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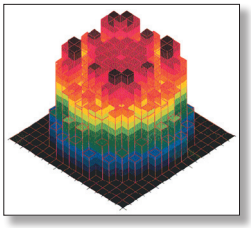
2013

Validation of the JEFF-3.1 Nuclear Data Library

JEFF Report 23



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Validation of the JEFF-3.1 Nuclear Data Library

JEFF Report 23

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NEA No. 7079

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Specific areas of competence of the NEA include the safety and regulation of nuclear activities, radioactive waste management, radiological protection, nuclear science, economic and technical analyses of the nuclear fuel cycle, nuclear law and liability, and public information.

The NEA Data Bank provides nuclear data and computer program services for participating countries. In these and related tasks, the NEA works in close collaboration with the International Atomic Energy Agency in Vienna, with which it has a Co-operation Agreement, as well as with other international organisations in the nuclear field.

Cover photos: Olkiluoto-3 under construction, Finland (TVO); Power distribution modelling in an advanced reactor, Switzerland (Paul Scherrer Institute).

Foreword

The Joint Evaluated Fission and Fusion (JEFF) Project is a collaborative effort among the member countries of the OECD Nuclear Energy Agency (NEA) Data Bank to develop a reference nuclear data library. The JEFF library contains sets of evaluated nuclear data, mainly for fission and fusion applications; it contains a number of different data types, including neutron and proton interaction data, radioactive decay data, fission yield data and thermal scattering law data.

The latest version of the JEFF library, JEFF-3.1, was released by the NEA in May 2005. JEFF-3.1 combines the efforts of the JEFF and European Fusion File/European Activation File (EFF/EAF) working groups. They have contributed to this combined fission and fusion file. The general purpose neutron library contains incident neutron data for 381 materials from ^{1}H to ^{255}Fm. The activation library (based on the European Activation File, EAF-2003) contains 774 different targets from ^{1}H to ^{257}Fm. The radioactive decay data file contains data for 3 852 isotopes, of which 226 are stable. The proton library contains incident proton data for 26 materials from ^{40}Ca to ^{209}Bi. The thermal scattering law data cover 9 materials, and the fission yield files cover 19 isotopes of neutron-induced fission yield from ^{232}Th to ^{245}Cm and 3 isotopes with spontaneous fission yields (^{242}Cm, ^{244}Cm and ^{252}Cf).

The JEF/DOC and EFFDOC working documents cited in the report are available online at www.oecd-nea.org/dbdata/nds_jefreports/jefreport-23/.

Acknowledgements

The NEA Data Bank would like to gratefully acknowledge the involvement of all the scientists who contributed to the JEFF Project and to the JEFF-3.1 files. In particular, the NEA Data Bank wishes to express its gratitude to all the researchers and experts from the different institutions who participated in JEFF meetings and contributed to the improvement of the JEFF library. The list of authors and contributors is found in Appendix A.

This report is dedicated to the memory of Christopher Dean, a long-term active member of the JEFF Project and co-author of this report, who passed away on 15 May 2012.

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1. Introduction

This report contains a validation of the last major release of the Joint Evaluated Fission and Fusion Project: JEFF-3.1. The JEFF Project is a collaborative effort among the member countries of the NEA Data Bank to develop a reference nuclear data library for a wide range of scientific and technical applications. The JEFF Project assesses the needs for nuclear data improvements and brings together experts in different areas such as experiments, data evaluations, verification and compilation of the data under strict quality assurance procedures, file processing and benchmarking. The JEFF-3.1 library was released by the NEA in May 2005 and consists of the following libraries:

- neutron general purpose library;
- neutron activation library;
- thermal scattering library;
- decay data library;
- fission yield data library;
- Proton special purpose library.

The detailed contents of these libraries have been described elsewhere [1] [2], while an overall summary of the contents, evaluation methods and performance in benchmarking has been described in [3] [4]. The present report essentially concerns the performance of the JEFF-3.1 library in various benchmarks, for various different nuclear applications. The JEFF-3.1.1 update is described in more detail in [5].

It is well known that the lack of accurate data for technical design and development of nuclear systems can lead to inefficiencies, lack of reliability and safety problems, all of which can be very costly. The JEFF-3.1 files were validated using a number of different processing and simulation codes in several organisations, e.g. SCK-CEN (Belgium) [6], NRG (Netherlands) [7][114][115], IJS (Slovenia) [8], CEA (France) [9][116-122], IRSN (France) [10], ENEA (Italy) [11] [12], BNFL/NNL (UK) [13], UKAEA/Serco (UK) [17], FZK/KIT (Germany) [83-88], UKAEA/CCFE (UK) [14], etc. In the present report, we have collected a selection of important validation work to illustrate the quality and reliability of the new library. To present the results, we have chosen to use the following categorisation: (1) thermal reactors, (2) fuel cycle, storage and reprocessing, (3) fusion and (4) other applications.

1.1 Thermal reactors

The safe, economical and reliable operation of current nuclear power reactors depends on the use of nuclear data to predict several important characteristics of plant operation. These characteristics include the desired energy production from a reactor core from the time it starts operation to the time it is ready to be refuelled, the rate at which heat is being generated in each of the fuel pins, the rate at which neutron bombardment of the pressure vessel leads to embrittlement, the shutdown of the reactor, the effect of the shielding to reduce the exposure of equipment and personnel to radiation, and requirements for fuel storage. Research institutes and nuclear industry make use of professional reactor-software to predict and analyse such characteristics. The results are only reliable if the underlying nuclear data libraries are of sufficient quality. In this report, therefore, we include a large suite of criticality and shielding

benchmarks, performed with both deterministic and Monte Carlo codes, to assess the quality of the JEFF-3.1 data library for application in reactor simulations. Also, the effect of improved fission product evaluations on reactivity worth values will be reported.

1.2 Fuel cycle, storage and reprocessing

The JEFF-3.1 library is important for the analysis of the back-end of the fuel cycle. This concerns mostly applications associated with handling spent fuels after irradiation. The validation includes the chemical and isotopic composition of spent fuel and resulting integral parameters including the three principle safety criteria radiogenic heat, gamma-ray and neutron radiation emitted and criticality. Also included will be results for decay heat and neutron emission immediately following reactor shutdown that are important for some safety studies.

1.3 Fusion reactors

The design of fusion devices such as ITER and IFMIF requires an extensive nuclear data library for the calculation of the fusion reaction rate in the plasma, prediction of neutron and photon transport in the primary energy conversion system (blanket), calculation of the tritium production rate in the blanket, calculation of nuclear heating, calculation of radioactivity and decay heat, and prediction of gas production rates and atomic displacements as indicators of radiation damage in materials. The safety margin in the design can become too large to make these fusion devices affordable if precise nuclear data are not available. Quantities such as radioactivity and decay heat must be available at a sufficient level of accuracy for approval of construction under current regulations. To assess the current quality of the data library, various material evaluations of JEFF-3.1 have been tested with 14 MeV shielding benchmarks. Also, measurements of the tritium production rate and neutron/gamma flux have been analysed with the new nuclear data library. Validation of the activation library JEFF-3.1/A (= EAF-2003) against integral data has been performed by means of direct comparison with measurements of sample materials under fusion- and IFMIF-relevant neutron spectra. A summary of the most important results is reported here.

1.4 Other applications

Although the JEFF project is mainly fission- and fusion-reactor driven, new and better nuclear data have been developed since the 1990s by other emerging applications that make use of the JEFF libraries. Examples are accelerator-driven systems, with an emphasis on energies above 20 MeV, and medical applications. Some examples of intermediate energy validation for lead and iron are reported here.

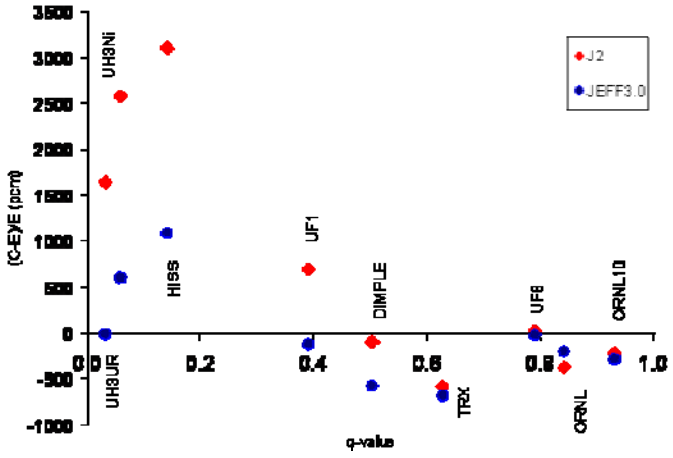
2. Validation studies for thermal systems

This chapter is concerned with the application of JEFF-3.1 [1] [3] to predict physics parameters for thermal systems. It includes application to criticality, reactor physics and shielding as reported after the release of the library in May 2005.

2.1 Pre-release validation

Development of the JEFF-3.0 [15] library included a new evaluation of ^{235}U [16] that increased neutron capture and dramatically improved predictions of reactivity for intermediate spectral uranium fuelled systems (Figure 2.1). See also [116].

Figure 2.1: Prediction of k-effective by the JEF-2.2 (J2) and JEFF-3.0 data libraries as a function of resonance escape (q)



The "q"-value is a measure of the number of fission neutrons reaching 2.6 eV. A low "q" represents a hard spectrum; the softest system, with no resonance absorption, has a "q" of 1. An overall key to the benchmarks considered is in Table 2.1. More details are given by Hanlon [17].

Unfortunately, in preserving existing data for ^{238}U the prediction for typical PWR lattices was lowered as shown for DIMPLE in Figure 2.1 and by Courcelle *et al.* in [116] [117].

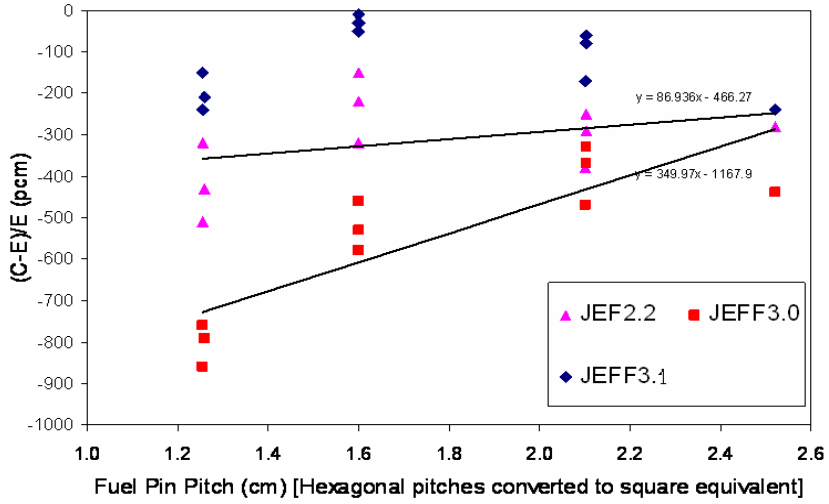
As a consequence, the international data community instigated a two-year programme to resolve the issue by developing a new evaluation for ^{238}U [18]. Over the two years, considerable validation of the developing contents of JEFF-3.1 was reported. The JEFF-3.1 library, including the new ^{238}U file, was released in May 2005 and comprises sets of evaluated nuclear data, including neutron and proton interaction data, thermal scattering law data, radioactive decay data and fission yield data. This period of development was reported by Koning [19] to the NEA Nuclear Science Committee. At the same time, the impact of the ^{238}U development was presented via predictions for VALDUC as reproduced in Figure 2.2. The VALDUC lattices cover the resonance escape (q) range of

0.5 to 0.9. However, the improvement in results is best seen via correlation with pin pitch. Here slopes with pitch have disappeared when JEFF-3.1 (see Section 2.2.3 for more details) is invoked.

Table 2.1: Lattices sensitive to uranium nuclear data

Identifier	Description	q value
UH3-UR	Uranium hydride TOPSY assembly – uranium reflector	0.031
UH3-NI	Uranium hydride TOPSY assembly – nickel reflector	0.058
HISS (HUG)	Homogeneous uranium/graphite mixture	0.141
U fluoride 1	Water-reflected uranium fluoride sphere (solution)	0.391
DIMPLE S01	Low enriched uranium lattice	0.503
TRX	Low enriched uranium lattice	0.628
U fluoride 6	Water-reflected uranium fluoride sphere (solution)	0.792
ORNL-1	Bare sphere of uranium nitrate (solution)	0.843
ORNL-10	Bare sphere of uranium nitrate (solution)	0.932

Figure 2.2: Predictions of reactivity for VALDUC (LEU-COMP-THERM-007)



2.2 Validation of uranium nuclear data

At the November 2005 JEFF meeting there were reports of successful application of the library to the benchmarking of many uranium fuelled thermal systems.

2.2.1 Uranium-235 eta

Haeck led the charge giving MCNPX results from some 80 benchmarks in a single slide [20]. This represents a huge data processing exercise since reactivity predictions are given for JEF-2.2, JEFF-3.0, JENDL-3.3, ENDF/B-VI.8 and JEFF-3.1. Due to the amount of data the overhead is difficult to read but his thesis [21] points to further open literature [6] where numerical values can be found. There are only 5 thermal benchmarks as indicated in Table 2.2 with results in Table 2.3.

Table 2.2: Haeck's thermal solutions

Name	Type	Description	CSEWG	ICSBEP [22]
usol13a	HEU ORNL-1	Unreflected sphere of uranyl (20.12 g/l) nitrate	T-1	HEU-SOL-THERM-013 Case 1
usol13b	HEU ORNL-2	Unreflected sphere of uranyl (23.53 g/l) nitrate with boron	T-2	HEU-SOL-THERM-013 Case 2
usol13c	HEU ORNL-3	Unreflected sphere of uranyl (26.77 g/l) nitrate with boron	T-3	HEU-SOL-THERM-013 Case 3
usol13d	HEU ORNL-4	Unreflected sphere of uranyl (28.45 g/l) nitrate with boron	T-4	HEU-SOL-THERM-013 Case 4
usol32	HEU ORNL-10	Unreflected sphere of uranyl (28.45 g/l) nitrate with boron	T-5	HEU-SOL-THERM-032

Table 2.3: Haeck's reactivity predictions with JEF(F) libraries

Name	Experiment	σ (pcm)	JEF-2.2	σ (pcm)	JEFF-3.0	σ (pcm)	JEFF-3.1	σ (pcm)
usol13a	1.00120	260	0.99904	7	0.99906	7	0.99907	7
usol13b	1.00070	360	0.99814	8	0.99813	8	0.99826	8
usol13c	1.00090	360	0.99482	9	0.99428	8	0.99439	8
usol13d	1.00030	360	0.99643	8	0.99598	8	0.99580	9
usol32	1.00150	260	-		0.99840	5	0.99886	5

The MONK [23] results for HEU ORNL-1 and HEU ORNL-10 for JEFF-3.0, shown in Figure 2.1, are somewhat lower than those from Haeck's study and there is more change with library when using MONK. However, the important feature is the reduction in k_{eff} as boron is introduced and compensated by uranium enrichment as indicated in Table 2.4.

