Uncertainty Analysis of Benchmark Experiments using MCBEND

Steve CHUCAS, Malcolm GRIMSTONE and Christopher DEAN

AEA Technology, Winfrith Technology Centre, Dorchester, Dorset DT2 8DH, UK

Differences between measurement and calculation for shielding benchmark experiments can arise from uncertainties in a number of areas including nuclear data, radiation transport modelling, source specification, geometry modelling, measurement, and calculation statistics. In order to understand the significance of these differences, detailed sensitivity analysis of these various uncertainties is required. This is of particular importance when considering the requirements for nuclear data improvements aimed at providing better agreement between calculation and measurement.

As part of a programme of validation activity associated with the international JEFF data project, the Monte Carlo code MCBEND has been used to analyse a range of benchmark experiments using JEF-2.2 based nuclear data together with modern dosimetry data.

This paper describes the detailed uncertainty analyses that have been performed for the following Winfrith material benchmark experiments: graphite, water, iron, graphite/steel and steel/water. Conclusions are reported and compared with calculations using other nuclear data libraries. In addition, the effect that nuclear data uncertainties have on the calculated results is discussed by making use of the data adjustment code DATAK. Requirements for further nuclear data evaluation arising from this work are identified.

KEYWORDS: Uncertainty analysis, benchmark experiments, Monte Carlo, nuclear data, validation, JEF-2.2

I. Introduction

MCBEND[(1)] is a general geometry Monte Carlo code developed within a collaborative agreement between AEA Technology and BNFL, and distributed by the ANSWERS Software Service of AEA Technology. For neutrons, MCBEND represents the nuclear data on a grid of 13,193 energy points with an exact treatment of the scattering laws, and can use data libraries based on the JEF-2.2, UKNDL, ENDF/B-VI and JENDL-3.2 evaluations. As part of a programme of validation activity associated with the international JEFF data project and funded by the UK's Health and Safety Executive/Industry Management Committee (HSE/IMC) programme, MCBEND has been used to analyse a range of benchmark experiments using JEF-2.2 based nuclear data[(2)] together with modern dosimetry data[(3)].

The experiments considered in this paper are the Winfrith graphite, water, iron, graphite/steel and steel/water benchmarks. The uncertainties in each analysis have been considered in detail, these being associated with nuclear data, radiation transport modelling, source specification, geometry modelling, measurement, and calculation statistics.

II. The Winfrith Benchmarks

The Winfrith graphite, iron, graphite/steel and steel/water benchmarks all have similar configurations, as illustrated schematically in **Fig. 1**.

The source is a highly enriched, circular fission plate powered by low energy neutrons leaking from the core of the NESTOR reactor. The shield configurations are as follows:

Graphite	177cm graphite
Iron	67cm iron
Graphite/steel	45cm graphite/30cm steel
Steel/water	12cm water/6cm steel/13cm water/ 23cm steel

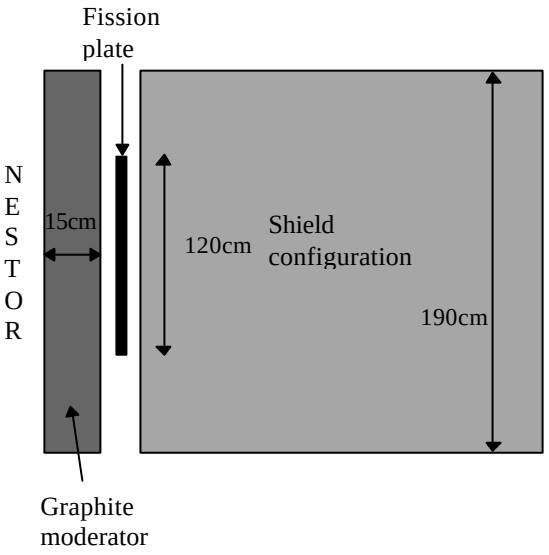

Fig. 1 Schematic Winfrith Benchmark

The measurements described in this paper were taken through the shield along the central axis of the system. The reaction-rates considered ranged from threshold detectors to epi-cadmium foils, namely $S^{32}(n,p)P^{32}$, $In^{115}(n,n')In^{115m}$, $Rh^{103}(n,n')Rh^{103m}$, $Au^{197}(n,\gamma)Au^{198}$/Cd and $Mn^{55}(n,\gamma)Mn^{56}$/ Cd. (Not all of these were associated with every benchmark.)

The water benchmark was somewhat different, and consisted of a tank containing a light support structure from which various Cf^{252} source configurations were suspended in a symmetric configuration around a central detector tube. The tank was large enough for the system to be considered an infinite sea of water. Only the $S^{32}(n,p)$ reaction was considered.

