST-4), and the other with unreflected cylinders, HEU-SOL-THERM-020 (HST-20) [14]. Both sets have high neutron leakage (~40%) and relatively large uncertainties for the benchmark k_{eff} (±3.3 to ±5.9 mk for HST-4 and ±7.7 to ±11.6 mk for HST-20). Since the HST-20 experiments required corrections (about 4.1 mk) for 'room return' of neutrons and the results for HST-4 deteriorated with the changes to deuterium in ENDF/B-VI.5, it was suspected that the ENDF/B-VI.4 $P(E,\mu)$ data were preferable for systems with high leakage.

In marked contrast, it was found that MCNP5 simulations of modern ZED-2 (Zero Energy Deuterium) critical experiments at AECL's (Atomic Energy of Canada Limited) Chalk River Laboratories (CRL) showed [15] little sensitivity (<1 mk) to the change in the deuterium data. The ZED-2 facility consists of a large cylindrical aluminum tank containing D_2O moderator and surrounded in the radial and lower axial directions by a graphite reflector. Vertical heterogeneous fuel assemblies are suspended within the tank on a regular lattice pitch to form lattice arrays. Criticality is achieved by raising the D_2O moderator level. The initial ZED-2 experiments studied were characterized by low neutron leakage (about 9% to 14% from the D_2O moderator surfaces), natural uranium (NU; 0.72 atom % ^{235}U) fuel and a highly thermalized spectrum (about 92% of fissions occur at neutron energies <0.625 eV).

Subsequent investigations [16] using a simple, two-region numerical benchmark consisting of an uranium metal sphere of either pure ^{235}U or NU surrounded by a D reflector (at the number density for D_2O) captured the basic features of both the HST and ZED-2 results.

The manner in which the sensitivity of k_{eff} to the change in the D data is reduced in going from HEU to NU is examined using MCNP5 calculated neutron-fission-yield tallies as a function of incident neutron energy for similar, highly simplified, non-reflected critical spheres containing either pure ^{235}U or NU mixed with D at a concentration equal to that of one of the HST-4 experiments (D-to-^{235}U atom ratio of 430). Since the sum of the fission-yield tallies equals the MCNP5 track-length estimator of k_{eff} [1, 17], the difference between two sets of tallies (one using D data from ENDF/B-VI.4 and the other using D data from ENDF/B-VII.0) shows how the net reactivity impact, Δk_{eff}, arises as a function of neutron energy. Figure 1 compares the differences in the fission-yield tallies using D data from ENDF/B-VI.4 to those obtained using ENDF/B-VII.0 D data for a 50.29-cm-radius HEU ^{235}U-D sphere, a 303.70-cm-radius NU-D sphere and a 167.93-cm-radius sphere (case labeled NU5-D) for which the ^{238}U is removed from the NU, keeping the ^{235}U number density unchanged. For the ^{235}U-D case, a large net Δk_{eff} of about +13 mk is obtained, resulting from a large increase in fission yields (~13.4 mk) at energies below about 0.1 MeV and a small decrease (~0.4 mk) at higher energies. For the NU-D case, the Δk_{eff} increase is very small (<0.5 mk) and results almost entirely from contributions at low energies $<10^{-6}$ MeV. The NU5-D case shows an intermediate Δk_{eff} gain of +1.7 mk and demonstrates that the dilution of ^{235}U to a D-to-^{235}U ratio of 59,700 corresponding to the NU-D case (and adjusting the radius of the sphere to maintain criticality) accounts for much of the loss of sensitivity of k_{eff} to the D data in going from HEU to NU.

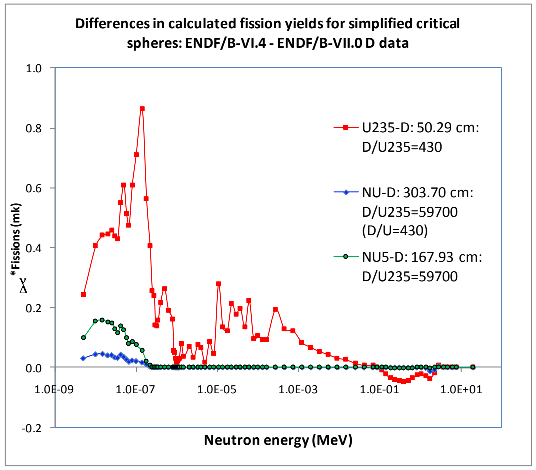

Figure 1 Comparison of differences in calculated fission yields for critical spheres using ENDF/B-VI.4 and ENDF/B-VII.0 D data.

