Application of JEFF3T Data to the Winfrith Iron Benchmark

A report produced for IMC

S.J.Chucas, C.J.Dean, R.J.Perry, W.V.Wright

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Executive Summary

The JEFF3 starter file (otherwise known as JEFF3T) includes a new evaluation of cross-section data for Fe⁵⁶. New measurements of inelastic data are included in the evaluation as well as transmission effects which together, improve the evaluation at MeV energies.

The new data have been added to the MCBEND JEF2.2-based nuclear data library, along with a previous evaluation known as the "Geel" data which only included transmission effects. The code has been used to analyse the Winfrith iron benchmark as this indicates the main effect of changing any Fe^{56} data. Three threshold detectors were considered, namely $S^{32}(n,p)P^{32}$, $In^{115}(n,n')In^{115m}$ and $Rh^{103}(n,n')Rh^{103m}$.

Analysis of calculated and measured reaction-rates throughout the system shows that the JEF-2.2, Geel and JEFF3T data predict the sulphur results with similar accuracy.

However, for indium and rhodium JEFF3T produces results which are generally slightly higher than those using the Geel data, with the JEF-2.2 results being the lowest. For indium, the values of C/E using JEFF3T are generally just below unity, while they hover around 1.1 for rhodium. Along with the sulphur results, JEFF3T is therefore predicting the reaction-rates with acceptable accuracy. Most notably, the trend towards underestimation of the JEF-2.2 indium results has been removed without unacceptable disruption to the other reactions.

Contents

1	INTRODUCTION	Page 1
2	LIBRARY GENERATION	2
3	THE CALCULATIONAL MODEL	3
4	RESULTS	4
5	COMPARISON OF THE JEF-2.2, GEEL AND JEFF3T DATA	7
6	SUMMARY	8
7	ACKNOWLEDGEMENTS	8
8	REFERENCES	9
Ta	ables	
1	CALCULATED AND MEASURED REACTION-RATES	Page 5
Fi	gures	
1	SCHEMATIC DIAGRAM OF THE IRON BENCHMARK	Page 3
2	RATIOS OF CALCULATED AND MEASURED REACTION-RATES	6

1 Introduction

The Winfrith iron benchmark experiment[1], which was performed in 1988, has been analysed using the Monte Carlo code MCBEND [2]. The code has been applied to the benchmark using nuclear data in the DICE format based JEF-2.2 in 13193 groups.[3]

JEF-2.2 has been found to give better agreement than the earlier UKNDL throughout the benchmark for the three threshold detectors $S^{32}(n,p)P^{32}$, $In^{115}(n,n')In^{115m}$ and $Rh^{103}(n,n')Rh^{103m}$ -termed sulphur, indium and rhodium in this report. However, the indium results are underpredicted and sensitivity analysis indicates that this is due to deficiencies in the cross-section data for Fe⁵⁶ between 0.6 and 1.74MeV. It is this underprediction which is the focus of this exercise.

A new evaluation of the cross-section data for Fe⁵⁶ was produced in 1997 by the Netherlands Energy Research Foundation at Petten. It was based on measurements made at the CEC-JRC Institute for Reference Materials and Measurements (IRMM) at Geel in Belgium, and is thus known as the "Geel" data or evaluation [4,5]. Application of the Geel data to the iron benchmark indicated that the Geel data provide better agreement between calculation and measurement than that achieved by the JEF-2.2 data.

The latest evaluation of the Fe⁵⁶ cross-section [6] is included on the starter file for JEFF3, known as JEFF3T. It was again based on measurements at Geel. (For consistency with previous analyses, the term "Geel data" will be used for the 1997 evaluation, and "JEFF3T" for the latest data.) Processing and adding the JEFF3T data to MCBEND's JEF2.2-based library has allowed another analysis of the Winfrith iron benchmark in order to assess the main effect of changing any Fe⁵⁶ data.

The generation of DICE data based on the JEFF3T evaluation is outlined in section 2. Section 3 describes the MCBEND calculations, section 4 presents the results, and section 5 considers any differences in results caused by the three evaluations.

2 Library Generation

This section describes the procedures used to generate 13,193 group DICE data from the JEFF3T Fe⁵⁶ evaluation.