III. Uncertainties

Various uncertainties are associated with the benchmark analyses, namely:

1) The source strength
2) The source spectrum
3) Transmission cross-sections
4) Detector cross-sections
5) Material compositions
6) Monte Carlo statistics
7) Measurement statistics
8) Geometry modelling

Uncertainties associated with transmission and detector cross-sections vary with detector and configuration, but the other uncertainties can be considered together for all the benchmarks.

Taking them in turn, the source strength in the fission plate has an associated uncertainty (at the one standard deviation level) of about 4%. The uncertainty associated with the fission spectrum has been assessed by interrogating the measurements of the spectrum which were used to provide the Watt-Cranberg fit used by MCBEND. The uncertainties in the spectrum were folded with the sensitivities of the reaction-rates to provide uncertainties in the calculated results, these being less than 5%. (For the Cf^{252} sources in the water benchmark, the equivalent uncertainties were 0.5% and 1% respectively.)

As for the statistics associated with the Monte Carlo calculation and with the measurements, in general these were both less than 5%.

Uncertainties associated with the tolerance on material densities and minor approximations in the modelling of the highly specified benchmarks were small, the greatest being 3%. To assist in the estimation of such uncertainties, MCBEND can calculate sensitivities to material densities and to the size and position of components within the geometry model.

Combining the above in quadrature, excluding the uncertainties associated with transmission and detector cross-sections therefore leaves an underlying uncertainty associated with the benchmark analyses of about 10%.

IV. Transmission Cross-sections

To determine the uncertainties associated with the nuclear data, variance-covariance data from JEF-2.2 were processed into a multi-group library consisting of 25 energy ranges. The uncertainty σ associated with a particular nuclide/reaction combination p is then determined from:

$$s^2 = G V_p G^t ,$$

where V_p is the variance-covariance matrix, and G is the sensitivity matrix which consists of items

$$g_i = \frac{p_i}{c}\frac{dc}{dp_i},$$

such that g is the sensitivity, i.e. the fractional change in the result c per fractional change in the parameter p - which in this case is the value of the cross-section.

MCBEND can calculate values of the sensitivity g in the same group scheme as the library of variance-covariance data, and a stand-alone module known as WINCOV was used to calculate σ for various nuclide/reaction combinations, namely the elastic and non-elastic cross-sections of the dominant materials in a given benchmark.

Values of the uncertainty in the calculation of the S^{32}(n,p) reaction-rate associated with nuclear data showed the following trends:

- In the graphite benchmark the reaction is sensitive to the inelastic cross-section of carbon, giving an uncertainty of 11% at 70cm penetration.
- In the iron benchmark it is highly sensitive to the Fe^{56} cross-section, giving uncertainties at 60cm penetration of 26% and 18% for the elastic and total inelastic cross-sections respectively.
- In the steel/water benchmark, uncertainties associated with the elastic and inelastic cross-section of Fe^{56} were 8% and 9% respectively at deep penetration.
- The graphite/steel benchmark shows a combination of the trends in the iron and graphite benchmarks, with uncertainties at deep penetration of 11% associated with both elastic and inelastic Fe^{56} data, and 6% for the carbon non-elastic cross-section.

Uncertainties associated with the In^{115}(n,n') and Rh^{103}(n,n') reactions followed the same trend, but to approximately half the extent. All uncertainties associated with the epi-cadmium reactions were less than 5%. Uncertainties associated with hydrogen and oxygen data in the water and steel/water benchmarks were small.

V. Detector Cross-sections

The WINCOV module was similarly used in combination with a variance-covariance library for detector cross-sections. In this case the sensitivity is the fractional contribution to the reaction-rate provided by a particular energy group, and again MCBEND can provide the required values. In most cases the resultant value of uncertainty was less than 5%.

The exception to this trend was the uncertainty associated with the Rh^{103}(n,n') cross-section which reached 16% at 60cm penetration in the iron benchmark, and 10% after 30cm penetration of steel in the graphite/steel benchmark. This is because at deep penetration in iron this result is most sensitive to the detector cross-section near the inelastic threshold - where the data carry a relatively high uncertainty.