While the initial ZED-2 k_{eff} results with NU fuel exhibited little sensitivity to the D nuclear data, they did show a small change in the D_2O coolant void reactivity (CVR) simulation bias (by about +0.6 mk using ENDF/B-VI.4 D data compared to ENDF/B-VII.0 D data), determined from the difference between the calculated k_{eff} values for critical core configurations with air-cooled fuel channels and corresponding configurations with D_2O-cooled channels. The estimated experimental uncertainty of the ZED-2 CVR bias is about ±0.3 mk (1 σ).

3. Deuterium nuclear data review

Subsequently, AECL contracted L.W. Townsend of the University of Tennessee to review [18] the experimental database supporting the angular distributions of elastic scattering $P(E,\mu)$. An example from this review is shown in Figure 2, which compares $\sigma(E,\mu)$ for D(n,n)D elastic scattering at 500 keV for data from the Adair [19] and Elwyn [20] measurements with values from the ENDF/B-VI.8 and JENDL-3.3 (Japanese Evaluated Nuclear Data Library) data libraries, the latter being based on solution of the Faddeev equation [21]. The review concluded that existing experimental data were old, sparse and inconsistent and recommended that new measurements be undertaken. In consequence, AECL submitted a measurement request to the OECD (Organization for Economic Cooperation and Development) - NEA's (Nuclear Energy Agency) High Priority Request List.

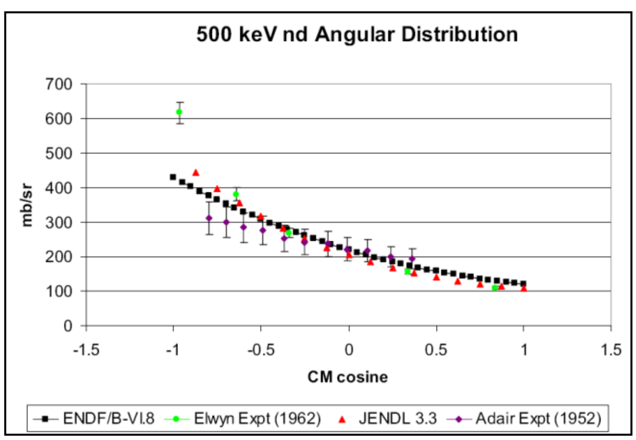

Figure 2 Comparison of D(n,n)D CM angular-distribution data at 500 keV.

4. Deuterium anisotropy comparison

A key feature of the D(n,n)D $P(E,\mu)$ distribution in the CM reference frame is the preference for backward scattering at energies below about 2.5 MeV, trending to isotropy as $E \rightarrow 0$. This anisotropy is compared in Figure 3 using the ratio of the cumulative backward-to-forward scattering probabilities extracted from the ACE files corresponding to the following evaluated nuclear data files for D, in addition to ENDF/BVII.0 and JENDL-3.3

- ENDF/B-IV based on the 1967 evaluation by B.R. Leonard and K.B. Stewart,
- Russian ROSFOND [22], which adopted the $P(E,\mu)$ from ENDF/B-VI.4,
- Chinese CENDL-3.1, based on a Faddeev calculation [23],
- Bonn-B nuclear-theory calculations (see section 5), and
- JENDL-4.0, based on a Faddeev calculation with the PEST (Paris EST expanded) potential.

Figure 3 indicates significant uncertainty in the $P(E,\mu)$ data for D and also reveals a numerical inadequacy in ENDF/B-VII.0, which has only one data table at 500 keV between 0.1 and 1.0 MeV. Refining the ENDF/B-VII.0 $P(E,\mu)$ using piecewise cubic polynomial interpolation increases the degree of backscatter and was found to increase the calculated k_{eff} for the HST-4 experiments by about 0.8 mk.