Table 2.4: JEFF-3.1 prediction of reactivity as a function of the introduction of boron

Type	B Conc. (g/l)	q	Haeck	Others
HEU ORNL-1	0	0.844	0.99907	0.99880
HEU ORNL-2	0.0935	0.840	0.99826	0.99791
HEU ORNL-3	0.187	0.838	0.99439	0.99416
HEU ORNL-4	0.230	0.837	0.99580	0.99591
HEU ORNL-10	0	0.933	0.99886	0.99855

The boron concentrations were taken from the 2007 ICSBEP DVD [22]. "q" values were calculated with MONK using its JEF-2.2 library. The k_{eff} values in the "Others" column are taken from Sublet's work [9] for HEU ORNL-1 to 4 and from van der Marck's study [7] for HEU ORNL-10.

It can be seen that the discrepancy in k_{eff} generally increases as the boron is introduced. The experiments determined eta (the number of fission neutrons produced per thermal neutron absorption by fuel) for ^{235}U. They are noted to be sensitive to H_2O fast scattering, and ^{235}U plus hydrogen absorption. Assuming there are no problems with the experiments, the results can be further improved by developing these data and most likely the ^{235}U data in the low energy range.

^{238}U data seem to have little influence on these enriched solutions since they have been developed from JEF-2.2 to JEFF-3.1 and Haeck reported very little change. The JEFF-3.1 ^{238}U data have improved results for low enriched uranium (LEU) systems with similar "q" values, as seen for VALDUC in Figure 2.2.

2.2.2 Steven van der Marck's database

Steven van der Marck delivered MCNP4C reactivity predictions for 126 HEU thermal benchmarks [7] at the November 2005 JEFF meeting. His overall database covers all systems, allocated into ICSBEP categories. He also gives overall descriptions of each series of experiments. This forms a strong database for analysis to be performed. Unfortunately, little analysis has been performed with the exception of producing overall graphs of C/E values. The collective category results suffer from interaction of effects from different materials. As noted earlier in JEF-2.2, mass analysis can lead to very incorrect assumptions (page 2 of [17]).

As an example, the mass analysis of van der Marck's HEU systems with JEFF-3.1 yields a variance weighted average C/E discrepancy of -103±32 pcm, which looks very good. However, the graphs show very high C/E values of ~1.04 for HEU-SOL-THERM-38 case 29 and HEU-SOL-THERM-39 case 5 with the whole HEU-SOL-THERM-39 series predicting C/E above 1.025. The Chi-squared per degree of freedom is 6 for the distribution when it is expected to be: $1 \pm 1/\sqrt{126} = 0.91 \div 1.09$

The ICSBEP DVD includes predictions of k_{eff} for the HEU-SOL-THERM-39 series [mixture of uranium (93%) hexafluoride and hydrofluoric acid (low H/U ratio) in a hot-water-reflected spherical tank]. These are reported in Table 2.5.

Table 2.5: k_{eff} predictions for HEU-SOL-THERM-39

Evaluation	ENDF/B-V	ENDF/B-VI.2	JENDL-3.2	JEF-2.2 (172 group)	JEFF-3.1
Case 1	1.0323	1.0512	1.0604	1.0596	1.03778
Case 2	1.0395	1.0537	1.0486	1.0499	1.02986
Case 3	1.0212	1.0367	1.0460	1.0439	1.02780
Case 4	1.0243	1.0365	1.0493	1.0457	1.03237
Case 5	1.0355	1.0475	1.0604	1.0555	1.04286
Case 6	1.0190	1.0276	1.0401	1.0351	1.02762

Prediction of these critical systems is poor with all data sets. The variation with cases is similar throughout. There is clearly an improvement in JEFF-3.1 relative to JEF-2.2. In-depth analysis is necessary to make a proper conclusion. The spectra in these systems are hard with 1-12% of neutrons below 0.625 eV (typical PWR fuel has ~13%; AGR ~28% and Magnox ~35%). Sublet [24] presents good predictions for other fluoride solutions that cover some of the spectral range for HEU-SOL-THERM-39 but examination indicates that these benchmarks contained much less fluorine. Duhamel [10] suggests that the fluorine data should be further investigated.

Van der Marck's results thus form a database of validating results which can be presented and then more fully analysed by others.

2.2.3 Low enriched uranium systems

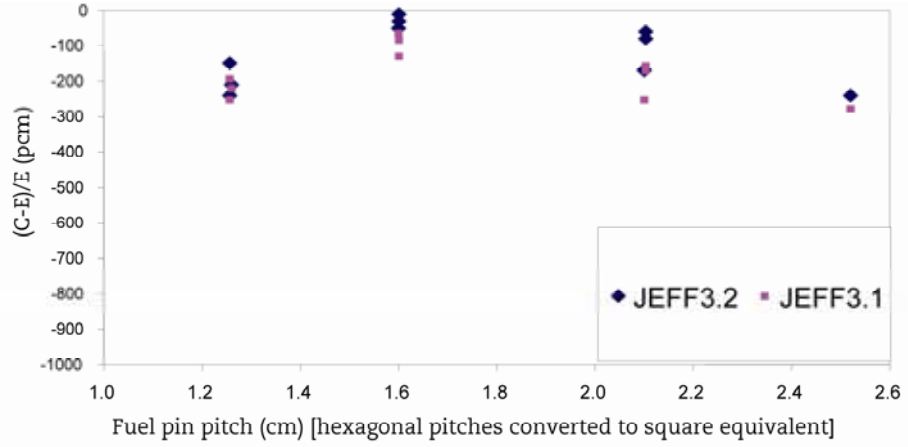
Sublet presented a considerable selection of results at the November 2005 meeting [25] and sustained this effort delivering updated results as TRIPOLI and his methods improved. A subsection of his results from his internal paper [24] was presented to JEFF [9] and replaced those from the earlier paper.

First, he reports a selection of LCT6 experiments. These are Japanese light-water-moderated lattices with 2.6 wt.% UO_2 fuel rods, arranged in a square array. The water-to-fuel volume ratio in the lattice cells ranged from 1.50 to 3.00.

The reactivity predictions for all eight benchmarks are well within 100 pcm of unity; the mean being 4 pcm high. Van der Marck's database includes all 18 assemblies and again reactivity predictions are all well within 100 pcm using the MCNP code. The largest difference between any of Sublet's results and van der Marck's is 105 pcm. This indicates that JEFF-3.1 gives really excellent results for these LEU benchmarks.

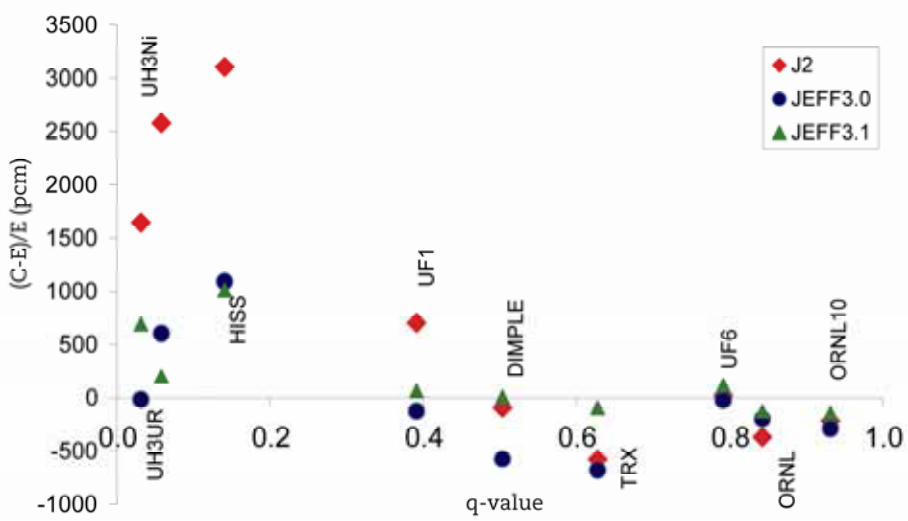
Next, Sublet presents results for LCT7, which are the VALDUC assemblies considered prior to release of JEFF-3.1 (see Figure 2.2). Again, van der Marck considered all 10 assemblies whereas Sublet considered a sub-set. Combining results from TRIPOLI (Sublet) with MCNP (van der Marck) indicates good but slightly lower results than the pre-release (Figure 2.3). These pre-release results (labelled as JEFF-3.2 in Figure 2.3) were obtained using a version of ^{238}U that became available only shortly before the official release of JEFF-3.1. This version of ^{238}U was not adopted for JEFF-3.1 as, at that time, it had not been fully validated. However, these results suggest that the final JEFF-3.2 release will further improve these validation studies.

Figure 2.3: Predictions of reactivity for LEU-COMP-THERM-007



It is possible to select JEFF-3.1 C/E values for reactivity of the benchmarks from Table 2.1 from values published by Sublet and van der Marck (inverse variance averaging where appropriate). These are plotted in Figure 2.4.

Figure 2.4: Improvement to thermal benchmarks with JEFF-3.1



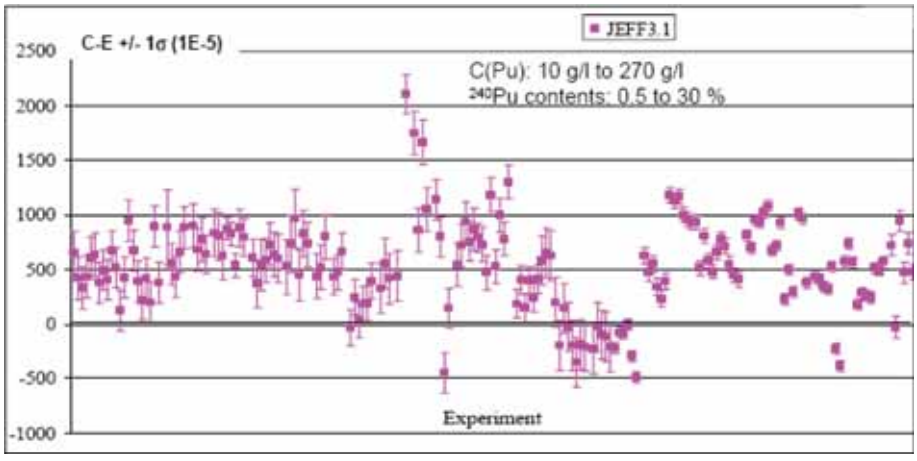
Over the thermal range (q > 0.4) all JEFF-3.1 results are within 150 pcm of unity. The three intermediate systems are within 1% of unity; a considerable improvement over JEF-2.2. The change between JEFF-3.0 and JEFF-3.1 is in the opposite direction for the Ni and uranium reflected TOPSY assemblies (UH3Ni and UH3UR, respectively). This may be caused by updates to the ^{238}U data affecting the reflector.

The practical impact of JEFF-3.1 on reactivity predictions for Uranium OXide (UOX) fuelled thermal reactors is studied by Litaize *et al.* [26]. They use the APOLLO code validated by TRIPOLI to study two whole cores from the EOLE zero-power research reactor. The fuel enrichment is 3.7%. The reactivity prediction for the EPICURE UH1.2 core with 1.26 cm pitch and 600 ppm boron improved from being 375 pcm high with JEF-2.2 to 225 pcm high with JEFF-3.1. The reactivity prediction for the MISTRAL 1 core with 1.32 cm pitch and 300 ppm boron improved from being 150 pcm high with JEF-2.2 to 140 pcm high with JEFF-3.1. Both results are good. The authors point out that the small improvements result from larger swings in reactivity worth from individual nuclides. They give a breakdown for MOX cores but not for UOX.

2.3 Validation of plutonium nuclear data

The application of JEFF-3.1 to plutonium fuel and hence MOX fuel leads to overprediction of reactivity by about +700 ±200 pcm for solution benchmarks with Pu concentrations of less than 80 g/l and by about +340 ±200 pcm for those above 80 g/l [5] [27]. This conclusion is formed from an analysis of van der Marck's database [7] and confirmed by Duhamel's work [10]. The overall need for improvement to plutonium data is suggested by Sublet [24] who has extended van der Marck's database. Duhamel's figure is reproduced as Figure 2.5 to illustrate the overprediction with APOLLO-MORET, confirmed by TRIPOLI. This overprediction clearly needs to be reduced, firstly by considering the ^{239}Pu file. Systematic JEFF-3.1 overestimation of whole core reactivity using Monte Carlo codes is reported by Litaize *et al.* [26]. They suggest ~700 pcm over prediction for a MOX core.

Figure 2.5: Reactivity predictions with JEFF-3.1 for plutonium solutions (^{239}Pu, ^{240}Pu)



Bernard *et al.* [5] [27] note that the CEA will develop Pu files via the NEA framework (HPRL, WPEC) [28]. In the meantime, a new evaluation for ^{239}Pu has been developed, by making "pragmatic" changes, for inclusion in JEFF-3.1.1. It has been processed for use with APOLLO. The resulting reactivity is well predicted at +200 ±200 pcm for solution benchmarks with Pu concentrations of less than 80 g/l and 0 ±200 pcm for those over 80 g/l.

2.4 Actinides

The accuracy of 2200 m/s cross-sections is summarised by Dupont *et al.* in JEF/DOC-1138 [29]. The Mini-INCA project measured the cross-sections in the ILL high flux reactor alongside an enriched fuel element within a D_2O tank using alpha and gamma spectroscopy. Cross-sections in barns are shown in the table below, together with their uncertainties and JEFF-3.1 values. In addition to the capture and fission cross-sections, the isomeric ratio (IR) of the $^{241}Am(n,\gamma)^{242m,g}Am$ reactions and the half-life of ^{244m}Am are considered.