VI. Comparison of Calculation with Measurement (C/M)

The various values of uncertainty were combined in quadrature and overlaid as error bars on values of C/M in order to assess the accuracy of the JEF-2.2 predictions of reaction-rate. In many cases, good agreement between calculation and measurement was evident as illustrated in **Fig. 2**. In others the values of C/M are relatively constant, which indicates that the rate of attenuation is being predicted accurately, but the error bars do not overlap unity which implies that some unknown systematic error is present. The range of results for which the rate of attenuation is predicted accurately is:

- Graphite - $S^{32}(n,p)$
- Iron - $Rh^{103}(n,n')$, $Au^{197}(n,\gamma)/Cd$
- Water - $S^{32}(n,p)$
- Steel/water - $S^{32}(n,p)$, $In^{115}(n,n')$, $Rh^{103}(n,n')$
- Graphite/steel - $S^{32}(n,p)$, $Au^{197}(n,\gamma)/Cd$

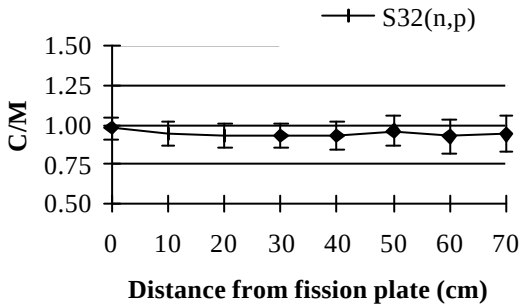

Fig. 2 C/M for $S^{32}(n,p)$ in the Graphite Benchmark

Less acceptable results are considered in the following sections.

1. $In^{115}(n,n')$ in the Iron Benchmark

The calculated rate of attenuation for this reaction is too great, leading to progressive underestimation which is not covered by the uncertainty analysis. This effect is known to be due to inaccuracies in the Fe^{56} cross-section data between 0.6 and 1.7MeV.

The starter file for the next generation of nuclear data, JEFF3T, includes a new evaluation of the elastic and inelastic cross-sections of Fe^{56} between 0.85 and 2MeV[4]. One of the features of the new evaluation is that, although the overall level of the cross-sections is similar to that of JEF-2.2, the new evaluation has much more detailed fluctuation in both the elastic and inelastic cross-section. The new data have been applied to the iron benchmark and the original and revised results are presented in **Fig. 3**, which indicates a great improvement in the agreement between calculation and measurement.

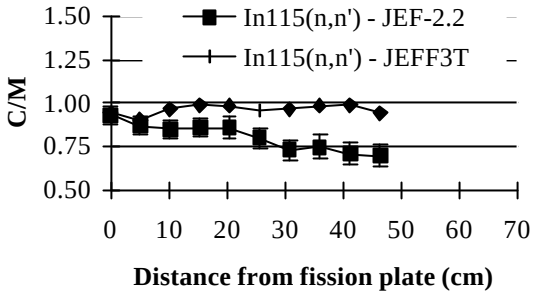

Fig. 3 C/M for $In^{115}(n,n')$ in the Iron Benchmark

The new evaluation does not affect the acceptability of the $Rh^{103}(n,n')$ results, a slight underprediction with JEF-2.2 becoming a slight overprediction with JEFF3T - in both cases the uncertainties lead to the error bars on C/M overlapping unity. The $S^{32}(n,p)$ results are unaffected because the reaction is insensitive to cross-section data below 2MeV.

Calculations for the iron benchmark have also been performed using the data libraries based on JENDL-3.2 and ENDF/B-VI. Results for the $In^{115}(n,n')$ reaction are presented in **Fig. 4**. This shows that the results obtained with these two libraries are in close agreement, and that they lie between those obtained with JEF-2.2 and JEFF3T. The same observations apply to the results for $Rh^{103}(n,n')$.

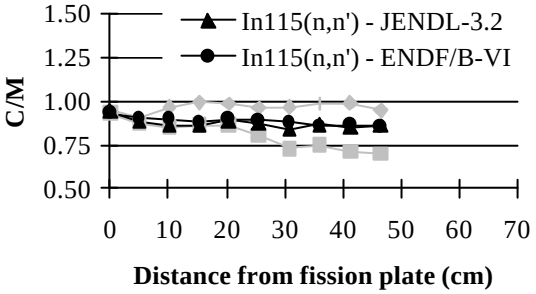

Fig. 4 C/M for $In^{115}(n,n')$ in the Iron Benchmark using JENDL-3.2 and ENDF/B-VI data

2. $Rh^{103}(n,n')$ in the Graphite Benchmark

The calculated rate of attenuation for this reaction is also too great, leading to unacceptable underestimation at deep penetration. In this case, the data adjustment program DATAK was presented with the calculated and measured results for the graphite benchmark along with all uncertainty and variance-covariance data, in order to adjust the elastic and inelastic cross-sections of carbon in an attempt to improve the level of C/M. For the elastic cross-section, DATAK determined that decreases of up to 2% were desirable in the energy range 1-5MeV. Furthermore, a large (35%) decrease in the inelastic cross-section near its threshold was required. (It is

known that the uncertainty in this range is high, which gives DATAK a lot of freedom to adjust it.)