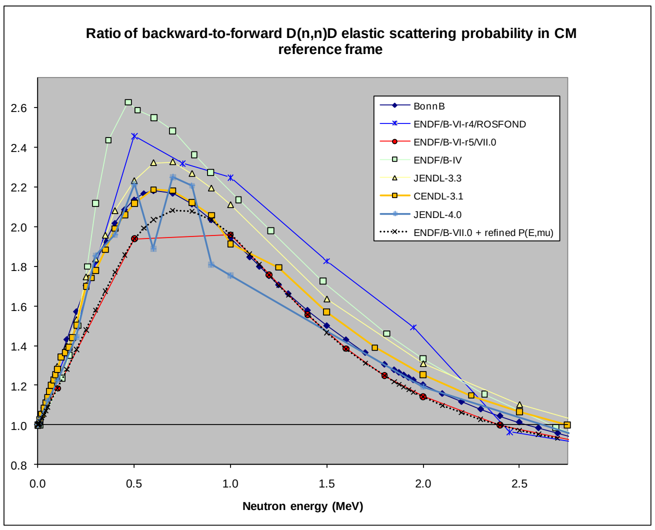

Figure 3 Ratio of backward-to-forward D(n,n)D scattering as a function of neutron energy.

5. Nuclear-theory calculations

In the absence of new measurements for D, AECL commissioned new nuclear-theory calculations by J.P. Svenne of the University of Manitoba and L. Canton of Università di Padova, using modern nucleon potentials and solution methods. In nuclear physics, neutron-deuteron scattering is important for testing three-nucleon forces, along with the ^{3}H and ^{3}He bound states and proton-deuteron scattering. Neutron-deuteron scattering and the triton, further offer a stage for testing models of the electro-magnetic interaction when direct Coulomb forces are absent. Theoretical studies are facilitated by the current detailed knowledge of the nucleon-nucleon (N-N) forces and the fact that the three-nucleon problem is sufficiently simple to be treated exactly. Initial results [24] were obtained for incident neutron energies from 50 keV to 3.0 MeV using the Bonn-B nucleon-nucleon interaction potential with the Alt-Grassberger-Sandhas (AGS) version of the three-body equations [25]. The results showed fair agreement with the $P(E,\mu)$ distribution from JENDL-3.3, and significant discrepancies with that from ENDF/B-VII.0.

The nuclear-theory calculations have been extended to include different nucleon-nucleon potentials (Bonn-B, CD-Bonn and AV18), alternate solution formalisms (AGS and Faddeev), three-nucleon forces (3NF) and the magnetic moment (MM) interaction between the neutron and the deuteron. The new data include tabulation of the differential cross section at 74 CM μ values (from –1.0 to +1.0) for the following eight combinations/variations

- Bonn-B nucleon-nucleon potential using the AGS equations (at 73 energies from 1 keV to 29 MeV).
- Bonn-B with 3NF (at 50 energies from 1 keV to 29 MeV)
- CD-Bonn potential using AGS (at 73 energies from 1 keV to 29 MeV)
- CD-Bonn with 3NF (at 51 energies from 1 keV to 29 MeV)
- Bonn-B with MM interaction (no 3NF; at 69 energies from 50 keV to 29 MeV)
- AV18 potential using Faddeev equations (at 32 energies from 20 keV to 3 MeV)
- Bonn-B using Faddeev (at 32 energies from 20 keV to 3 MeV)
- CD-Bonn using Faddeev (at 32 energies from 20 keV to 3 MeV)

The angular distributions for these eight variations are compared with those from JENDL-3.3 and ENDF/B-VII.0 at 1 MeV in Figure 4.