Table 2.6: Thermal cross-sections for actinides

Reaction	Measurement (barns)	Uncertainty, σ (barns)	JEFF-3.1 (barns)	(C-E)/E (%)	(C-E)/σ (no dim)
^{209}Bi (n,γ) ^{210g}Bi	0.0179	0.0008	0.0285	59	13.3
^{209}Bi (n,γ) ^{210m}Bi	0.017	0.002	0.0054	-68	-5.9
^{232}Th (n,γ) ^{233}Th	7.4	0.3	7.4	0	0.0
^{233}Pa (n,γ) ^{234}Pa	40	1	41	3	1.0
^{233}U (n,γ) ^{234}U	39	1.6	45	15	3.8
^{234}U (n,γ) ^{235}U	104	3.5	100	-4	-1.1
^{235}U (n,γ) ^{236}U	98	13	99	1	0.1
^{237}Np (n,γ) ^{238}Np	180	5	162	-10	-3.6
^{238}Np (n,f)	2165	70	2027	-6	-2.0
^{238}Np (n,γ) ^{239}Np	1035	250	203	-80	-3.3
^{238}Pu (n,γ) ^{239}Pu	476	33	540	13	1.9
^{242}Pu (n,γ) ^{243}Pu	22.5	1.1	18.8	-16	-3.4
^{241}Am (n,γ) ^{242}Am	696	48	647	-7	-1.0
^{241}Am (n,γ) IR g/g+m	0.914 no dim	0.007 no dim	0.91 no dim	0	-0.6
^{242g}Am (n,γ) ^{243}Am	330	50	219	-34	-2.2
^{242m}Am (n,γ) ^{243}Am	1173	107	1231	5	0.5
^{242g}Am (n,f)	1735	87	2094	21	4.1
^{242m}Am (n,f)	6263	313	6398	2	0.4
^{243}Am (n,γ) ^{244}Am	81.8	3.6	76.7	-6	-1.4
^{243}Am (n,γ) ^{244g}Am	5.2	1.6	4.7	-8	-0.3
^{244m}Am Half-life	25.9 min	0.9 min	26 min	0	0.1
^{242}Cm (n,γ) ^{243}Cm	22.6	2	15.9	-30	-3.4

As can be seen from the last column, 14 quantities are within 3 standard deviation leaving ^{209}Bi and $^{242g}Am(n,f)$ in dire need of attention, followed by $^{233}U(n,\gamma)$, $^{237}Np(n,\gamma)$, $^{238}Np(n,\gamma)$, $^{242}Pu(n,\gamma)$ and $^{242}Cm(n,\gamma)$.

Bernard *et al.* [30] describe the Oscillation in MINERVE of isotopes in "Eupraxic" spectra (OSMOSE) programme measuring reactivity worths of UO_2 pellets doped with minor actinides, in collaboration with EDF and the US-DOE. Minor actinides worths were calculated with the CEA APOLLO2 and ANL DRAGON codes using JEF-2.2, JEFF-3.1 and

ENDF/B-VI.8 libraries. A PWR spectral core was considered. (C-E)/E values are given in Table 2.7 below.

Table 2.7: (C-E)/E for reactivity worths of selected actinides

Nuclide	JEF-2.2 (%)	JEFF-3.1 (%)	CEA uncertainty (%)	ENDF/B-VI.8 (%)	ANL uncertainty (%)
^{234}U	0.8	-6.7	2.0	4.3	2.5
^{239}Pu	-2.0	-0.5	1.8	0.5	2.3
^{242}Pu	0.7	0.4	2.1	3.6	2.5
^{237}Np/Sample1	-9.9	-14.4	2.2	5.3	2.6
^{237}Np/Sample2	-7.3	-12.2	1.8	13.5	2.3

This work [30] indicates that JEFF-3.1 data for ^{234}U and ^{237}Np need development. The ^{237}Np results were presented in JEF/DOC-1144 [5] [31] where it is suggested that JEF-2.2 data should be re-adopted. In JEF/DOC-1174 [32] the authors note a rescaling by 1.07 of the most recent thermal measurement, which may explain the lower value initially adopted in JEFF-3.1.

2.5 Thorium, uranium-233

Trkov [8] assesses JEFF-3.1 thorium data for fast, intermediate and thermal systems together with high energy shielding using MCNP with available libraries. The light-water breeder reactor (LWBR) thermal system results are given in Table 2.8 below.

Table 2.8: (C-E)/E for k_{eff} in Shippingport seed assemblies

Identifier	Fuel	Blanket	k_{eff}	σ (pcm)	JEFF-3.1 (pcm)	ENDF/B-VI.8 (pcm)	ENDF/B-VII.β+ (pcm)
SB-1	93%$^{235}UO_2$+ZrO_2,	ThO_2	1.00060	270	-365	-410	-34
SB-5	93%$^{235}UO_2$+ZrO_2,	ThO_2	1.00150	280	-400	-316	-178
SB-2	97%$^{233}UO_2$+ZrO_2,	ThO_2	1.00150	250	-352	-204	132
SB-2½	97%$^{233}UO_2$+ZrO_2,	none	1.00000	240	-312	-175	255
SB-3	97%$^{233}UO_2$+ZrO_2,	UO_2+ThO_2	1.00070	250	-675	-618	51
SB-4	97%$^{233}UO_2$+ZrO_2,	UO_2+ThO_2	1.00150	260	-636	-690	-102
SB-6	97%$^{233}UO_2$+ZrO_2,	ThO_2	0.99950	270	-185	111	304
SB-7	97%$^{233}UO_2$+ZrO_2,	UO_2+ThO_2	1.00040	280	-	-397	15

Specifications are from HEU-COMP-THERM-015 for SB-1 and 5 with ^{235}U fuel and from ^{233}U-COMP-THERM-001 for the other ^{233}U fuelled systems; all taken from the ICSBEP handbook [22]. All but one of the JEFF-3.1 (C-E)/E values exceed the experimental uncertainty σ. For SB-3 and SB-4, the excess is more than two standard deviations. In contrast, for ENDF/B-VII.β+, all (C-E)/E, except two, are within one standard deviation. Evidence on the accuracy of the thermal cross-section in thorium cycle nuclides is given in [29] and reported below.

Table 2.9: Thermal cross-sections for nuclides in the Th-U fuel cycle

Reaction	Measurement (barns)	Uncertainty, σ (barns)	JEFF-3.1 (barns)	(C-E)/E (%)	(C-E)/σ (no dim)
^{232}Th (n,γ) ^{233}Th	7.4	0.3	7.4	0	0.0
^{233}Pa (n,γ) ^{234}Pa	40	1	41	3	1.0
^{233}U (n,γ) ^{234}U	39	1.6	45	15	3.8
^{234}U (n,γ) ^{235}U	104	3.5	100	-4	-1.1
^{235}U (n,γ) ^{236}U	98	13	99	1	0.1

The thermal capture cross-section of ^{233}U in ENDF/B-VII is also 45 barns, so it is not the reason for improvements in ENDF/B-VII results.

2.6 Fission products

Fission product benchmarking in JEF(F) has concentrated on the absorption data for individual leading nuclides (rather than overall fission product absorption), e.g. through the CERES programme [118]. Through WPEC Subgroup 21 [33] and Subgroup 23 [34] significant evaluation effort led to new files being included in ENDF/B-VII. In [35] Dean *et al.* reanalysed the fission product absorption using JEFF-3.1 and ENDF/B-VII. Since the CERES programme took place in the UK and French reactors and were analysed by both countries, it was important to have JEFF-3.1 analysed with the CEA codes. These results are reported by Gruel *et al.* [36] but using JEFF-3.1.1 data for four spectra. New data for ^{103}Ru, ^{99}Tc, ^{148g}Pm, ^{93}Zr, ^{147}Pm, ^{154}Eu and ^{135}Cs [5] [37] are included in JEFF-3.1.1 but of these only the ^{99}Tc is measured in the CERES programme. The CEA oscillation programme in MINERVE continues to the present but sadly the DIMPLE reactor in the UK has been decommissioned back to a green field site. The CEA programme covers four different spectra: PWR-UO_2 (R1UO_2 lattice), PWR-MOX (R1MOX lattice), BWR (REB lattice) and thermal spectrum (R2UO_2 lattice). The assembly with the thermal spectrum differs somewhat from the core in DIMPLE leaving the PWR-UO_2 assembly suitable for comparison. JEFF-3.1 trends are shown in the table below.

Table 2.10: (C-E)/E for reactivity worth of fission products

	DIMPLE	MINERVE	
Isotope	(C-E)/E (%)	(C-E)/E (%)	σ(Exp) (%)
Mo-95	~0	+1	2
Tc-99	+8	+9	3
Rh-103	+6	+8	2
Ag-109	+2	+5	4
Cs-133	+10	+7	1
Nd-143	-3	-2	1
Nd-145	+1	+2	1
Sm-147	+4	+7	1
Sm-149	-4	~0	1
Sm-152	~0	+2	1
Eu-153	-6	-11	1
Gd-155	+3	~0	1

The uncertainty on reactivity worth in the initial CERES programme was said to be 4% but further work by the CEA has improved the accuracy estimation and their new values are given in the final column of the above table. It is noticeable that the reactivity worth varies significantly between the French and UK analyses suggesting that further investigation of this benchmark is required.

2.7 Absorbers

2.7.1 Gadolinium

Sublet [38] assesses the status of Gd-evaluated data following new (post JEFF-3.1) measurements at Rensselaer Polytechnic Institute – RPI [39]. The RPI measurements result in a 9.1% decrease in the natural gadolinium thermal cross-section and a 2.3% increase in the resonance integral relative to the JEFF-3.1 values of 48 627 and 388 barns, respectively.

Sublet shows that JEFF-3.1 criticality predictions for the BASALA-C (MOX) and CAMELEON (UOX) assemblies are relative to measurements in the EOLE reactor. The MOX assemblies are predicted to be ~700 pcm high and the UOX ~100 pcm high using TRIPOLI-4.5 with JEFF-3.1 data. Changing to the new RPI data had a minimal effect indicating that the k_{eff} has little sensitivity to Gd data.

Next, he considers cases from the ICSBEP [22] noting he used the 2007 edition.

First he analysed a high (~89%) enriched uranium solution poisoned with Gd and reflected by water – high enriched uranium solution – thermal (HST14). Results with all libraries were high by ~1% and he considers this benchmark "unreliable".

Next, he considers two arrays of uranium oxide pins in solutions poisoned with Gd to varying extents including zero. The one assembly from low enriched uranium compound thermal (LCT14) has 0.064 g/l of Gd and yields k_{eff} low by ~450 pcm with JEFF-3.1. Two cases without Gd are predicted within 70 pcm and changing to the new RPI data brings the poisoned case within 70 pcm indicating a possible problem with the JEFF-3.1 Gd data.

However, he goes on to analyse the LCT5 series of uranium oxide assemblies. He notes that the Gd worth is greatest for the tightest pitch series. The case without Gd is predicted some 250 pcm high with JEFF-3.1 whereas the two cases with 0.068 and 0.438 g(Gd)/l are predicted almost exactly. A case with 0.482 g(Gd)/l is low by ~150 pcm. When the new RPI data are applied, results become significantly high even if one assumes the other nuclides contribute +250 pcm. This gives confidence in the existing JEFF-3.1 Gd data and makes the new measurements questionable.

Overall, Sublet recognises that more benchmarks are required, or more analysis, to be definitive about the Gd developments.

He pursues this goal in a paper [40] published in Nuclear Science and Engineering. Fission rates for Gd poisoned pins, measured in three elevations of BWR assemblies during the LWR-Proteus programme, are improved noticeably when the JEFF-3.1 evaluation is replaced by the new RPI data. Mean C/E discrepancies reduce from -2.3% to -0.5%, from -2% to -0.6% and from -1.1% to 0.3%. Further, the poisoned pin discrepancies tend to be within the overall fission rate discrepancy distributions rather than being extreme values. Unfortunately, the same is not true of the measurements of capture in ^{238}U relative to total fissions. These become slightly worse.

There is further evidence in favour of the reduction of the Gd thermal cross-section. The ~9% reduction is mainly from an 11% reduction in the ^{157}Gd thermal value. At the November 2010 CSEWG meeting [41] Mughabghab included two slides showing the capture cross-section of ^{157}Gd. He has found low temperature measurements at ~10 m/s [42] between 2.3 10^{-8} eV and 1 10^{-6} eV. When the current JEFF-3.1 evaluation is processed it

gives values 11% higher than this experiment. He also lists other cold experiments that indicate this kind of reduction is necessary.

2.7.2 Hafnium

The status of Hf data is clearly described in the OECD/NEA High Priority Request List [28]. The entry by Noguere (request ID #5) notes that "Interpretations of critical experiments with UOX fuel conducted by CEA in the AZUR zero-power reactors has shown systematic underestimation of the reactivity worth that may be attributed to an overestimated natural hafnium capture cross-section in the epi-thermal energy range" [43] [44].

The entry points out that "Neither the JENDL-3.3 nor the JEFF-3.1 libraries, that were recently issued, solve the problem. In fact, this was observed for JENDL-3.3 before the JEFF-3.1 file was constructed. As a result, the JEFF-3.1 file has been produced with this problem in mind and taken into consideration the recent data from Trbovich *et al.* obtained at RPI [45]. Finally, a 400 pcm underestimation remains that is likely due to interfering isotopic contributions in the resolved energy region. New high resolution measurements appear needed, and would be particularly valuable if they can distinguish the contributions of different isotopes."

Noguere's technical note [45] points to results from the EOLE and AZUR critical experiments [46] [47]. It also points to overestimation of JENDL-3.2 Hf in the epithermal region from the STEK experiment [48]. This report defines C/E-values of infinitely dilute sample reactivities in STEK, normalised to the C/E-value of boron-10, obtained with the JNC standard route in 70 energy groups. The various STEK facilities increasingly soften the spectrum through STEK-500 (hardest) via 1 000, 2 000, 3 000, to STEK-4000 with the softest spectrum. The C/E values for Hf were very close to unity for all but the softest system where a value of 1.27±11% is obtained. This tends to indicate too large a capture cross-section with JENDL-3.2 data but by far more than 4%. It is noticeable that many other nuclides are more discrepant than Hf.

The CEA has investigated the representation of Hf data in the APOLLO code showing an improvement with the SHEM energy mesh [49]. They consider JEFF-3.1 application to the BASALA BWR mock-up. The reactivity worth is quoted to be within 1% with the SHEM mesh rather than 1.5% with the XMAS scheme. Although capture is overpredicted with JEFF-3.1 in this assembly, it is within acceptable limits rather than being 3% high as reported elsewhere.

At PHYSOR-2010, the CEA authors re-analysed the CAMELEON results [50] this time using both APOLLO with the SHEM mesh and TRIPOLI in continuous energy. Here they consider the reactivity worths of 9, 17 and 25 absorber pins within a 17×17 PWR assembly. Results are measured relative to boron concentration. The Hf absorption is overpredicted by 2.5 to 3.4% using TRIPOLI. The code predicts the rod worths for Ag, In, Cd rods high are by 1-3% with JEFF-3.1 and the boron rods by 1%.

