International Conference on Nuclear Data for Science and Technology 2007
DOI: 10.1051/ndata:07445

On the observation of discrepancies in the $^{16}O(n,\alpha)$ data between different evaluated nuclear data files

A. Vasiliev, H. Ferroukhi, M.A. Zimmermann, and E. Kolbe[a]

Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Abstract. The disagreement of calculational results on the fast neutron flux at the pressure vessel of a pressurized water reactor obtained with modern neutron data libraries based on ENDF/B-VI.8, JEF-2.2 and JENDL-3.3 evaluations and using MCNPX Monte Carlo neutron transport code is analysed. Comparison of the neutron cross sections data important for the considered study and taken from these libraries has indicated that the observed results disagreement could be explained by differences in the $^{16}O(n,\alpha)$ data and this is examined and discussed in the paper. The major conclusion of the given study is that presently the uncertainties in the $^{16}O(n,\alpha)$ data could be considered as an important contribution to the overall fast neutron fluence calculational uncertainty.

1 Introduction

Based on observations drawn from the modelling of fast neutron transport using the MCNPX code, discrepancies in the $^{16}O(n,\alpha)$ reaction cross sections have been found between JENDL-3.3 [1] and ENDF/B-VI.8 [2] and JEF-2.2 [3] (based on the ENDF/B-VI evaluation) standard libraries. The observed discrepancy is found to be non-negligible with respect to the water absorption cross section in the energy range above ~4 MeV. In this paper, the impact of such discrepancy is illustrated with regards to the calculations of the fast neutron fluence (E >1 MeV) at the Reactor Pressure Vessel (RPV) for Pressurized Water Reactors (PWRs).

The presented study consists in a RPV fluence analysis of an operating PWR based on a realistic modelling of the actual reactor operation history and using the CASMO-4/SIMULATE-3/MCNPX-2.4.0 system of codes. A particular advantage of this study is that the calculated results are compared to "reference" fast neutron fluence (FNF) data that were evaluated from scraping tests performed on the RPV of the given reactor after ten cycles of operation.

It is shown that with the ENDF/B-VI.8 (JEF-2.2) library, the agreement between the calculated FNF and the reference data is around ±5% which can be considered as very satisfactory. On the other hand, using the JENDL-3.3 library leads to an overestimation of the FNF by around +10% compared to the ENDF/B-VI.8 and JEF-2.2 results. This is found to be due to a lower neutron absorption in the water (−30% in the (n,α) reaction rate) when using the JENDL-3.3 library.

The discussed cross section differences could potentially lead to more sizable discrepancies for other applications, and thus need to be brought to the attention of neutron data evaluators and users.

[a] Presenting author, e-mail: edwin.kolbe@psi.ch

2 Fast neutron flux modelling

2.1 Methodology and validation studies

The development, at the Paul Scherrer Institut (PSI), of a CASMO/SIMULATE/MCNPX calculation scheme for FNF modelling, as also its validation against a reactor pressure vessel (RPV) scraping test using JEF-2.2 library, were reported recently [4,5]. The applied methodology is based on the conversion of power distribution and fuel composition results from deterministic CASMO-4/SIMULATE-3 core-follow calculations into a axially distributed pin-by-pin 3D volumetric fixed neutron source for ex-core neutron transport simulations using the Monte Carlo code MCNPX.

The reference fluence estimates considered in the given paper are based on a previously performed activity analysis of RPV scraping samples, taken after ten cycles of operation of the nuclear power plant [6]. The steel samples were taken from the PWR RPV from two different azimuthal segments, corresponding to diagonally opposite locations. The total relative error in the fluence estimations has been stated as ~10% [6]. For the validation study presented here, symmetry has been assumed for the reactor core, so that only a single 90°-symmetric sector has been modelled with MCNPX. Based on this assumption, the experimentally-estimated FNF data for both sectors was averaged, providing reduced uncertainties of the weighted-average FNF estimations, compared to the initial data [5] (see also fig. 1).

In order to identify the influence of choice of nuclear data library used in conjunction with the Monte Carlo code on the calculational results, test calculations with three different standard cross section libraries distributed by the OECD/NEA Data Bank [1–3] have been performed.