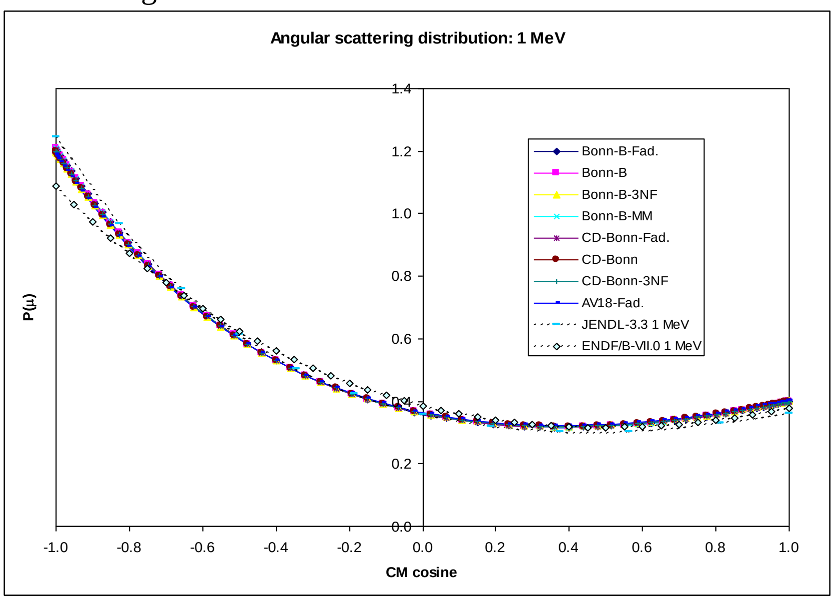

Figure 4 Comparison of D(n,n)D CM angular-distribution data at 1 MeV.

The new nuclear-theory results agree very well with each other, differing by less than about 0.9% at the extreme values of $\mu=\pm1.0$, but show more backscatter than ENDF/B-VII.0 near $\mu=-1.0$. At 1 keV, where $P(\mu)$ is essentially isotropic in the CM reference frame (see also Figure 3), the nuclear-theory results agree with each other to within about 0.002%, but still show consistently more backscatter than ENDF/B-VII.0.

6. Low-energy elastic scattering cross section

Nuclear theory was also used to calculate the (n,2n) cross section and $\sigma_s(E)$, the latter down to as low as 1 keV in some cases. The low-energy $\sigma_s(E)$ results are compared in Figure 5 with those from evaluated data libraries and the value of 3.390 ± 0.012 b (±0.35%; 3 σ) derived from Dilg's 1971 measurements [26] at 130 eV of the (total) cross sections for D_2O, SiO_2 and Si. Figure 5 shows that the nuclear-theory values are a bit high when extended to low energy and would require scaling to match measurement; Bonn-B provides the best agreement.

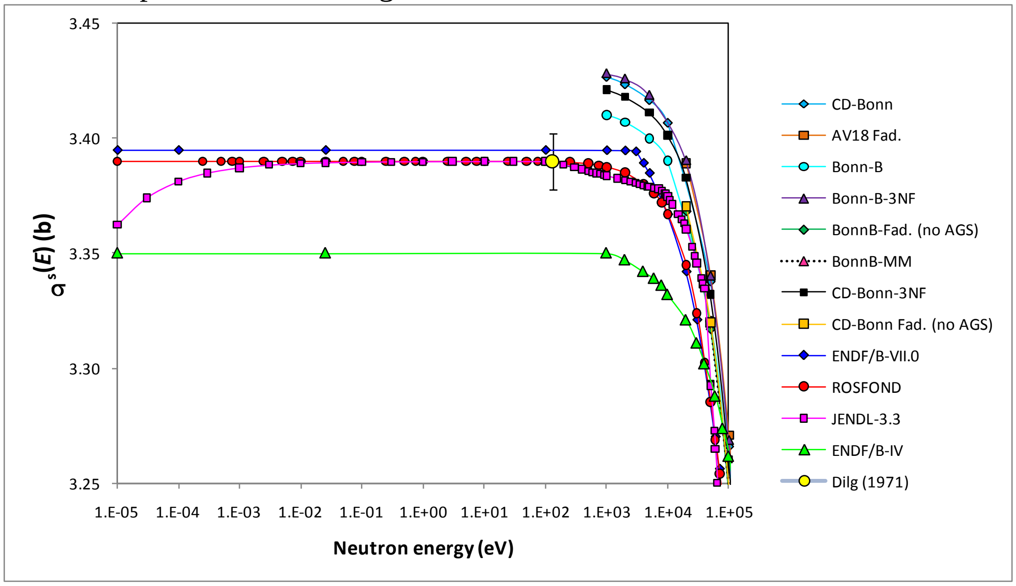

Figure 5 Comparison of low-energy D(n,n)D elastic-scattering cross-section data (at $T \rightarrow 0$ K).

The 3NF included in the present calculations, has a one-pion-exchange character and is designed specifically to take into account low-energy n-d scattering effects, in particular the spin-dependent observables (such as, e.g., the famous Ay puzzle). This 3NF has a small, but noticeable, impact also in the angular distributions. Another 3NF model, the so-called two-pion exchange, is needed to account for the scaling of the cross-section with respect to the triton binding energy.