Recently new Hf data have been measured [51] [52] and files for future JEFF libraries have been assembled [53]. The latter document includes results from two room temperature critical experiments. Large blocks of Hf are surrounded by high enriched fuel to give a harder spectrum than in most PWRs. The block size differed in the two cases. MONK Monte Carlo calculations were converged to an accuracy of 20 pcm. Results show the benchmark with the small block of Hf predicted supercritical by 110 pcm with JEFF-3.1. The case with the larger block was high by 260 pcm.

The benchmark results from Ware and Dean's work seem different from those of CEA [50]. TRIPOLI predicts criticality for the reference case devoid of absorber high by 150 pcm whereas the case with 25 absorber pins is predicted low by about the same amount.

It is the Cadarache study of different absorbers that leads to the statement about over-absorption by JEFF-3.1 Hf data. It is worth noting that further study of the integral results may be necessary as well as developing the differential data.

2.8 Zirconium and oxygen

Bernard *et al.* [5] [54] describe the effects of JEFF-3.2 beta evaluations for Zr and O. (C-E)/E discrepancies are shown in the table below.

Table 2.11: (C-E)/E discrepancies with JEFF-3.1 and JEFF-3.2 beta for Zr and O evaluations

Core	JEFF-3.1 (pcm)	JEFF-3.2β (pcm)	Experimental uncertainty (pcm)
LCT	-120	-70	200
Mock-up	+180	+280	250
Operating PWR	-500	-350	350
Operating BWR	-450	-250	400

Here "LCT" represents results from van der Marck's work [7] for low enriched uranium compound thermal benchmarks from the ICSBEP benchmark database [22]. "Mock-up" represents average results from UO_2-light-water reactor-mock-ups in EOLE uranium oxide cores: EPICURE UH1.2 and MISTRAL 1 [26].

Predictions of reactivity with JEFF-3.1 for operating conditions are just outside of the overall uncertainty. The 150-200 pcm increase in reactivity from the new evaluations of Zr and O removes some of this but unfortunately introduces slightly high results for the 3.7% UO_2 mock-up cores UH1.2 and MISTRAL1 although the paper [26] concludes that these are satisfactory.

The improvements are achieved by adopting O(n,α) from the work by Giorginnis [55] following a new evaluation suggested by WPEC Subgroup 22 [18] and presented at the November 2007 JEFF meeting by Gilles Noguere *et al.* [5] [56].

Also, revised resonance parameters for the 292.4 eV resonance in ^{91}Zr and the 301.1 eV resonance in ^{96}Zr were inserted into the JEFF-3.1 files by Noguere [5] [57]. These are based on Mughabghab's Atlas of Neutron Resonances [58]. The JEFF-3.1 files with these resonance parameters included form JEFF-3.1.1 evaluations of the two nuclides. Suggestions for new Zr measurements are made, but, as yet, not included in the High Priority Request List. It is likely the JEFF-3.1 capture width for the 292.4 eV resonance in ^{91}Zr was mistakenly typed as 170 instead of 107. During the study, Noguere notes that Brusegan *et al.* [59] and Salah [60] confirmed change of spin from 2^+ to 3^+ for the 292.4 eV resonance in ^{91}Zr.

3. Fuel cycle, storage and reprocessing

The properties of spent nuclear fuel are all dependent upon the composition of the fuel and the number densities of the nuclides present. All fuel cycle operations will depend on this (including handling, storage, transport, chemical and physical processing, fuel fabrication from recycled components, waste management and disposal). It must be stressed that together with the heavy elements and fission products, the activation products of the fuel additives and impurities, and the cladding and structural materials must also be considered. This will allow a fully quantified fuel cycle to be developed with a detailed description of the wastes.

The safety procedures for any part of the fuel cycle will depend on the operation concerned, its specific hazards, the material involved and a detailed risk analysis. However, in all operations, there are two nuclear physics issues. First, irradiated material will contain radioactive nuclides that emit radiation. These radiations will either be absorbed locally resulting in heating, ionisation and possible nuclear reactions, or will travel outwards giving a radiation dose to the surrounding structures and any personnel. For practical applications in the current nuclear energy industry, neutrons and higher energy photons are the only radiations to travel any significant distance. Also associated with decay are nuclear reactions producing neutrons by alpha particles reactions (α,n) that need to be considered. These neutron sources, spontaneous fission for example, are a direct result of radioactive decay. Second, it is necessary to consider neutron multiplication within the fuel. If sufficient fissile material is present, it can result in a criticality releasing significant neutron and photon radiation and in some situations enough heat to boil liquids or adversely effect containment. This could potentially result in the release of radionuclides. Thus to operate safely, it is necessary to contain the radioactive material, keep the amount of fissile material significantly below that which would cause a criticality event and to have sufficient cooling that the heat can be safely removed without causing damage. Sufficient radiation shielding should be present such that personnel and the wider environment receive only safe radiation doses.

This chapter considers the available validation of JEFF-3.1 for fuel cycle applications associated with handling spent fuels after irradiation. It includes the nuclide inventory of spent fuel and the resulting integral parameters including the three principle safety criteria; radiogenic heating, gamma-ray and neutron radiation emitted and criticality. Where available, the effect of the update to the radioactive decay data, JEFF-3.1.1 [2], will be described and its effects considered.

3.1 Spent fuel inventories

The general form of the differential equation governing the number density of a nuclide with time is given by:

$$\frac{dN_i}{dt} = -\lambda_i N_i + \sum_j \lambda_j N_j B_{j,i} + \sum_k N_k \sigma_{f,k} \phi Y_{k,i} - \sum_l N_i \sigma_{i,l} \phi + \sum_m N_m \sigma_{m,i} \phi$$

The first two terms of this equation are those developed by Bateman [61] to describe a chain of radioactive decays. Here the first term is the decay of the nuclide i and the second term is the decay of direct precursor nuclides (given as the set of nuclides j) to i. N_x is the

number density of a nuclide x, λ_x is the decay constant of x, and $B_{x,y}$ is the branching fraction of decays of x that lead to y. The last three terms describe the general form for neutron reactions using, for simplicity, a flux integrated over all energies and the cross-sections given as one group flux weighted average cross-sections. The third term is the production of fission product nuclides i from the neutron induced fission of nuclides, k, where $\sigma_{f,k}$ is the fission cross-section of nuclide k, ϕ is the scalar neutron flux and $Y_{k,i}$ is the independent yield of nuclide i from the fission of nuclide k. The fourth term is the destruction of nuclide i by all possible neutron reactions to a set of nuclides l, where $\sigma_{i,l}$ is the cross-section of i leading to l. The fifth term describes the product of nuclide i by neutron reactions on all nuclides that lead to i by one reaction step given as the set of nuclides m.

3.1.1 Thermal reactors

There are currently two sets of validation results published in this area. The first is a set of CEA comparisons; mean results from three fuel samples from UOX assemblies with initial ^{235}U enrichments of 4.5 wt% and irradiated in the French Gravelines PWR to about 60 GWd/t [62], analysis of a 64 GWd/t sample from Gravelines 5 and a 33 GWd/t sample of BWR fuel from Gundremmingen [63]. The first set used JEF-2.2 and JEFF-3.1 data, and the other data used JEFF-3.1.1. These results are shown in Table 3.1.

The other set of data compared with JEF-2.2, JEFF-3.1 and JEFF-3.1.1 calculations contains 3 UOX samples from the Gösgen PWR, which was part of the ARIANE programme. These were analysed at the Institute for Transuranium Elements (ITU) and the Belgian Nuclear Research Centre (SCK-CEN) during the late 1990s [64]. The samples are referred to as GU1 (analysed at SCK-CEN), GU3 and GU4 (ITU). The solution derived from sample GU3 was divided and analysed at both laboratories. These results are identified as GU3' (SCK-CEN) and GU3 (ITU). Enrichments were 3.5% and 4.1%, and sample irradiations ranged from 29 to 60 GWd/t. The average C/E ratios for these samples using WIMS, TRAIL, FISPIN10 with JEFF-3.1.1, JEFF-3.1 and JEF-2.2 based libraries are shown in Table 3.2 [65].

To date only PWR UOX validation has been published. It can be seen that using JEFF-3.1.1/JEFF-3.1 data gives some improvements to the results of those using JEF-2.2, but the trends differ between the two published sets of results.

It would be useful to include other validated published results from PWR and BWR samples for both UOX and MOX and to validate other thermal systems such as graphite and heavy water-moderated reactors. Published validation data exist for samples irradiated in the graphite moderated Magnox and AGR reactors through the NEA Expert Group on Assay Data of Spent Nuclear Fuel [63]. This would be useful both to confirm the JEFF-3.1 nuclear data for applications and test the cross-section data in the thermal and lower energy resonance region that are important in some innovative advanced reactor designs being developed.

Table 3.1: Results from CEA comparison between spent fuel radiochemical assays and calculations

Measured ratio	Gravelines PWR ^{235}U 4.5%(w/o) 60 GWd/t			Gravelines PWR 64 GWd/t		Gundremmingen BWR 33 GWd/t
	C/E -1 (%)		± ΔE/E (%)	C/E -1 (%)	± ΔE/E (%)	C/E -1 (%)
	JEF-2.2	JEFF-3.1		JEFF-3.1.1		JEFF-3.1.1
^{234}U/^{238}U	1.8	4.3	3.0	1.7	2.0	-
^{235}U/^{238}U	4.6	2.1	3.5	8.0	6.1	5.1 ± 4.1
^{236}U/^{238}U	-4.2	-0.7	0.6	-0.9	1.1	0.1 ± 1.6
^{237}Np/^{238}U	-6.5	-1.3	3.2	1.4	2.7	-4.5 ± 3.1
^{238}Pu/^{238}U	-10.2	-9.0	3.7	-3.9	4.1	-2.6 ± 4.4
^{239}Pu/^{238}U	1.4	0.4	1.3	5.7	1.6	3.0 ± 0.9
^{240}Pu/^{238}U	-0.7	0.4	1.1	4.2	1.3	2.3 ± 1.7
^{241}Pu/^{238}U	-2.3	-3.0	1.6	1.7	1.7	1.1 ± 1.6
^{242}Pu/^{238}U	-8.6	-3.1	2.8	-2.5	3.9	-1.4 ± 4.4
^{241}Am/^{238}U	-	-	-	2.4	5	-
^{241}Am/^{238}U EOC	5.8	0.1	5.0	8.7	9	-0.4 ± 2.1
^{242m}Am/^{238}U	-21.6	2.3	7.1	7.2	7	-4.7 ± 2.3
^{243}Am/^{238}U	-8.7	-2.4	4.4	-0.2	5.5	-1.4 ± 6.1
^{243}Cm/^{238}U	-19.2	-26.5	6.3	-19.9	12	-13.0 ± 5.9
^{244}Cm/^{238}U	-16.8	-11.2	4.3	-8.4	10	0.9 ± 8.2
^{245}Cm/^{238}U	-17.8	-17.9	5.9	-5.4	11	-4.6 ± 9.3
^{246}Cm/^{238}U	-29.2	-32.2	7.0	-21.5	14	-19.5 ± 12.6
^{247}Cm/^{238}U	-16.0	-1.3	9.6	-17.4	16	-9.8 ± 15.2
^{143}Nd/^{238}U	-1.4	-0.7	1.2	2.1	1.1	0.6 ± 1.4
^{144}Nd/^{238}U	-2.1	-0.5	3.1	-2.4	2.9	-2.0 ± 2.3
^{145}Nd/^{238}U	-0.4	-0.4	1.5	-0.7	1.5	-0.2 ± 1.5
^{146}Nd/^{238}U	0.9	1.3	2.4	-0.4	2.4	-0.5 ± 1.8
^{148}Nd/^{238}U	1.5	1.4	2.1	0.2	2.1	0.2 ± 1.8
^{150}Nd/^{238}U	0.7	0.7	2.3	-0.5	2.3	-0.4 ± 1.8
^{133}Cs/^{238}U	-4.4	-3.2	1.3	-	-	-
^{134}Cs/^{238}U	-0.7	-1.9	2.4	-	-	-
^{135}Cs/^{238}U	-3.8	-4.9	2.6	-	-	-
^{137}Cs/^{238}U	-5.8	-6.4	2.1	-	-	-

Table 3.2: Ariane Gösgen UOX nuclide inventory C/E ratios using JEFF-3.1 and JEF-2.2 data