An MCNPX reactor model representing averaged reactor conditions (neutron source and coolant density data) over all 10 cycles was applied for the sake of simplicity. Such a simplified approach was found quite adequate for the purpose of the given study by comparison with the detailed cycle-by-cycle calculations. Differences between results from the two

Article available at http://nd2007.edpsciences.org or http://dx.doi.org/10.1051/ndata:07445

approaches, for the FNF at individual azimuthal locations of the RPV, were found to be within the relative statistical error of the simplified calculation, viz., ~2%.

2.2 Test calculations

Results obtained for the scraping test analysis using the JEF-2.2, JENDL-3.3 and ENDF/B-VI.8 libraries are presented in figure 1. The azimuthal distributions of the FNF at the core mid-plane are shown in each case. Also shown, for comparison, are the corresponding reference results, viz., the FNF values derived from the RPV scraping test measurements and their estimated uncertainties (for more details see refs. [4–6]).

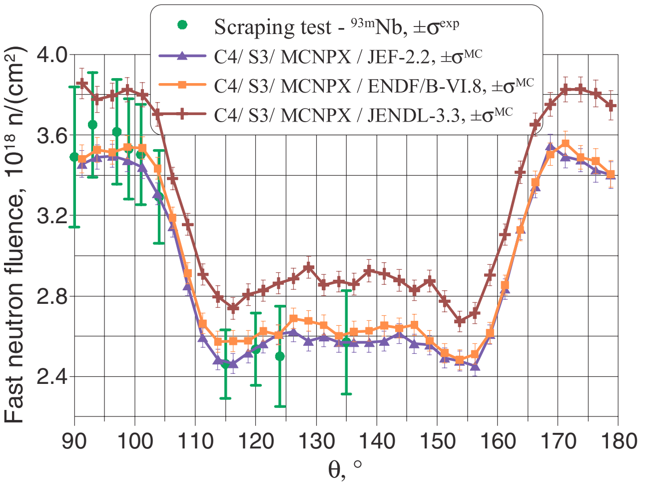

Fig. 1. Fast neutron fluence calculation results, obtained with the three different data libraries, along with the reference values derived from the RPV scraping test measurements.

It is seen clearly that the calculation results obtained with the JEF-2.2 and the ENDF/B-VI.8 libraries are almost identical and agree very well with the reference, experiment-based values, while the results with JENDL-3.3 are larger by ~10%. The possible reasons for this inconsistency are examined more closely in the following section.

2.3 Analysis of calculational results

To identify possible sources of the presented calculational results discrepancy, analysis of cross sections of important reactor materials, i.e., water and steel, have been performed.

No sizable differences in the total cross sections were found. This is not surprising in the case of the JEF-2.2 and ENDF/B-VI.8 total cross sections for water, since the neutron data for ^{16}O and ^{1}H in JEF-2.2 are known to have been originally taken from the ENDF/B-VI and ENDF/B-V evaluations respectively. Even with respect to JENDL-3.3, only very slight differences could be detected for these data.

The total cross sections contributors, however, need to be examined in greater detail. Thus, the main constituents are the scattering cross sections – elastic in the case of water, and both elastic and inelastic in the case of steel. In general, these cross sections, for the various nuclides concerned (i.e., hydrogen, oxygen, iron, etc.), have been found to be very similar in the three libraries.

Important for the present analysis is the fact that, from the viewpoint of single interactions, high energy neutrons lose only a fraction of their energy when this interaction is scattering, whether elastic or inelastic, and in this case are likely to remain above the energy bound of interest for RPV FNF assessment (~1 MeV). On the other hand, the absorption of a high energy neutron, even if its probability is small, has a direct impact in terms of reducing the fast flux. Clearly, an inspection of the partial neutron cross sections is needed in this context.

Among the considered nuclides, only ^{16}O absorbs fast neutrons significantly due to its (n,α) reaction. As for the inelastic cross section of the ^{16}O nuclide, it becomes significant only at neutron energies above 6 MeV, where the fractional neutron flux is relatively small. Figure 2 gives the comparison of the neutron data files for the ^{16}O(n,α) cross section between the JENDL-3.3 and the ENDF/B-VI.8 libraries (data is taken from [7]). It is clearly seen that the JENDL-3.3 values are significantly lower over the important energy range.