The data produced by the experiment were for natural iron. The Fe⁵⁶ data were derived such that, when combined with ENDF/B-VI Fe⁵⁴ data and EFF2.4 Fe⁵⁷ and Fe⁵⁸ data, the original natural iron data would be reproduced. Thus, data for Fe⁵⁴, Fe⁵⁷ and Fe⁵⁸ from the above sources were also processed and added to the otherwise JEF2.2 based library.

To construct DICE libraries, the evaluated files are processed by NJOY94.62W [7] to generate group cross-sections and by a package consisting of ACER/CNMONK/MOULD [8] to process the secondary angle and energy data. These are combined with the cross-sections from NJOY to produce a DICE format file.

The DICE data for Fe⁵⁴, Fe⁵⁷ and Fe⁵⁸ were generated using the above procedures and did not require any special actions to be taken.

In generating the Fe⁵⁶ DICE data, however, the standard production route had to be extended to consider the following aspects:

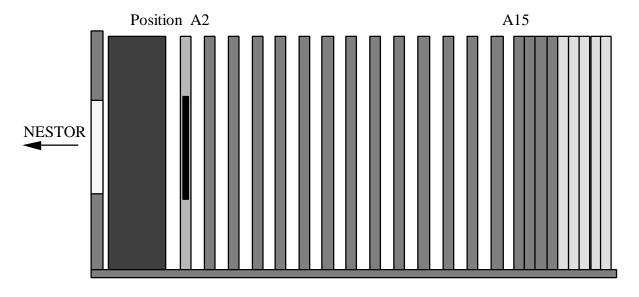
- i. The evaluation contained combined secondary energy/angle data. The DICE generation codes cannot cope with secondary data in this form and so the file was processed by the code SIXPAK [9] in order to split the combined data into separate sections for angle and energy data.
- ii. Previous Fe⁵⁶ evaluations had included an overlapping region where resonance structure was defined by both unresolved resonance parameters and structure in the cross-section data. This overlap was not present in the new file.
- iii. The data fluctuations are applied to all the inelastic levels requiring that resonance shielding data be produced for all the inelastic levels.
- iv. Nuclides which use subgroup data up to high energies should use a WIMS flux spectrum to condense the subgroup data rather than the standard 1/E weighting.

The last two points required the use of special versions of NJOY and ACER/CNMONK/MOULD that had been modified to carry out the necessary processing. These code versions were created to process the Geel Fe⁵⁶ file.

The new data, for all the iron isotopes, were added to a copy of the JEF2.2 based DICE library.

3 The Calculational Model

A schematic diagram of the MCBEND model of the iron benchmark is shown in Figure 1. The source is a fission plate powered by low energy neutrons leaking from the core of the NESTOR reactor. The thirteen slabs of iron give a total penetration of 67cm, with activation foils being positioned between them. Measurements were taken along the axis of the system at positions known as A2-A15.



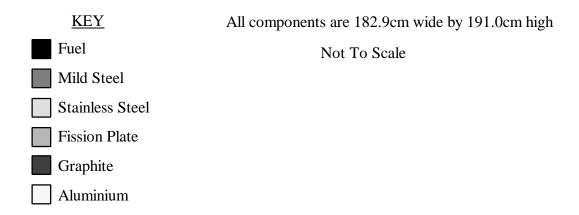


Figure 1: Schematic Diagram of the Iron Benchmark

Calculations have been performed with MCBEND9D for the three threshold detectors used in the benchmark, the calculations being identical except for the use of JEF-2.2, Geel or JEFF3T cross-section data for iron throughout the system. Detector response functions were taken from the code's response library, which is based on IRDF-90 [10].

4 Results

Table 1 presents the measured and the latest calculated reaction-rates for the three threshold detectors, along with the calculated/experiment (C/E) ratio for all three evaluations.

The values of C/E are also presented graphically in Figure 2. Since the aim of this exercise is to compare calculations using different sets of nuclear data, rather than a general uncertainty assessment, error bars at the one standard deviation level are associated only with the Monte Carlo statistics.

The values of C/E indicate that all three evaluations predict the sulphur results with similar accuracy.