Nuclide	JEFF-3.1.1 Mean ± SD	JEFF-3.1 Mean ± SD	JEF-2.2 Mean ± SD
Sr90	0.94 ± 0.12	0.94 ± 0.12	0.96 ± 0.12
Mo95	0.95 ± 0.05	0.95 ± 0.05	0.95 ± 0.05
Tc99	1.06 ± 0.15	1.04 ± 0.15	1.05 ± 0.15
Ru101	0.96 ± 0.08	0.96 ± 0.08	0.96 ± 0.08
Ru106	0.82 ± 0.25	0.81 ± 0.25	0.80 ± 0.25
Rh103	1.11 ± 0.10	1.11 ± 0.10	1.11 ± 0.10
Ag109	1.64 ± 0.77	1.60 ± 0.75	1.45 ± 0.67
Sb125	1.94 ± 0.05	1.93 ± 0.05	2.90 ± 0.09
I129	0.96 ± 0.05	0.95 ± 0.05	1.00 ± 0.04
Cs133	1.00 ± 0.04	0.98 ± 0.04	0.98 ± 0.04
Cs134	0.98 ± 0.10	1.07 ± 0.10	1.06 ± 0.10
Cs135	1.07 ± 0.05	1.07 ± 0.05	1.06 ± 0.05
Cs137	0.99 ± 0.05	0.99 ± 0.05	1.00 ± 0.05
Ce144	1.07 ± 0.01	1.07 ± 0.01	1.06 ± 0.01
Nd142	1.01 ± 0.08	1.00 ± 0.08	0.99 ± 0.08
Nd143	1.07 ± 0.07	1.07 ± 0.07	1.07 ± 0.07
Nd144	0.95 ± 0.02	0.95 ± 0.02	0.95 ± 0.02
Nd145	1.00 ± 0.02	1.01 ± 0.02	1.01 ± 0.02
Nd146	0.990 ± 0.008	0.983 ± 0.006	0.979 ± 0.005
Nd148[1]	1.000 ± 0.000	1.000 ± 0.001	1.001 ± 0.002
Nd150	0.97 ± 0.03	0.97 ± 0.03	0.97 ± 0.03
Pm147	1.10 ± 0.27	1.04 ± 0.25	1.05 ± 0.25
Sm147	1.00 ± 0.05	0.96 ± 0.06	0.97 ± 0.06
Sm148	0.91 ± 0.07	0.94 ± 0.08	0.95 ± 0.08
Sm149	1.16 ± 0.16	1.17 ± 0.17	1.17 ± 0.17
Sm150	1.04 ± 0.03	1.03 ± 0.03	1.03 ± 0.03
Sm151	1.29 ± 0.04	1.36 ± 0.05	1.35 ± 0.05
Sm152	1.11 ± 0.06	1.23 ± 0.07	1.22 ± 0.07
Sm154	1.07 ± 0.07	1.06 ± 0.07	1.07 ± 0.07
Eu151	0.67 ± 0.14	0.71 ± 0.15	0.71 ± 0.15
Eu153	1.09 ± 0.04	1.08 ± 0.05	1.09 ± 0.05
Eu154	1.81 ± 0.32	1.76 ± 0.33	1.77 ± 0.33
Eu155	0.96 ± 0.08	0.98 ± 0.08	1.05 ± 0.09
Gd155	1.01 ± 0.24	1.02 ± 0.25	1.04 ± 0.24
U234	1.35 ± 0.12	1.34 ± 0.12	1.34 ± 0.12
U235	1.21 ± 0.15	1.24 ± 0.16	1.24 ± 0.17
U236	1.01 ± 0.01	0.99 ± 0.01	0.99 ± 0.01
U238	0.996 ± 0.001	0.996 ± 0.001	0.996 ± 0.001
Np237	0.82 ± 0.08	0.78 ± 0.07	0.78 ± 0.07
Pu238	0.98 ± 0.06	0.94 ± 0.07	0.94 ± 0.07
Pu239	1.08 ± 0.07	1.11 ± 0.06	1.11 ± 0.06
Pu240	0.99 ± 0.03	0.96 ± 0.02	0.96 ± 0.02
Pu241	1.10 ± 0.03	1.09 ± 0.04	1.09 ± 0.04
Pu242	0.96 ± 0.06	0.88 ± 0.06	0.87 ± 0.06
Pu244	0.62 ± 0.10	0.60 ± 0.11	0.60 ± 0.11
Am241	1.20 ± 0.10	1.20 ± 0.10	1.20 ± 0.10
Am242m	1.08 ± 0.22	1.11 ± 0.23	1.10 ± 0.23
Am243	1.00 ± 0.12	0.96 ± 0.11	0.95 ± 0.11
Cm242	0.96 ± 0.03	0.96 ± 0.04	0.95 ± 0.04
Cm243	2.16 ± 1.38	2.14 ± 1.38	2.11 ± 1.35
Cm244	0.78 ± 0.14	0.76 ± 0.15	0.76 ± 0.15
Cm245	0.84 ± 0.20	0.75 ± 0.20	0.74 ± 0.19
Cm246	0.71 ± 0.03	0.62 ± 0.00	0.62 ± 0.01
Pu[2]	1.05 ± 0.04	1.04 ± 0.03	1.04 ± 0.03

1. Irradiation determined using the ^{148}Nd/U ratio.
2. Derived in this work by summing the isotopic results.

3.1.2 Fast reactors

To date, there are no published comparisons between assays of irradiated fast reactor fuel and inventory calculations using JEFF-3.1. Many of the improvements in JEFF-3.1 have been driven by the needs of the fast reactor programme, especially criticality benchmarks. Since then it has been proposed for reasons of nuclear energy sustainability to move to fast reactor systems, and/or similar fast spectra advanced reactors. Therefore, it is important that inventory calculations of the fuel and any breeder blankets can be validated so that well quantified fuel cycles can be developed and their impacts properly studied.

3.2 Spent fuel integral parameters

3.2.1 Decay heat from PWR assemblies

Schmittroth reported measurements of the decay heat from irradiated PWR assemblies together with comparisons against ORIGEN2 [66]. This included 20 measurements with cooling times between 2.4 and 8.2 years for irradiations between 25 and 40 GWd/t; note that 4 measurements reported as suspect were ignored. The assemblies came from the San Onofre, Point Beach and Turkey Point reactors. The stainless steel cladding from San Onofre did not have a measured value for the cobalt impurity and, as this results in 10 to 20% of the heat in these cases, they could not be used for validation. Results from decay heat calculations were carried out [65] using the WIMS, TRAIL and FISPIN10 with JEF-1, JEF-2.2, JEFF-3.1 and JEFF-3.1.1 based libraries [65] [67]. The reactor physics models were based on design data reported in the World Nuclear Industry Handbook [68]. The experimental decay heats and the FISPIN results are compared in Table 3.3 for several of the JEFF files.

These results show good agreement between experiment and calculations, all within ±5%. The overall mean C/E was 1.00 ± 0.03. It is noted that the uncertainties on the measurements were ±2%. However, this type of analysis is only valid for fuels measured. In a recent work [69], it has been shown using nuclide inventory validation, sensitivity studies and the nuclear data uncertainties from JEFF-3.1 that the biases on decay heat results should be less than 0.5% and the expected uncertainty about 5% for the cooling times of these assemblies.

It should be noted that calculations using JEFF-3.1.1 gave no difference in the decay heat results. It is known that most improvements in the JEFF-3.1.1 radioactive decay data library were driven by decay heat issues associated with nuclides having half-lives of less than a day, and thus no significant changes were expected.

Table 3.3: Comparison of PWR assembly decay heat measurements with calculations using the JEF/JEFF libraries

Reactor	Initial ^{235}U (Wt%)	Burn-up (GWd/t)	Cooling (days)	Measured heat (W)	JEF-1 C/E	JEF-2.2 C/E	JEFF-3.1 C/E	JEFF-3.1.1 C/E
Point beach	3.397	31.914	1 635	724	1.04	0.98	0.97	0.97
	3.397	31.914	1 635	723	1.04	0.98	0.97	0.97
	3.397	38.917	1 634	921	1.04	1.01	1.00	1.00
	3.397	39.384	1 633	931	1.04	1.01	1.00	1.00
	3.397	35.433	1 630	846	1.03	0.97	0.96	0.96
	3.397	38.946	1 629	934	1.03	1.00	0.99	0.99
	3.397	37.057	1 630	874	1.04	1.00	0.99	0.99
Turkey point	2.556	28.430	962	1423	1.05	1.05	1.04	1.04
	2.556	28.430	2 077	625	1.02	1.03	1.01	1.01
	2.556	26.485	963	1284	1.06	1.06	1.05	1.05
	2.556	27.863	864	1550	1.07	1.06	1.05	1.05
	2.559	25.595	1 782	637	0.99	1.00	0.98	0.98
Mean and standard deviation of C/E values				Point beach	1.04 ± 0.01	0.99± 0.02	0.98± 0.02	0.983 ± 0.016
				Turkey point	1.04 ± 0.03	1.04 ± 0.03	1.02 ± 0.03	1.026 ± 0.030
				Combined	1.04 ± 0.02	1.01 ± 0.03	1.00 ± 0.03	1.001 ± 0.031

Recently, new measurements have been made by the Swedish Nuclear Fuel and Waste Management Company (SKB). These calorimetric measurements of decay heat from BWR and PWR assemblies were carried out at the Swedish Interim Spent Fuel Storage Facility, CLAB, at Oskarshamn [70]. These include 43 measurements of decay heat from PWR spent fuel and 66 from BWR. The PWR measurements range in enrichment between 2.1 to 3.4%, irradiation of 19.7 to 51.0 GWd/t and cooling of 13 to 23 years. The BWR measurements range in enrichment between 2.1 to 3.1%, irradiation of 14.5 to 46.6 GWd/t and cooling of 11 to 27 years. This considerably extends the current FISPIN decay heat validation in irradiation and cooling. The measured heat and the calculated/experimental ratios (C/E) are given with details of the reactor, assembly, irradiation, enrichment and cooling in Tables 3.4 and 3.5, and the results summarised in Table 3.6.

Table 3.4: Comparison of existing PWR assembly decay heat measurements with calculations using JEFF data

Assembly	Reactor	Enrichment (%^{235}U)	Burn-up (MWd/t)	Cooling (days)	Measured decay heat (W)	C/E values (JEF-2.2)	C/E values (JEFF-3.1.1)
C01	Ringhals 2	3.10	36 688	8 468	415.8	1.048	1.034
C12		3.10	36 385	8 403	410.3	1.050	1.036
C20		3.10	35 720	6 950	415.8	1.077	1.064
				6 951	426.1	1.051	1.038
				6 952	428.9	1.044	1.031
				6 959	435.6	1.028	1.015
C42		3.10	35 639	5 803	442.3	1.033	1.020
				5 804	448.4	1.019	1.006
D27		3.25	39 676	7 669	456.1	1.035	1.022
D38		3.25	39 403	8 005	442.3	1.045	1.031
E38		3.20	33 973	7 999	376.3	1.032	1.017
E38				8 000	374.3	1.038	1.023
E40		3.20	34 339	8 075	381.3	1.029	1.015
F14		3.20	34 009	7 722	381.3	1.042	1.026
F21		3.20	36 273	7 376	420.9	1.031	1.017
F25		3.20	35 352	7 725	396.7	1.049	1.035
F32		3.20	50 962	5 860	692	1.045	1.034
G11		3.19	35 463	6 990	416.4	1.030	1.016
G23		3.21	35 633	6 984	420.6	1.034	1.019
I09		3.20	40 188	5 849	507.9	1.053	1.039
I20		3.20	34 313	6 588	403.5	1.022	1.007
I24		3.20	34 294	6 601	410.1	1.018	1.003
I25		3.20	36 859	6 198	445.8	1.048	1.035
0C9	Ringhals 3	3.10	38 442	6 551	491.2	1.051	1.038
0E2		3.10	41 628	5 823	587.9	1.026	1.014
0E6		3.10	35 993	5 829	487.8	1.031	1.018
1C2		3.10	33 318	6 559	417.7	1.044	1.029
1C5		3.10	38 484	6 593	499.2	1.034	1.021
1E5		3.10	34 638	5 818	468.8	1.030	1.015
2A5		2.10	20 107	7 297	233.8	1.049	1.033
2C2		3.10	36 577	6 550	466.5	1.047	1.033
3C1		3.10	36 572	6 545	470.2	1.037	1.023
3C4		3.10	38 447	6 544	497.3	1.036	1.023
3C5		3.10	38 373	6 543	501.4	1.031	1.018
3C9		3.10	36 560	6 552	468.4	1.041	1.027
4C4		3.10	33 333	6 572	422	1.034	1.019
4C7		3.10	38 370	6 550	498.7	1.035	1.022
5A3		2.10	19 699	6 972	237.7	1.023	1.007
5A3		2.10		6 975	236.6	1.028	1.012
5A3		2.10		6 977	243.4	0.999	0.983
5A3		2.10		7 291	230.9	1.038	1.022
5A3		2.10		7 304	230.2	1.041	1.024
5F2		3.40	47 308	4 724	714.1	1.031	1.033

Table 3.5: Comparison of existing BWR assembly decay heat measurements with calculations using JEFF data

Assembly	Reactor	Enrichment (%^{235}U)	Burn-up (MWd/t)	Cooling (days)	Measured decay heat (W)	C/E values (JEF-2.2)	C/E values (JEFF-3.1.1)
14076	Barseback 2	3.15	40 010	4 177	240.3	0.883	0.869
2014	Barseback 1	2.33	19 648	8 992	82.7	0.925	0.906
2018		2.33	20 605	8 469	84.3	0.962	0.943
2048		2.33	22 559	8 986	94.6	0.930	0.912
2074		2.33	22 923	8 475	97.8	0.930	0.912
2118		2.50	20 654	7 840	98.3	0.834	0.817
9329		2.92	41 094	5 371	222.8	0.893	0.880
				5 373	224.3	0.887	0.873
				5 542	218.6	0.899	0.886
10288		2.95	35 180	5 534	185.8	0.900	0.884
3838	Forsmark 1	2.09	25 669	4 170	126.8	1.035	1.020
				4 171	126	1.041	1.027
KU0100		2.98	34 193	4 893	185.3	0.931	0.916
KU0269		2.94	35 113	4 903	192.7	0.941	0.926
KU0278		2.94	35 323	4 595	195.4	0.952	0.938
KU0282		2.94	37 896	4 574	218.5	0.925	0.910
5535	Forsmark 2	2.10	19 944	5 634	84.6	1.083	1.065
11494		2.92	32 431	5 618	166	0.950	0.933
11495		2.91	32 431	5 593	167.6	0.943	0.926
13847	Forsmark 3	2.77	31 275	4 871	170.3	0.947	0.931
				4 872	169.6	0.951	0.935
13848		2.77	31 275	4 882	170.7	0.944	0.928
1377	Oskarshamn 2	2.20	14 546	9 750	56.2	1.040	1.019
1389		2.20	19 481	8 171	83.9	0.994	0.977
1546		2.20	24 470	7 455	108.1	1.017	1.001
1696		2.20	20 870	7 411	92.4	0.995	0.979
1704		2.20	19 437	7 808	84	0.997	0.980
2995		2.70	29 987	8 211	130.5	0.988	0.972
3054		2.89	34 891	7 453	141	1.002	0.987
3058		2.89	31 987	7 423	126.7	1.009	0.993
3064		2.89	30 391	7 844	121.7	0.979	0.963
6350		2.88	27 675	6 754	126.9	0.995	0.978
				6 755	129.4	0.976	0.959

Assembly	Reactor	Enrichment (%^{235}U)	Burn-up (MWd/t)	Cooling (days)	Measured decay heat (W)	C/E values (JEF-2.2)	C/E values (JEFF-3.1.1)
12684		2.90	46 648	4 519	282.7	0.931	0.919
12078	Oskarshamn 3	2.58	25 160	5 611	120.2	1.014	0.995
13268		2.71	35 619	4 581	194	0.975	0.961
13630		2.71	40 363	4 554	235.7	0.944	0.931
582	Ringhals 1	2.26	21 270	8 623	91.7	0.949	0.932
596		2.26	22 256	8 631	88.3	1.032	1.014
				8 632	91.2	0.999	0.982
710		2.26	22 614	7 869	96.3	0.973	0.957
				7 914	92.9	1.006	0.990
				7 915	92.3	1.013	0.996
900		2.26	23 152	7 881	96.5	1.001	0.985
1136		2.26	22 230	7 541	95.2	0.957	0.942
				7 542	95.8	0.951	0.936
1177		2.65	36 242	6 690	177.9	0.974	0.960
1186		2.65	30 498	6 674	140.8	1.003	0.988
5829		2.71	44 861	5 988	210.7	0.945	0.934
6423		2.90	35 109	5 263	174.2	1.013	0.998
6432		2.89	36 861	5 421	185.4	0.994	0.981
				5 423	189.5	0.973	0.959
				5 669	184.4	0.985	0.970
				5 679	183.2	0.990	0.977
				5 680	184.9	0.981	0.968
				5 686	181.3	1.001	0.986
				5 687	181.9	0.998	0.983
6454		2.90	37 236	6 395	186.3	0.959	0.945
6478		2.90	35 183	6 394	121.5	0.982	0.967
8327		2.90	37 851	6 417	196.9	0.901	0.888
8331		2.91	35 903	4 598	187	1.014	0.999
8332		2.90	34 977	5 284	168.7	1.034	1.018
8338		2.97	34 830	5 694	169.5	1.000	0.985
8341		2.89	34 099	5 697	164.9	0.985	0.970
				5 700	162.9	0.997	0.982