DATAK presents the change in calculated result associated with the nuclear data adjustment, and the values of C/M using the original and adjusted data are presented in **Fig. 5** which illustrates the degree of improvement which data adjustment could provide.

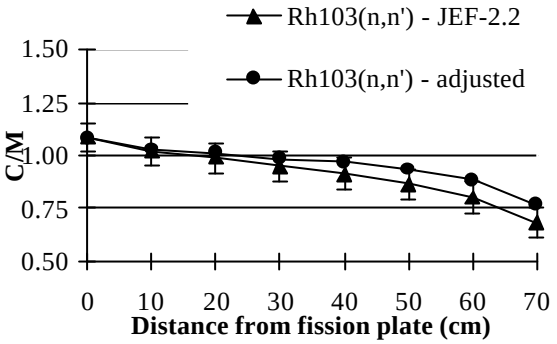

Fig. 5 C/M for Rh^{103}(n,n') in the Graphite Benchmark

The data adjustments also improved the In^{115}(n,n') results, although these had not shown such large discrepancies as those for Rh^{103}(n,n').

A similar problem with Rh^{103}(n,n') was observed in the graphite/steel benchmark, although the error was smaller because of the shorter penetration of graphite. In this case, the Rh^{103}(n,n') and In^{115}(n,n') results also improved when the carbon data were adjusted. For both benchmarks, the acceptability of the S^{32}(n,p) results was not affected.

For the graphite benchmark, calculations have also been performed using the data libraries based on JENDL-3.2 and ENDF/B-VI. The cross-sections for carbon in ENDF/B-VI are very similar to those in JEF-2.2, except for small differences for inelastic scattering. Differences between the JENDL-3.2 and JEF-2.2 evaluations are somewhat larger. In spite of this, the Rh^{103}(n,n'), In^{115}(n,n') and S^{32}(n,p) results obtained with both JENDL-3.2 and ENDF/B-VI were very close to those obtained using unadjusted JEF-2.2 data.

3. S^{32}(n,p) in the Iron Benchmark

This final example illustrates the highest levels of uncertainty observed in the analyses. As noted in Section IV this reaction is highly sensitive to the Fe^{56} elastic and inelastic cross-sections, to the extent that at 60cm penetration the overall level of uncertainty is some 30% as shown in **Fig. 6**. However, although the rate of attenuation seems to be underpredicted over such deep penetration, it is rare that such thicknesses of iron are analysed, and the rate of attenuation over more common thicknesses, say 20cm for the pressure vessel of a PWR, is predicted accurately.

A calculation using JENDL-3.2 data overpredicted the attenuation over 60cm by about 10%, while a calculation with ENDF/B-VI predicted the attenuation very accurately.

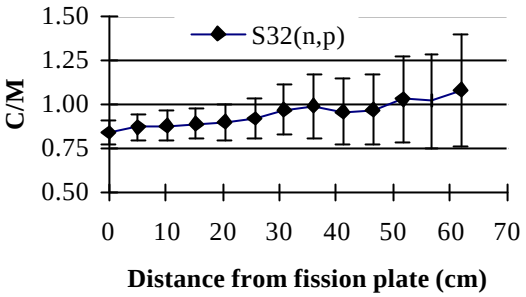

Fig. 6 C/M for S^{32}(n,p) in the Iron Benchmark

VII. Summary

Detailed uncertainties in the calculated reaction-rates associated with material and detector cross-sections have been combined with other uncertainties in the analysis of a particular benchmark, such as those associated with the source strength and with Monte Carlo and experimental counting statistics. Such uncertainty analyses have been performed for the graphite, iron, water, steel/water and graphite/steel experimental benchmarks, all of which were performed at Winfrith.

Overall, it is considered that agreement between calculations using JEF-2.2 and measurement is good, with rates of attenuation being predicted well. However, there are two occasions when this is not the case.

Firstly, the attenuation through iron of neutrons of energies of about 1MeV, as measured by the In^{115}(n,n') reaction, is overestimated. Indications are that this problem will be relieved when JEFF3 becomes available. However, this is not expected to solve the problem with the underestimation of the attenuation of neutrons at higher energies, as measured by the S(n,p) reaction.

Secondly, JEF-2.2 underpredicts some reaction-rates in carbon. A study into the carbon cross-sections indicates that adjustments to the elastic cross-section above 1MeV and to the inelastic cross-section at its threshold would improve agreement between calculation and measurement.

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