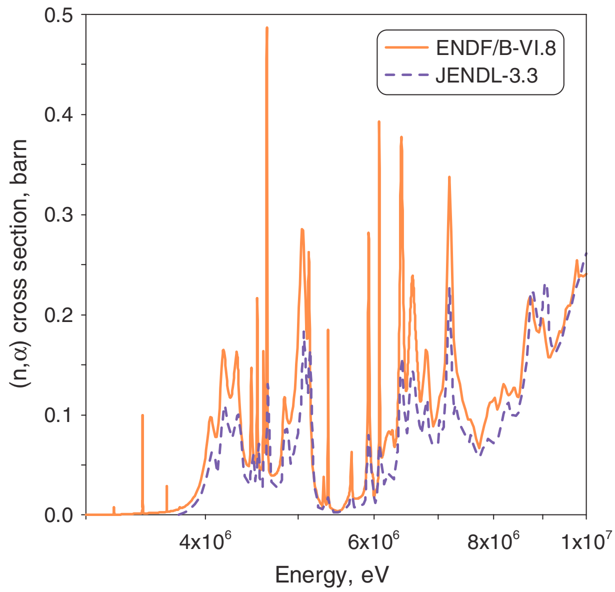

Fig. 2. Comparison of the ^{16}O(n,α) data from JENDL-3.3 and ENDF/B-VI.8.

As regards the ^{16}O elastic scattering cross section within the considered energy range, it was noted that there are slight differences in the JENDL-3.3 and the ENDF/B-VI.8 libraries, but these are not systematic. Furthermore, one needs to bear in mind that the manner in which the elastic and total cross sections have been evaluated is quite different in the two libraries [7].

It should in fact be noted that, at the time of the study, these two evaluations for ^{16}O were the only ones which are truly independent. As mentioned earlier, the corresponding JEF-2.2 (as well as JEFF-3.0 and JEFF-3.1) data are based

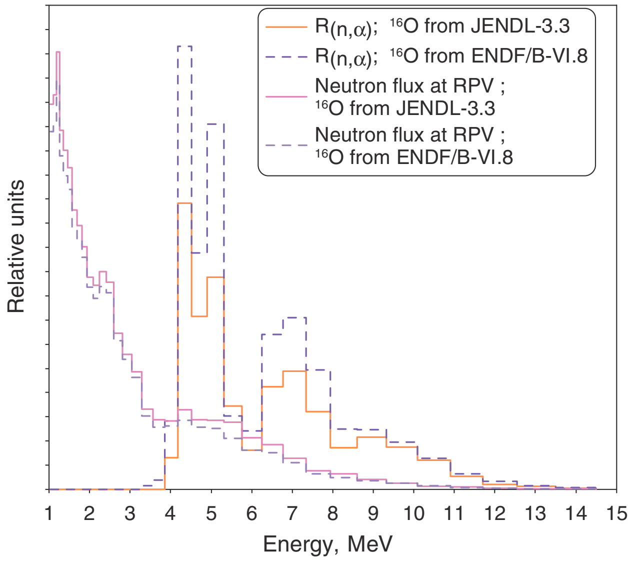

Fig. 3. Impact of ^{16}O cross section data on the (n,α) reaction rate in the downcomer region and the fast neutron flux at the inner surface of the RPV.

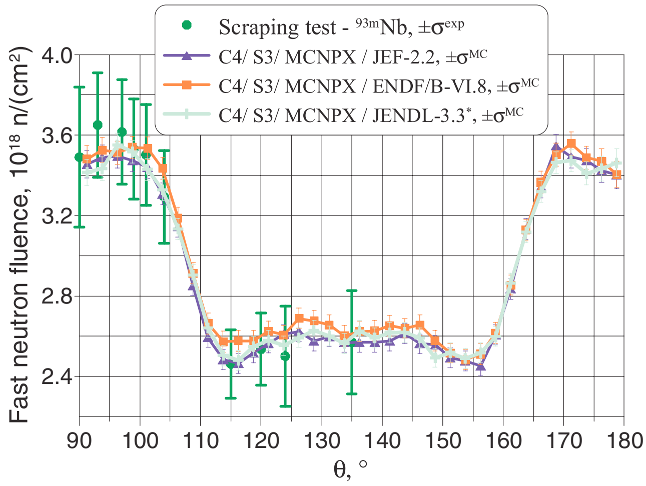

Fig. 4. Comparison of the fast neutron fluence calculation results (marked JENDL-3.3*), obtained using JENDL-3.3 data for all nuclides except ^{16}O (for which ENDF/B-VI.8 data were used).

on ENDF/B-VI. Furthermore, the CENDL-2 ^{16}O(n,α) cross sections [7] are very similar to the ENDF/B-VI data up to ~6 MeV, while the BROND-2.2 cross sections [7] have been taken from the corresponding ENDF/B-IV file for this reaction.