However, for indium and rhodium JEFF3T produces results which are generally slightly higher than those using the Geel data, with the JEF-2.2 results being the lowest. For indium, the values of C/E using JEFF3T are generally just below unity, while they hover around 1.1 for rhodium. Along with the sulphur results, JEFF3T is therefore predicting the reaction-rates with acceptable accuracy. Most notably, the trend towards underestimation of the JEF-2.2 indium results has been removed without unacceptable disruption to the other reactions.

Sulphur

Sulphui					
Penetration (cm)	Experiment	sd(%)	JEFF3T	sd(%)	
					JEF2.2
0.00 (A2)	2.02E+7	1.0	1.69E+7	2.0	0.84
5.10	4.29E+6	1.0	3.72E+6	2.3	0.87
10.22	1.40E+6	1.0	1.30E+6	2.5	0.88
15.34	5.12E+5	1.0	4.82E+5	2.7	0.89
20.44	1.91E+5	1.0	1.84E+5	2.8	0.90
25.64	7.13E+4	1.0	7.14E+4	2.8	0.92
30.79	2.70E+4	1.5	2.76E+4	3.0	0.97
35.99	1.03E+4	1.0	1.04E+4	3.0	0.99
41.19	3.93E+3	1.0	4.17E+3	3.2	0.96
46.44	1.49E+3	1.0	1.58E+3	3.4	0.97
51.62	5.73E+2	1.0	6.52E+2	4.1	1.03
56.69	2.27E+2	2.5	2.47E+2	4.0	1.02
61.81 (A14)	8.53E+1	5.7	9.47E+1	3.9	1.08

	C/E	
JEF2.2	Geel	JEFF3T
0.84	0.85	0.83
0.87	0.87	0.87
0.88	0.91	0.93
0.89	0.92	0.94
0.90	0.94	0.96
0.92	0.96	1.00
0.97	0.99	1.02
0.99	0.96	1.01
0.96	0.99	1.06
0.97	1.01	1.06
1.03	1.01	1.14
1.02	1.08	1.09
1.08	1.18	1.11

Indium

Penetration (cm)	Experiment	sd(%)	JEFF3T	sd(%)
0.00	7.02E+7	1.0	6.63E+7	2.3
5.10	2.40E+7	1.0	2.17E+7	2.4
10.22	1.06E+7	1.0	1.02E+7	2.7
15.34	5.14E+6	1.0	5.09E+6	3.0
20.44	2.53E+6	1.0	2.49E+6	3.1
25.64	1.32E+6	1.0	1.27E+6	2.7
30.79	7.21E+5	1.0	6.96E+5	3.0
35.99	3.93E+5	1.2	3.87E+5	2.9
41.19	2.21E+5	1.4	2.18E+5	3.4
46.44	1.28E+5	1.7	1.21E+5	4.4

	C/E	
JEF2.2	Geel	JEFF3T
0.93	0.90	0.94
0.87	0.91	0.90
0.85	0.92	0.97
0.86	0.90	0.99
0.86	0.95	0.98
0.80	0.91	0.96
0.73	0.85	0.96
0.75	0.89	0.99
0.71	0.86	0.99
0.70	0.87	0.95

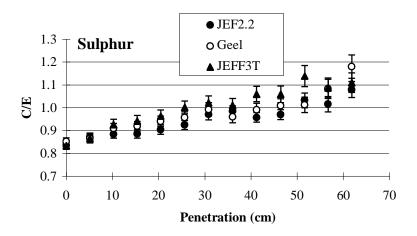
Rhodium

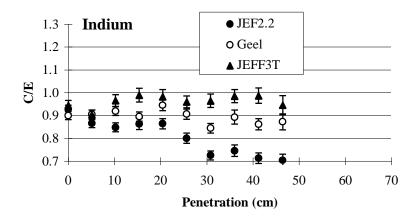
Penetration (cm)	Experiment	sd(%)	JEFF3T	sd(%)
0.00	3.35E+8	1.0	3.21E+8	1.8
5.10	1.42E+8	1.5	1.41E+8	1.8
10.22	7.78E+7	1.0	8.19E+7	1.7
15.34	4.70E+7	1.0	4.99E+7	1.7
20.44	2.86E+7	1.5	3.14E+7	1.8
25.64	1.82E+7	1.0	1.98E+7	1.5
30.79	1.20E+7	1.0	1.32E+7	1.6
35.99	7.97E+6	1.5	8.96E+6	1.6
41.19	5.48E+6	1.5	6.19E+6	1.8
46.44	3.84E+6	1.5	4.29E+6	2.3
51.62	2.68E+6	1.0	2.97E+6	2.1
56.69	1.89E+6	1.5	2.05E+6	2.0
61.81	1.34E+6	1.0	1.49E+6	2.7