Table 3.6: Summary of new validation results

Reactor	C/E values (JEF-2.2)	C/E values (JEFF-3.1.1)
PWR results		
Ringhals 2	1.039 ± 0.013	1.025 ± 0.014
Ringhals 3	1.034 ± 0.011	1.021 ± 0.012
BWR results		
Barseback 2	0.883 (only 1 value)	0.869 (only 1 value)
Barseback 1	0.907 ± 0.036	0.890 ± 0.035
Forsmark 1	0.971 ± 0.053	0.956 ± 0.053
Forsmark 2	0.992 ± 0.079	0.975 ± 0.078
Forsmark 3	0.947 ± 0.004	0.931 ± 0.003
Oskarshamn 2	0.994 ± 0.026	0.977 ± 0.025
Oskarshamn 3	0.978 ± 0.035	0.962 ± 0.032
Ringhals 1	0.986 ± 0.029	0.975 ± 0.028

The results show that PWR decay heat in this work is overestimated with JEF-2.2 by around 4% and with JEFF-3.1.1 by around 2% with a 1 standard deviation scatter of about 1%. The BWR results are more scattered and tend to underpredict decay heat by about 3% for JEF-2.2 and 5% for JEFF-3.1.1 with a 1 standard deviation scatter of about 5%. It is hypothesised that the BWR underprediction and scatter are due to the much more complicated neutronics of the modelling with each assembly having varying enrichment in the pins and experiencing varying void fractions and control blade insertion during their irradiation which are probably not well approximated by the 2D modelling assumptions used in this work.

3.2.2 Neutron emission from fabricated and irradiated fuel samples

In a recent validation report [71], work in the early 1980s by Lees and West measuring the neutron emission from some well characterised plutonium and mixed oxide fuel samples [72] [73] were compared to calculations using FISPIN with the existing JEF-2.2 and new JEFF-3.1 and JEFF-3.1.1 libraries. The following results were obtained for these samples.

These results show very good agreement with experiment, the calculations being within 2% of the measurement. The neutron emission values calculated using all the libraries are very similar, with the JEFF-3.1 and JEFF-3.1.1 results being practically identical. It should be noted that in these calculations the JEFF-3.1 data include a correction to the ^{238}U spontaneous fission branching ratio from radioactive decay that was incorrect in the library. This error was corrected in the JEFF-3.1.1 library release.

The neutron emission from irradiated fuel samples is dominated by the ^{242}Cm and ^{244}Cm activities. These nuclides usually have large uncertainties in their inventories, often greater than 30%, when comparing calculations with measurements of irradiated samples. In 1989, measurements of CAGR samples were made in the UKAEA research reactor DIMPLE to determine the neutron output and then these samples underwent destructive analysis to determine their heavy element composition [74]. It should be noted that it was estimated that the measured nuclides represented about 99% of neutron emission. The results of using the existing JEF-2.2 and new JEFF-3.1 and JEFF-3.1.1 data in these calculations are shown in Table 3.8.

Table 3.7: Comparison of measured and calculated neutron emission from fabricated plutonium fuels

Sample	Measured neutron emission (n/s)	Library	Neutron emission			
			SF	(α,n)	Total	C/E
M120 Fast reactor MOX	1 648±16	JEF-2.2	1 190	460	1 650	1.001
		JEFF-3.1	1 190	460	1 650	1.001
		JEFF-3.1.1	1 190	460	1 650	1.001
0671 Zebra Mk XIV Pu metal plate	10 024±161	JEF-2.2	10 198	6	10 203	1.018
		JEFF-3.1	10 198	6	10 203	1.018
		JEFF-3.1.1	10 198	6	10 203	1.018
IV/R/3467 Zebra Mk IV Pu/U oxide plate	5 116±86	JEF-2.2	3 022	2 008	5 029	0.983
		JEFF-3.1	3 021	2 004	5 025	0.982
		JEFF-3.1.1	3 021	2 004	5 025	0.982
ZMC 1616B Zebra Type "D" Pu/U oxide pin	3 949±49	JEF-2.2	2 669	1 286	3 956	1.002
		JEFF-3.1	2 669	1 283	3 953	1.001
		JEFF-3.1.1	2 669	1 283	3 953	1.001

Overall these results show good agreement, all being within 10% of the measured values. The JEFF-3.1 and JEFF-3.1.1 results show approximately a 2% increase in neutron emission above the JEF-2.2 results and hence a slight improvement overall. However, the differences between JEFF-3.1 and JEFF-3.1.1 results were small with only the Sample 31 case showing a difference in the above table.

3.2.3 Gamma-ray emission for shielding

To date, there are no published comparisons between gamma-ray emissions from irradiated thermal or fast reactor fuels using JEFF-3.1 to validate the irradiated fuel source terms for gamma-ray shielding. There is, however, work that identifies important nuclides which can be compared with the inventory results above to study the agreement between calculated and actual emissions.

For the development of novel fuel cycles, where no practical shielding validation of spent fuel currently exists, it will be important to justify to regulators the spent fuel inventory and hence its effect on shielding requirements so that well quantified fuel cycles can be developed and their impact properly studied.

Table 3.8: Comparison of neutron emission from irradiated AGR fuel samples

Sample	Measured neutron emission (n/s)	Library	Calculated neutron emission			
			SF	(α,n)	Total	C/E
31	10 306±206	JEF-2.2	9 501	454	9 955	0.966
		JEFF-3.1	9 723	456	10 179	0.988
		JEFF-3.1.1	9 723	456	10 180	0.988
33	19 282±386	JEF-2.2	18 867	746	19 613	1.017
		JEFF-3.1	19 295	753	20 048	1.040
		JEFF-3.1.1	19 295	753	20 048	1.040
34	4 845±97	JEF-2.2	4 153	299	4 452	0.919
		JEFF-3.1	4 236	300	4 536	0.936
		JEFF-3.1.1	4 236	300	4 536	0.936
35	6 091±122	JEF-2.2	5 365	331	5 696	0.935
		JEFF-3.1	5 479	333	5 812	0.954
		JEFF-3.1.1	5 479	333	5 812	0.954

3.2.4 Burn-up effects on criticality calculations

The calculation of criticality coefficients from spent nuclear fuel depends on the fuel composition. It is thus important to validate the concentrations of important nuclides, both the fissile materials and neutron absorbers, present in irradiated fuels. The results above could be used with published studies to investigate the likely effects of burn-up on criticality calculations.

For the development of novel fuel cycles, where no practical criticality validation of spent fuel currently exists, it will be important to justify to regulators the spent fuel inventory and hence its effect on criticality requirements so that well quantified fuel cycles can be developed and their impact properly studied.

4. Benchmarking for fusion technology applications

This section is devoted to the benchmark effort conducted in the frame of the European Fusion Technology Programme to validate the JEFF-3.1 general purpose and activation cross-section data for dedicated fusion technology applications [75-82].

4.1 Neutron cross-section data for fusion technology applications

Fusion technology applications require neutron cross-section data for all nuclides constituting the materials to be used in a fusion device, including the breeders, neutron multipliers, coolants, shielding, structure, magnets and insulators, with special emphasis on high-quality data around 14 MeV. A major feature is the importance of inelastic neutron reactions, which require the use of double-differential cross-section data to properly describe the energy-angle distributions of emitted secondary neutrons. Photon production and interaction data must be included in the nuclear data libraries for use in coupled neutron-photon transport calculations. In addition, specific nuclear response data are required such as tritium production, kerma factors, gas production and radiation damage data. Activation and transmutation cross-section data must also be provided for the isotopes of all stable elements that may be present as impurities in materials and for radioactive targets that are involved in multi-step pathways.

For practical applications, data evaluations must be complete i.e. they must include all data types and nuclear reactions which are required for neutron and photon transport simulations as well as the calculation of relevant nuclear responses. On the other hand, for activation calculations a full set of data for all potential target nuclides must be available.

Materials of interest to fusion applications include breeder materials such as Pb-Li, Li, Li_4SiO_4, Li_2O, Li_2TiO_3, neutron multipliers (Be, Pb), coolants (He, H_2O, or liquid metals), structural materials (in particular reduced activation steels such as Eurofer, but also SS-316, SiC, and others), shielding materials W, WC, B_4C as well as many other materials of minor importance.

4.2 General purpose data for transport calculations

The nuclear design of any kind of fusion device relies on the results of particle transport calculations which provide the neutron/photon flux spectra and form the basis for the calculation of nuclear responses of interest when convoluted with the related nuclear data. Complete general purpose data evaluations including secondary angle and energy distributions are required for performing the transport calculations. Prior to their use in design calculations, these data need to be validated through integral benchmark experiments and their computational analyses.

A variety of integral 14 MeV neutron benchmark experiments, suitable for checking fusion relevant neutron transport calculations, is available and has been used for benchmarking JEFF-3.1 general purpose data. In such experiments, material assemblies are irradiated with 14 MeV neutrons and nuclear responses of interest are measured and compared to calculations which simulate the experiment by modelling the experimental set-up as close as possible. As a general rule, the benchmark analyses include cross-

checks with other data evaluations such as FENDL-1, -2 and ENDF/B-VI, -VII as well as data checks of processed data with measured cross-sections.

4.2.1 Be, Ti, V, Ta, W and Pb

A series of benchmark analyses has been performed on the cross-sections of Be, Ti, V, Ta, W and Pb with the objective to check and validate the related recent data evaluations for neutron transport calculations. Available integral benchmark experiments have been analysed on the basis of Monte Carlo calculations with the MCNP Monte Carlo code using mainly EFF-3/JEFF-3.1 and FENDL-2.0/2.1 data evaluations. Major results of these benchmark analyses are summarised here.

Beryllium: The ^{9}Be EFF-3.1 data evaluation provides a unique decomposition of the (n,2n) reaction into 16 partial channels. Extensive benchmark tests have been performed at various stages of the data file preparation and its processing requiring special care. The KANT transmission experiment on spherical beryllium shells and the FNS/JAERI time-of-flight experiments on beryllium slabs were used for the benchmarking. Significant improvements over the existing Be data evaluations could be obtained due to the better description of the energy-angle distributions of neutrons emitted through the different 16 reaction channels. As an example, Figure 4.1 compares angular neutron leakage spectra calculated for the FNS time-of-flight experiment on a 15.24 cm thick slab at an angle of 66.8 degree. See EFFDOC-782 [95], -788 [96], -932 [97].

Titanium: The benchmark analyses on titanium showed significant discrepancies for all available Ti data evaluations. This is true for both the neutron emission spectra at 14 MeV incident neutron energy, shown in Figure 4.2, and the neutron leakage spectra calculated for a spherical shell transmission experiment performed at the OKTAVIAN facility of the University of Osaka, Japan. See EFFDOC-930 [84].

Vanadium: The JEFF-3.1 vanadium evaluation, which originates from ENDF/B-VI, was shown to better reproduce the measurements of the neutron flux spectra than the other available data evaluations while the photon flux spectra are significantly overestimated, see e.g. Figure 4.3 for the experiment performed at FNS Tokai-mura, Japan, on a rectangular vanadium block. See EFFDOC-999 [88].

Tantalum: Only two independent Ta data evaluations up to 20 MeV do currently exist which are included in the American ENDF/B-VI, -VII and the Japanese JENDL-3.3 data library, respectively. The ENDF/B-VI, -VII Ta evaluation is an obsolete evaluation performed in 1972 for ENDF/B-IV. The JEFF-3.1 library has adopted the JENDL-3.3 evaluation. The benchmark analyses on Ta indicate, however, the need for updating the Ta data evaluations with special focus on the energy spectra of neutrons emitted through the Ta(n,xn) reactions. A new ^{181}Ta data evaluation has been provided in the meantime as part of the ongoing EFF evaluation effort. Preliminary results, denoted as JEFF-3.2T are included in Figure 4.4 comparing neutron leakage spectra for the transmission experiments on two Ta spherical shells performed the Lawrence Livermore National Laboratory (LLNL), US, with a central 14 MeV neutron source and Figure 4.5 showing the neutron emission spectra at 14.1 MeV incident neutron energy. See EFFDOC-952 [85], -973 [86], -1009 [87].

Tungsten: The JEFF-3.1 W data evaluations originating from JENDL-3.3 were shown to give a severe underestimation of the fast ($E > 1$ MeV) neutron flux measured in the benchmark experiment on a tungsten assembly at the Frascati Neutron Generator (FNG), see Figure 4.6. It was thus concluded that a genuine JEFF evaluation of the W isotopes is required. This evaluation is underway for JEFF-3.2. See EFFDOC-885 [89], -897 [90], -994 [91], -1004 [92], -1016 [93], -1051 [94].

Lead: The new JEFF-3.1 lead evaluation was shown to underestimate measured neutron multiplication factors (Figure 4.7) and neutron leakage spectra as well as the photon emission and leakage spectra (Figure 4.8). It was concluded that the evaluation needs to be updated for fusion technology applications, see EFFDOC-929 [83].