After identification of this principal cause for the differences in the water absorption cross sections between JENDL-3.3 and the other libraries, the RPV FNF calculations were repeated using the JENDL-3.3 cross sections for all nuclides except ^{16}O, for which the data were taken from ENDF/B-VI.8. The results obtained are presented in figure 3, in terms of (a) the ^{16}O(n,α) reaction rate R(n,α) in the PWR downcomer region and (b) the RPV fast neutron flux. Comparison is also made of the corresponding results obtained using JENDL-3.3 data for all the nuclides. The relative differences in the integral values, induced by the usage of the JENDL-3.3 ^{16}O cross sections (instead of the ENDF/B-VI.8 data), are −30% for the (n,α) reaction rate and +10% in the fast neutron flux at the RPV.

Independently from the present study, similar differences, e.g., ~–30%, were observed for fast neutron absorptions in ^{16}O, between JENDL-3.3 and ENDF-B/VI-8 (JEF-2.2) based results, in the framework of MCNPX analyses [8] of the set of "low-enriched, thermal, compound uranium benchmarks" from 'International Handbook Of Evaluated Criticality Safety Benchmark Experiments' [9].

Figure 4 shows the new results for the azimuthal distribution of the FNF, marked as JENDL-3.3*, and its seen that these are now indeed very close to those obtained with the other two data libraries.

Thus, the differences in the ^{16}O cross sections between the JENDL-3.3 and ENDF-B-VI.8 data libraries, largely explain the differences between the corresponding calculated FNF values.

3 Discussion

The difference between the ^{16}O(n,α) cross sections from ENDF/B-VI.8 (JEFF-3.0) and JENDL-3.3 has also been discussed in a recent NEA publication [10] concerning thermal criticality benchmarks, even though the effect of this difference on the neutron multiplication factor for thermal systems is very small (~50 pcm) [10].

It is interesting to note that a proposal given in this recent report has been to decrease the ^{16}O(n,α) cross section in the ENDF/B-VII library, "placing the level of the cross section close to that of JENDL". A preliminary evaluation made in this sense, for the ENDF/B-VII.β2 library, is shown for energies up to 4.8 MeV [10]. However, all other important, general purpose libraries, e.g., JEFF (JEF), BROND and CENDL, have continued yet to preserve their ENDF/B-IV and VI based data for this reaction.

Finally, in the latest publication, announcing the newest ENDF/B-VII.0 library release [11] it is confirmed that the ^{16}O(n,α) cross section between 2.4 and 8.9 MeV has been reduced by 32%; additionally, the elastic cross section has been adjusted (increased) to conserve the total cross section.

Obviously, this means that if the FNF calculations would be performed with the ENDF/B-VII.0 library, the results could be closer to the results obtained with JENDL-3.3; but the magnitude of effect in the FNF is difficult to predict because decrease in the neutron absorption due to reduced ^{16}O(n,α) cross section may be compensated to some extend by increase slowing down of neutrons and their removal under 1 MeV energy bound. The test calculations with the ENDF/B-VII.0 library are of a high interest in this context.

Comparing the ENDF/B-VI and JENDL-3.3 files [7] one can also observe sizeable differences in the ^{16}O inelastic cross sections. Even though these have a low impact on the current analysis of the FNF above 1 MeV, the differences could be important for other cases, e.g. in analyzing the response of high-threshold detectors such as ^{27}Al(n,α) (sensitive to neutrons above ~6 MeV).

By all means, the present study should not be considered as a validation of evaluated neutron data libraries. Also, despite the fact that the ENDF/B-VI.8 and JEF-2.2 libraries provided the best comparison between calculational and experimental results comparing to JENDL-3.3, the recent updates in the ^{16}O(n,α) cross section in ENDF/B-VII.0 may worsen the currently obtained very good calculations-to-measurements agreement.

It should be mentioned also that there remain certain approximations made in the currently developed FNF calculation methodology which perhaps deserve further investigations in terms of quantifying their possible impact [4,5], even though these approximations are currently considered to be of relatively minor importance. Moreover, considering that accepted requirements on the accuracy of state-of-the art FNF evaluations are ~±20% [12], and that the referred scraping test experimental uncertainty is reported to be within 10%, the calculational results obtained with all the three libraries, including JENDL-3.3 can be considered as quite satisfactory.