The feasibility of obtaining a reliable value for $\sigma_s(E \rightarrow 0)$ from nuclear theory appears to be confirmed by Reference [27], which presents doublet and quartet scattering lengths derived from 48 variations of nucleon-nucleon interactions. Combining these to determine $\sigma_s(E \rightarrow 0)$ yields values ranging from 3.364 to 3.445 b with a mean of 3.390 b, which agrees with a weighted mean of 3.392 ± 0.012 b determined by A. Plompen of IRMM (Institute for Reference Materials and Measurements) from a review of experimental transmission measurements of the (total) cross section, with Dilg's value and with the value 3.390 ± 0.012 b adopted by the Atlas of Neutron Resonances [28].

However, it is noted that applying modern values of the scattering cross section for ^{16}O would reduce the derived $\sigma_s(E \rightarrow 0)$ for D by about 1.3% to 3.344 b, about the same as used in ENDF/B-IV. Such a value reduces the calculated k_{eff} by as much as 7 mk in MCNP5 simulations of the HST-4 experiments. But, in the absence of new precise σ_t measurements for D, ^{16}O or D_2O, it appears that a value close Dilg's value of 3.390 b for D should be retained. In particular, it is consistent with a modern precise measurement of the coherent neutron scattering length in deuterium, b_{nd} [29], suggesting that the $\sigma_s(E \rightarrow 0)$ for ^{16}O might instead need reexamination.

Indeed, σ_t(130 eV) from ENDF/B-VII.0 for ^{16}O is about 3.852 b, which disagrees with Dilg's value of 3.761 ± 0.007 b by about thirteen standard deviations (+2.4%). Similarly, it was noted [6] that the value of 5.875 fm for the ^{16}O coherent scattering length, b_{coh}, derived from ENDF/B-VII.0, disagrees by about fourteen standard deviations (+1.2%) with Koester's 1991 recommended value of 5.805 ± 0.005 fm [30], the latter of which agrees with Dilg's earlier value of 5.804 ± 0.007 fm and was adopted by the Atlas [28].

7. New deuterium measurements

7.1 Neutron scattering on C_6D_6

In response to AECL's data request, new D(n,n)D angular-scattering measurements were undertaken using the GELINA (Geel Linear Accelerator) neutron time-of-flight facility at the European Commission's (EC) Joint Research Centre (JRC) IRMM under the auspices of the Canada-EURATOM (European Atomic Energy Community) agreement for cooperation in nuclear research. A new experimental setup was established to detect scattered neutrons initially from a 10.2-mm-thick C_6D_6 target 80-mm in diameter inside an Al container. The choice of neutron detectors was difficult in the desired energy range as most show low efficiency, high sensitivity to gamma rays and poor stability. It was decided to use two coaxial HPGe detectors with a $^{10}B_4C$ converter placed in front of each detector.

Preliminary results for the ratio of the neutrons scattered at 150º from the target to those scattered at 120º in the LAB reference frame after one week of beam time at the 300-m scattering room are shown in Figure 6 [31] and compared with MCNP simulation results using ENDF/B-VII.0. The results in Figure 6 indicate less backscatter than predicted by ENDF/VII.0, especially at 600 keV, in contrast to the nuclear-theory calculations, which predict greater backscatter than ENDF/B-VII.0. However, with a C_6D_6 target the contributions from C as well as from the Al sample container suppress the D contribution significantly. Although Figure 3 shows a peak in the relative amount of backscatter from D near 600 keV in the CM reference frame, this is removed when estimating the ratio of 150º-to-120º scattering for C_6D_6 from just the data libraries for C and D, as a result of the transformation to the LAB reference frame. Instead, the calculated ratios vary smoothly with energy.