	C/E	
JEF2.2	Geel	JEFF3T
0.94	0.93	0.96
0.94	0.99	1.00
0.93	1.03	1.05
0.94	1.02	1.06
0.95	1.07	1.10
0.93	1.06	1.09
0.90	1.04	1.10
0.92	1.09	1.12
0.89	1.06	1.13
0.85	1.02	1.12
0.87	1.01	1.11
0.88	1.06	1.08
0.87	1.05	1.11

Note: Units are 10^{24} reactions/atom/s for a NESTOR power of 30kW.

Table 1: Calculated and Measured Reaction-rates





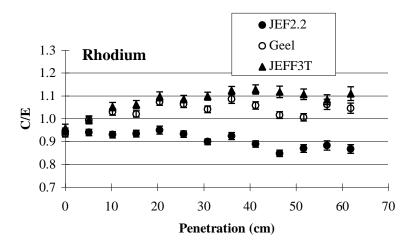


Figure 2: Ratios of Calculated and Measured Reaction-rates

5 Comparison of the JEF-2.2, Geel and JEFF3T Data

The reasons for the differences between the JEF-2.2 and Geel results are, between 0.85 and 2MeV the Geel elastic cross-section for Fe⁵⁶ is about 5% higher than JEF-2.2, with the Geel inelastic cross-section being about 9% lower than JEF-2.2. Sensitivity analysis concluded that any increase in result caused by the smaller Geel inelastic cross-section is balanced by a decrease caused by its larger elastic cross-section, but that only some of the difference between the two sets of results could be attributed to the overall magnitude of the cross-section data. It was postulated that the majority of the difference may be due to the greater fluctuation between peaks and troughs in the Geel cross-sections compared with JEF-2.2. Neutron penetration is aided by deeper troughs, thus the Geel data lead to the higher results. However, no firm conclusions were reached.

In the Geel evaluation, the fluctuations observed in the total cross-section had been applied to all reactions, i.e. elastic, inelastic and other threshold reactions. Although both Geel and JEFF3T data take their overall level of cross-section from the same evaluation, different fluctuations in the inelastic cross-section were applied in JEFF3T. Since not all the resonance shape in the total cross-section is present in the inelastic cross-section, less fluctuation in this reaction is evident in JEFF3T as compared with the Geel data. Given the argument regarding neutron penetration being aided by greater fluctuations, it may be expected that with a smoother variation in the inelastic cross-section JEFF3T would provide lower results than the Geel data; but this is not observed.

The detailed reasons for the differences in results when using the JEF-2.2, Geel or JEFF3T data are therefore unknown at present.

6 Summary

To assess the effect of using different evaluations for the cross-section data of Fe⁵⁶, the Winfrith iron benchmark has been re-analysed using the Monte Carlo code MCBEND with the JEF2.2 13193 group DICE library supplemented with cross-section data from the JEFF3T file and the so-called "Geel" evaluation.

S³²(n,p)P³², In¹¹⁵(n,n')In^{115m} and Rh¹⁰³(n,n')Rh^{103m} reaction-rates throughout the system have been determined, these having been measured in the experiment. The values of C/E indicate that all three evaluations predict the sulphur results with similar accuracy. The sulphur response is sensitive to the energy range above 1.74MeV.

However, for indium and rhodium JEFF3T produces results which are generally slightly higher than those using the Geel data, with the JEF-2.2 results being the lowest. For indium, the values of C/E using JEFF3T are generally just below unity, while they hover around 1.1 for rhodium. Along with the sulphur results, JEFF3T is therefore predicting the reaction-rates with acceptable accuracy. Most notably, the trend towards underestimation of the JEF-2.2 indium results has been removed without unacceptable disruption to the other reactions.

7 Acknowledgements

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