Figure 4.1: Angular neutron leakage spectra as calculated and measured for the FNS time-of-flight experiment on a 15.24 cm thick Be slab at an angle of 66.8 degree

(EFF-3.05 denotes the evaluation adopted in the final JEFF-3.1 data file)

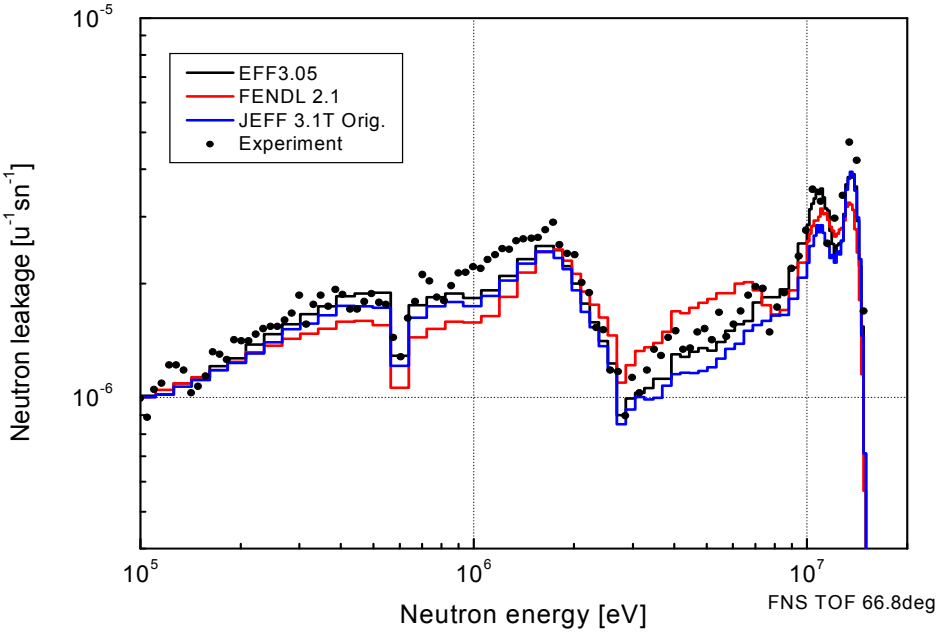


Figure 4.2: Comparison of Ti neutron emission spectra at 14 MeV incident neutron energy

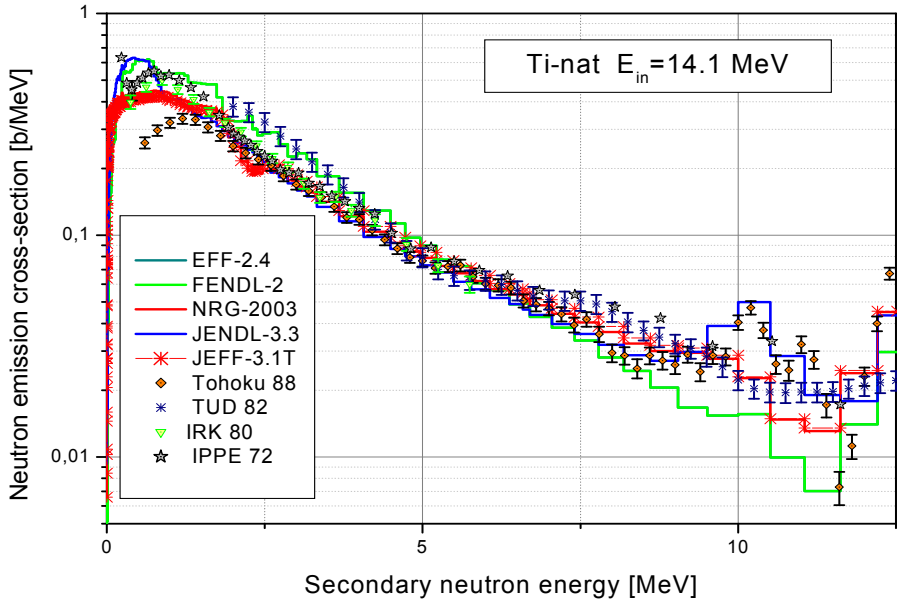


Figure 4.3: Neutron (left) and photon (right) flux spectra as measured and calculated for a detector position inside a rectangular Vanadium block

(FNS experiment with external 14 MeV neutron source)

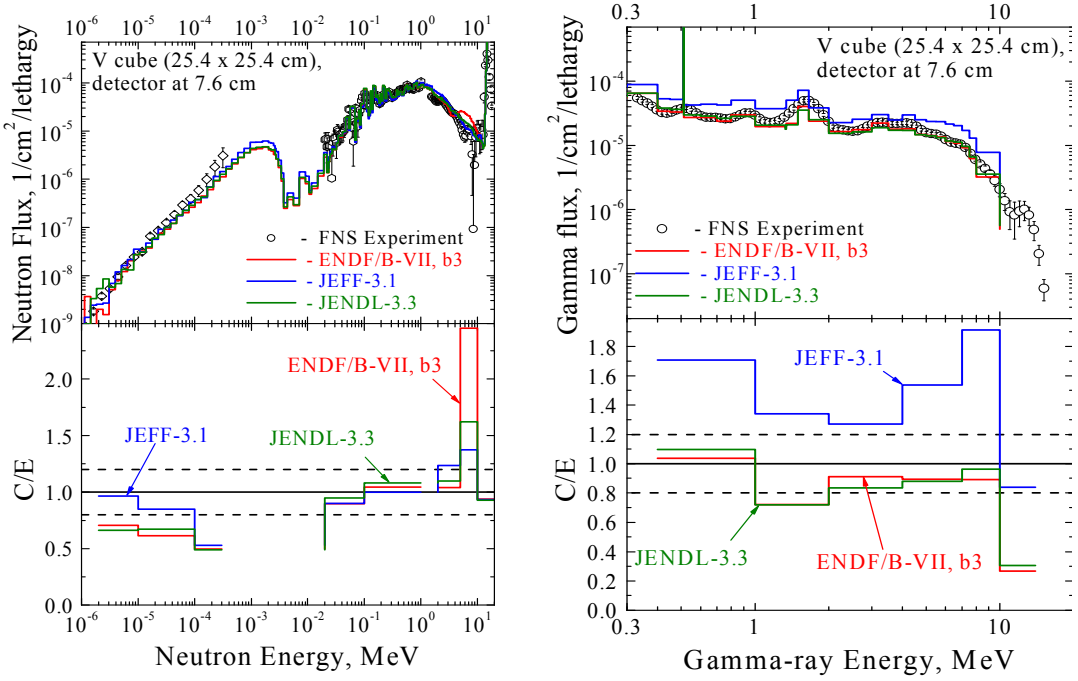


Figure 4.4: Comparison of measured and calculated neutron leakage spectra

(LLNL spherical Ta shell experiment with central 14 MeV neutron source)

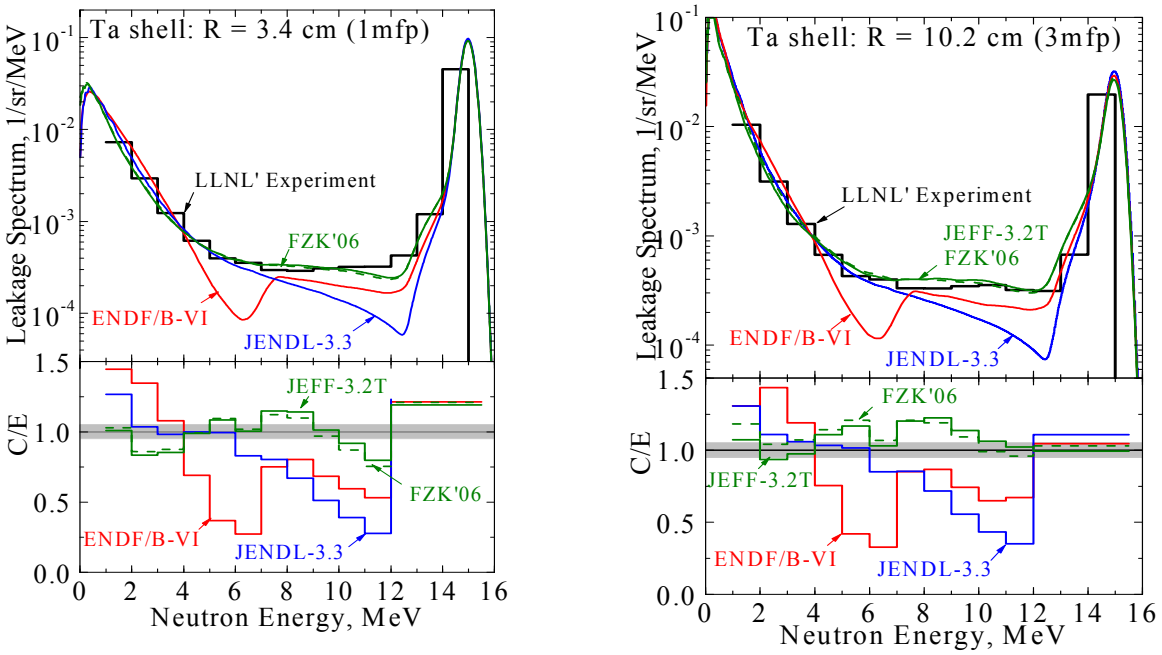


Figure 4.5: Comparison of Ta neutron emission spectra at 14.1 MeV incident neutron energy

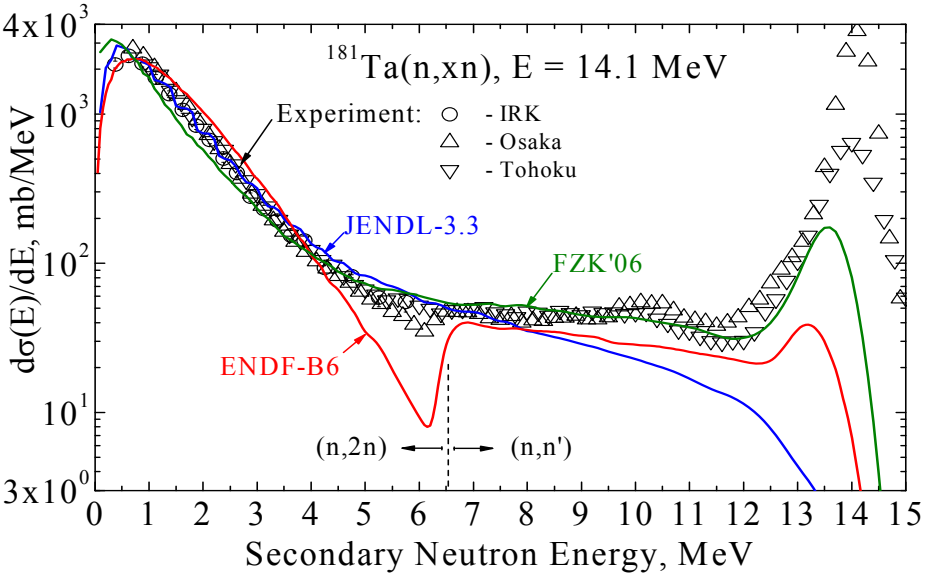


Figure 4.6: Comparison of calculated and measured neutron flux integrals (E > 12.5 MeV left, E> 1 MeV, right) at four detector positions in the W assembly irradiated at the Frascati Neutron Generator (FNG) with 14 MeV neutrons

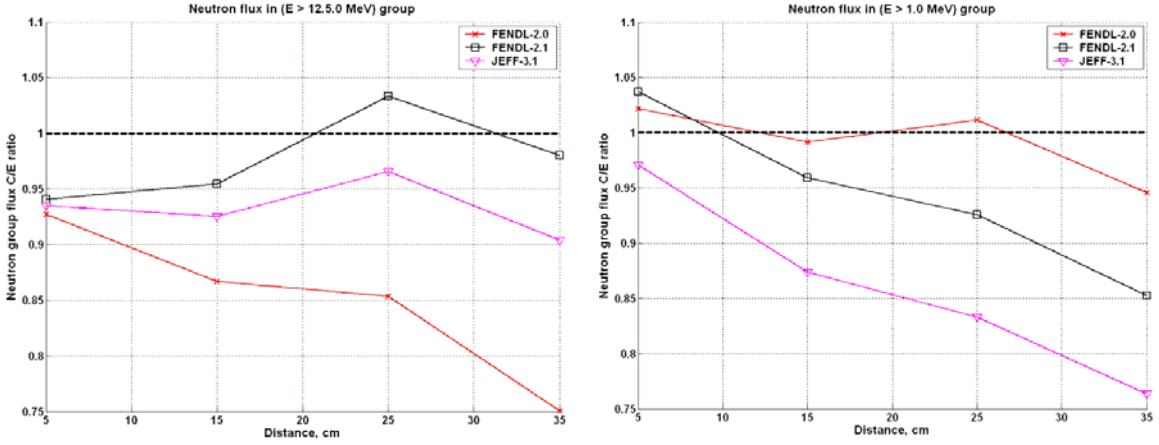


Figure 4.7: Neutron multiplication of spherical lead shells with central 14 MeV neutron source

(KIAE, TUD and OKTAVIAN experiments)

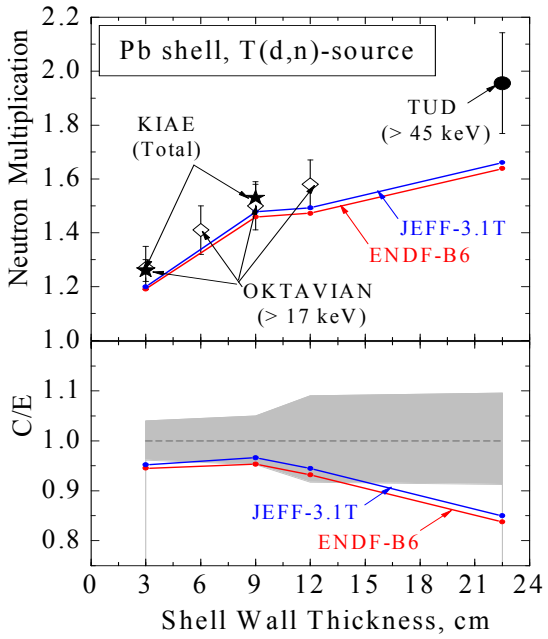
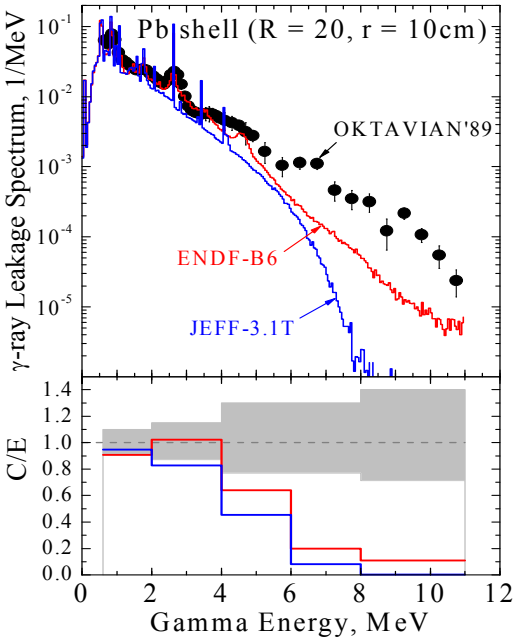


Figure 4.8: Photon leakage spectra from 10 cm thick spherical Pb shell with central 14 MeV neutron source

(OKTAVIAN experiment)



4.2.2 *ITER bulk shield and streaming experiments*

The benchmark experiments performed at the Frascati Neutron Generator (FNG) on mock-ups of the ITER inboard shield system have been re-analysed with JEFF-3.1 and FENDL-2.1 data. No significant differences were obtained for the calculated neutron and photon flux spectra, and the measured reaction rates when comparing results obtained with FENDL-2.0/2.1 and JEFF-3.1 data. There is a general trend for underestimating the fast neutron flux with increasing penetration depths, see Figure 4.9. The nuclear heating is underestimated throughout by about 10%. Examples of neutron and photon flux spectra are shown in Figure 4.10 for the streaming experiment. See EFFDOC-994 [91], -1004 [92].