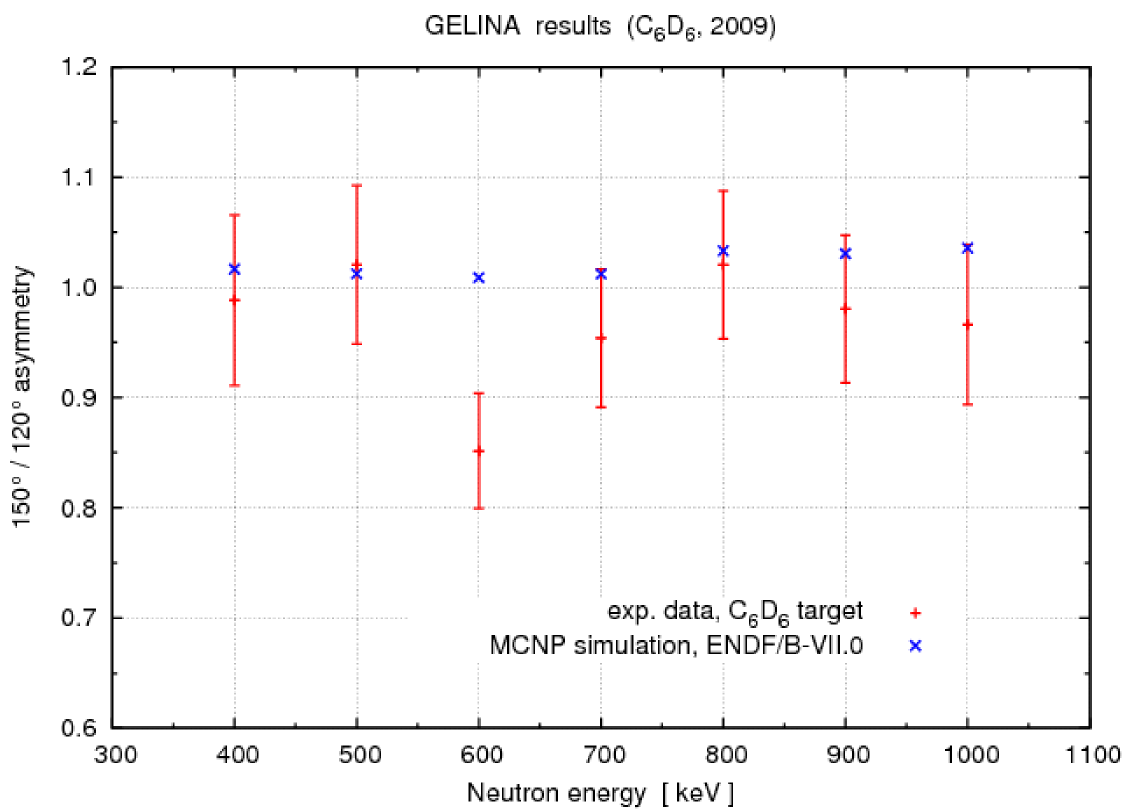

Figure 6 Ratio of LAB 150º/120º D(n,n)D scattering as a function of energy.

7.2 Neutron scattering on CD_2

To improve upon the C_6D_6 results, a higher D-to-C atom ratio is needed along with the absence of an Al container. Consequently, a 3-mm-thick deuterated polyethylene (CD_2; 99.999% D) target 70-mm in diameter was provided by AECL.

An initial attempt was made at increasing the data collection rate by moving to a more intense 30-m scattering position. However, this turned out to be forbiddingly difficult as a result of electronic noise induced by the GELINA modulators in the first 2-3 μs following each pulse. The setup was reinstalled at the 300-m position.

In parallel work, preliminary MCNP5 simulations were made to test the sensitivity of the CD_2 experimental setup with HPGe detectors to different deuterium data files, specifically ENDF/B-VII.0, JENDL-3.3 and Bonn-B. It was found that good discrimination in calculated detector signal ratios was obtained (about 15% between JENDL-3.3 and ENDF/B-VII.0) at 0.6 MeV using detectors placed at more extreme forward (25º) and backward (155º) angular scattering positions in the LAB reference frame.

Subsequently, a new experimental setup was installed at GELINA using two sets of four Li-glass neutron detectors placed at forward and backward scattering angles of 15º and 165º, respectively. New data have been collected using this setup, but the preliminary results are inconclusive due to low count rates. Additional measurements are planned.

Simplified MCNP5 simulations were performed for the 165º /15º CD_2 setup using virtual neutron detectors (in place of Li-glass neutron detectors) to test its sensitivity to various D data files. The results shown in Figure 7 indicate peak differences of up to about 36% (at 1.8 MeV) between the ratios calculated using different D data files and >22% over the energy range from 0.3 to 2.0 MeV.