It is worth to mention here, that even when recent efforts have been made to improve the ^{16}O(n,α) evaluations, attention in the corresponding references was paid only to its influence on the criticality calculation results. The problem considered in the given study is that the ^{16}O(n,α) reaction plays an important role in determining the RPV FNF.

The present findings are interesting also from the viewpoint that it is usually cross section data for iron and hydrogen that are primarily considered as sources of uncertainties for FNF modelling (at least in comparison to the role of ^{16}O) [13,14]. Currently, the iron and hydrogen cross sections appear to be quite similar in the three modern data libraries considered. Only the ^{16}O(n,α) data have been found to be noticeably different (and of relevance) between different evaluations, indicating that it is for this reaction that significant uncertainties or deficiencies continue to exist.

4 Conclusions

Based on a comparison of results obtained from fast neutron transport modelling using the MCNPX code, discrepancies in the ^{16}O(n,α) reaction cross sections have been found between the JENDL-3.3 and the ENDF/B-VI.8 (JEF-2.2) standard libraries distributed by the NEA/OECD Data Bank.

It has been shown that the agreement, between calculated FNF values and reference results based on a PWR RPV scraping test, is within about ±5% when the ENDF/B-VI.8 (JEF-2.2) library is used, which can be considered as very satisfactory. On the other hand, using the JENDL-3.3 library leads to an overestimation of the FNF by ~10%, compared to both the ENDF/B-VI.8 (JEF-2.2) based results and the reference values. As discussed in the paper, this can be attributed to the lower neutron absorption in water (~30% lower ^{16}O(n,α) reaction rate in the downcomer region), as calculated with the JENDL-3.3 library.

A particular feature of this study has been that the calculated results for the FNF are based on a realistic modelling of the actual PWR operational history, achieved by applying a realistic CASMO/SIMULATE/MCNPX calculation scheme, and that these have been compared with experiment-based values. Nevertheless, the presented comparisons should not be construed as a validation of the ^{16}O(n,α) cross section, the declared experimental uncertainty on the reference FNF values being ±10%, i.e., very similar to the differences in calculated results between the different libraries. Obviously, analysis of available experiments dedicated for benchmarking of fast neutron transport in water is desirable to provide greater confidence in the presented observation.

The main conclusion to be drawn is that the observed discrepancy is indeed worthy of being addressed in greater depth by the nuclear data community. Furthermore, the ^{16}O(n,α) and elastic scattering cross sections were recently reviewed and updated in the ENDF/B-VII.0 library and calculation of the FNF effects associated with these changes should be of interest for further studies.

References

1. ZZ FSXLIBJ33, NEA-1424/04, OECD/NEA Data Bank Computer Program Services (2003).
2. ZZ MCB-ENDF/B6.8, NEA-1669/03, *ibid.* (2004).
3. ZZ MCJEF22NEA.BOLIB, NEA-1616/04, *ibid.* (2001).
4. A. Vasiliev, H. Ferroukhi, M.A. Zimmermann, in *Proceedings of the ANS Topical Meeting on Reactor Physics (Physor-2006), Vancouver, BC, Canada, 2006*, on CD-ROM, paper B136.
5. A. Vasiliev, H. Ferroukhi, M.A. Zimmermann, R. Chawla, Ann. Nucl. Energy (to be published).
6. F. Holzgrewe, F. Hegedues, J.M. Paratte, Nucl. Technol. **109**, 383 (1995).
7. T-2 Nuclear Information Service, LANL; (online) available from http://t2.lanl.gov/data/data.html (2003).
8. E. Kolbe, A. Vasiliev, M.A. Zimmermann, in *Proceedings of the ANS Topical Meeting on Reactor Physics (Physor-2006), Vancouver, BC, Canada, 2006*, on CD-ROM, paper D081.
9. NEA/NSC/DOC(95)03, on CD-ROM, OECD/NEA (2003).
10. NEA/WPEC-22, ISBN 92-64-02317-8, OECD/NEA (2006).
11. M.B. Chadwick et al., Nucl. Data Sheets **107**, 2931 (2006).
12. Regulatory Guide 1.190, US NRC (2001).
13. NEA/NSC/DOC(96)5, OECD/NEA (1996).
14. I. Kodeli, E. Sartori, in *Proceedings of the International Conference "Nuclear Energy in Central Europe'98", Terme Catez, 1998*, p. 115.