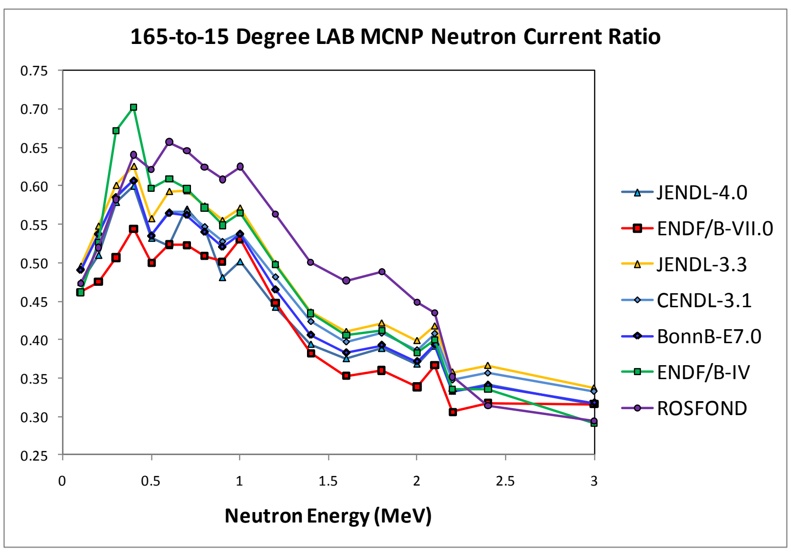

Figure 7 Comparison of 165-to-15 degree LAB MCNP5 neutron current ratios.

7.3 D recoil measurements

IRMM staff have also performed new neutron-deuteron scattering experiments that simultaneously measure the position, direction and energy of the recoiling deuterium nucleus using a state-of-the-art

TPC (Time Projection Chamber) detector filled with a deuterated P10 (90% Ar and 10% deuterated methane CD_4) gas mixture. The measurements were performed using the quasi mono-energetic neutron beam of the AIFIRA (Applications Interdisciplinaires de Faisceaux d'Ions en Région Aquitaine) facility at CENBG (Le Centre d'Etudes Nucléaires de Bordeaux Gradignan) in Bordeaux, France. The measurements were performed at 0.3, 0.5 and 0.7 MeV. The gas pressure was varied with the incident neutron energy so that the maximum range of a recoil is about 30 mm and the maximum recoil angle with a useful track length (10 mm) is 60° in the LAB reference frame. Analysis of these data and comparison data for neutron-proton scattering using P10 (Ar90(CH_4)10) is in progress.

7.4 Potential HEU ZED-2 experiments

Preliminary investigations were undertaken to see if new integral critical experiments could be performed in ZED-2 that would enhance the reactivity sensitivity to the D data. MCNP5 simulations were performed for a hypothetical compact critical core arrangement consisting of 46 annular Zr-alloy fuel elements, containing HEU UO_2 powder, on an hexagonal lattice pitch of 5 cm. Calculated k_{eff} values differed by up to 8.9 mk, being largest using the CENDL-3.1 D data and lowest using ENDF/B-IV. Thermal neutron flux tallies also showed small differences of up to ~0.9 % in the height of the relative flux peak in the radial D_2O neutron reflector and up to ~3 mm in the radial location of the flux peak, but these differences would likely be too small to detect using current techniques. If further investigation proves favorable, including reanalysis of similar HEU fuel assembly measurements performed in ZED-2 in the early 1980s, fuel-substitution-type measurements of HEU fuel elements into a reference lattice would likely be proposed. Such measurements should be reproducible to within about ±0.3 mk (1 σ).

8. Conclusion

The status of the deuterium nuclear data used in the simulation of HWRs was reviewed, emphasizing aspects that have noticeable reactivity impact, namely the $P(E,\mu)$ angular distributions for elastic scattering at energies <3.2 MeV, the value of the scattering cross section $\sigma_s(E)$ at very low energies and the numerical adequacy of their representation in evaluated nuclear data libraries. The progress of ongoing investigations by a multidisciplinary, international collaboration to reduce associated uncertainties was outlined along three paths, including nuclear-theory calculations, new neutron scattering measurements and potential new integral experiments. It is expected that the completion of this work will contribute to an improved evaluation for D to be incorporated in a future release of ENDF/B-VII and, hence, to improved accuracy in the simulation of HWRs. At the same time, the work of this collaboration provides an example of how progress in basic nuclear science continues to have an impact on nuclear systems having substantial practical applications.

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