4.2.3 *Breeder blanket mock-up experiment*

A special benchmark effort has been devoted to the test blanket module (TBM) under development for irradiation tests in ITER. A dedicated experiment has been performed on a TBM mock-up of the HCPB (helium–cooled pebble bed) breeder blanket at FNG to check and validate the capability of the neutronic codes and nuclear data to predict the tritium production. The tritium generated during irradiation in a series of Li_2CO_3 pellets located at different penetration depths in the mock-up was found to be underestimated in the calculations by 5 to 10% on average, see Figure 4.11. The same trend was obtained for other data evaluations such as FENDL-2.0 and – 2.1. These results indicate that design calculations for the tritium breeding ratio (TBR) of fusion power reactors employing a HCPB type breeder blanket are conservative.

Figure 4.9: Calculated (C) over experimental (E) ratios for the 58Ni(n,p) reaction rate (left), indicating the fast neutron flux, and the nuclear heating (right) in the ITER bulk shield experiment

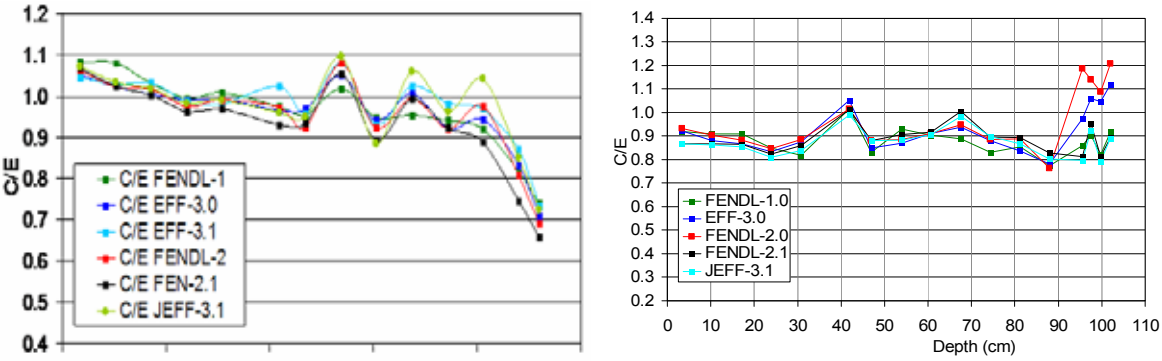
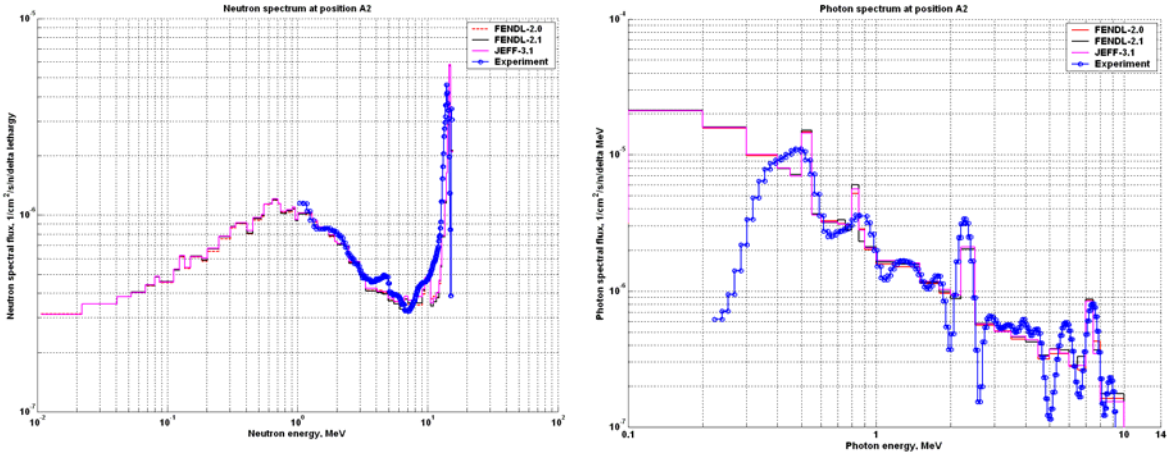


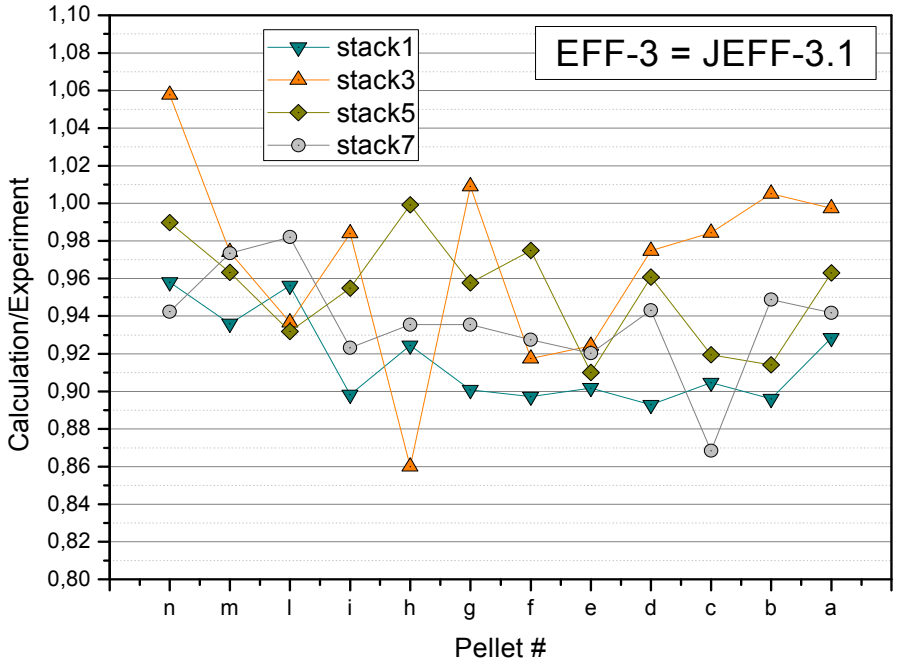
Figure 4.10: ITER streaming experiment: neutron (left) and photon (right) spectra calculated and measured at a dedicated position inside the shield assembly



The neutron flux across the breeder mock-up is well predicted within the total combined uncertainties of about ±5%. No significant differences between FENDL-2.0/2.1 and JEFF-3.1 data were observed. Behind the mock-up the fast neutron flux (E > 1 MeV) was found to be slightly overestimated by about 10%. This indicates that shielding calculations for the HCPB blanket are conservative. The γ-ray flux is underestimated by about 10% at the back of the mock-up. The slow neutron flux investigated by time-of-arrival spectroscopy is underestimated in the mock-up by about 20%.

A Monte Carlo based sensitivity/uncertainty analysis was performed for the TBM mock-up neutronics experiment to assess the uncertainties of calculated tritium production rates and track them down to specific nuclides and reaction cross-sections. The dominant tritium production from ^{6}Li, e.g. was shown to be mainly sensitive to the Be cross-sections for the elastic scattering (1.7 – 2.1 %/%) and the (n, 2n) reaction (0.7 %/%). The uncertainties of the total tritium production rate (TPR) due to uncertainties of the reaction cross-sections are at 4% (2σ confidence level) and are dominated by the ^{9}Be uncertainties. See EFFDOC-938 [98], -950 [99], -954 [100], -981 [101], -987 [102] and -994 [91], -1004 [92].

Figure 4.11: HCPB breeder mock-up experiment: ratios of calculated (C) and experimental (E) tritium activities in different pellet stacks of the mock-up



4.3 Activation cross-sections

Activation and transmutation cross-section data for fusion technology applications must be provided for the isotopes of all stable elements that may be present as initial constituents, impurities or tramp elements in the materials, or as transmutation products.

Accordingly, a major evaluation effort on the production of a qualified activation data library for fusion inventory calculations has been conducted in the frame of the EU fusion technology programme. This has led to various versions of the European Activation File (EAF), with the version EAF-2007 having an extended energy range up to 60 MeV. The previous version, EAF-2003 with neutron-induced cross-sections up to 20 MeV, has been adopted as the FENDL-2.1/A and JEFF-3.1/A activation data libraries.

4.3.1 *Fusion neutron irradiations*

A major experimental effort has been conducted on the validation of fusion relevant activation cross-section data. Various fusion candidate materials such as the steels SS-316, MANET, F82H and Eurofer, different vanadium alloys, pure elements (Al, V, Ni, Cu, Cr, Fe, Hf, Nb, Mo, La, Sn, Y, Pb, W, Ta), CuCrZr, SiC and the Li_4SiO_4 breeder ceramics have been irradiated at 14 MeV neutron generators and analysed using the FISPACT code with EAF data. In addition to these measurements funded by EFDA, it has also been possible to use results from the literature in a ^{252}Cf spontaneous fission spectrum and from experiments carried out at the JAERI FNS facility.

Measurements give the activity of various nuclides at various times following neutron irradiation (E). Calculations with EASY give the predictions for the activity of these nuclides (C) and the ratio C/E can be formed. The pathway method in FISPACT is able to determine how these nuclides have been formed and by determining the library value of the reaction cross-section in the particular neutron spectrum, the effective cross-section, it is possible to calculate the measured effective cross-section. These effective cross-sections, rather

than the nuclide activities are stored in SAFEPAQ-II and used in all the validation studies. Reference [14] gives the results of the validation of EAF-2003 (=JEFF-3.1/A) and this should be consulted for details of the original measurements, methodology of calculation of effective cross-sections and graphs for all reactions. Here the summary table of integral data for all reactions and some example plots are shown.

Table 4.1: Summary of reactions with integral data

Spectrum − the irradiation spectrum, # indicates new results included after the EAF-2003 release. QS − the quality score, scores in (brackets) indicate that the total cross-section is measured in the integral experiment and only partial data exist in the EAF file.

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
B-10(n,t)	6	cf252_flux_1#	5.00E-02	2.50E-02	1.093
N-14(n,2n)	6	fns_5min	8.08E-03	1.21E-03	0.862
N-14(n,γ)	5	cf252_flux_1#	4.80E-06	2.40E-06	26.92
O-16(n,p)	6	fns_5min	3.29E-02	1.40E-03	1.000
F-19(n,2n)	6	fns_5min	4.82E-02	2.41E-03	0.911
		cf252_flux_1#	1.08E-05	1.60E-06	1.639
		cf252_flux_1#	1.63E-05	5.00E-07	1.086
F-19(n,p)	6	fns_5min	1.54E-02	7.70E-04	1.064
Na-23(n,2n)	6	fns_7hour	3.80E-02	1.90E-03	0.861
		fzk_1	4.60E-03	2.76E-03	1.286
Na-23(n,γ)	6	cf252_flux_1#	3.35E-04	1.50E-05	0.663
Na-23(n,p)	5	fns_5min	2.29E-02	6.88E-04	1.397
Mg-24(n,p)	(6)	fns_5min	1.54E-01	1.69E-02	1.043
		cf252_flux_1#	1.94E-03	9.29E-05	1.124
		cf252_flux_1#	2.01E-03	6.00E-05	1.085
Mg-25(n,p)	6	fns_5min	4.98E-02	5.47E-03	1.146
Mg-26(n,α)	5	fns_5min	3.47E-02	3.82E-03	1.097
		fng_heat#	8.69E-02	9.56E-03	0.450
Al-27(n,p)	6	fns_5min	5.71E-02	2.86E-03	1.075
		cf252_flux_1#	4.89E-03	1.79E-04	1.092
		cf252_flux_1#	4.80E-03	9.00E-05	1.113
Al-27(n,α)	(6)	fzk_1	3.40E-02	6.80E-03	0.876
		fng_vanad	9.46E-02	8.92E-03	0.869
		sneg_1	1.25E-01	2.25E-02	0.874
		sneg_2	1.35E-01	2.29E-02	0.870
		fng_f82h	6.66E-02	6.86E-03	1.470
		cf252_flux_1#	1.01E-03	2.20E-05	1.044
		cf252_flux_1#	8.60E-04	5.00E-05	1.220
Si-28(n,p)	6	fns_5min	1.98E-01	1.78E-02	1.078
		fng_SiC	2.10E-01	6.29E-03	0.993
		fzk_1	6.30E-02	1.57E-02	1.529
		sneg_1	2.79E-01	1.24E-02	0.817
		cf252_flux_1#	7.12E-03	2.35E-04	1.035
		cf252_flux_1#	9.66E-03	5.50E-04	0.763
Si-29(n,p)	6	fns_5min	1.11E-01	8.92E-03	1.047
		fng_SiC	1.16E-01	5.79E-03	0.989
		fzk_1	3.20E-02	4.80E-03	1.213
		sneg_1	1.32E-01	4.11E-03	0.970
		cf252_flux_1#	1.79E-03	7.90E-04	2.028
Si-29(n,2p)	5	fzk_1	8.60E-06	1.03E-06	0.403
Si-30(n,α)	6	fns_5min	5.93E-02	4.74E-03	1.042
		fng_SiC	5.47E-02	2.19E-03	1.114
		sneg_1	7.36E-02	4.42E-03	0.949
P-31(n,p)	6	cf252_flux_1#	3.35E-02	2.00E-03	0.918
P-31(n,α)	6	fns_5min	1.22E-01	1.82E-02	0.865
S-32(n,p)	6	fns_7hour	2.30E-01	1.38E-02	0.952

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		cf252_flux_1#	6.46E-02	3.80E-03	1.092
		cf252_flux_1#	7.25E-02	2.95E-03	0.973
		cf252_flux_1#	6.84E-02	3.42E-04	1.031
S-32(n,t)	5	fns_5min	6.32E-05	5.69E-06	0.675
S-34(n,α)	5	fns_5min	1.37E-01	9.60E-03	0.863
Cl-35(n,2n)m	6	fns_5min	6.70E-03	3.35E-04	1.057
Cl-37(n,p)	5	fns_5min	1.60E-02	9.61E-04	1.209
Cl-37(n,α)	6	fns_5min	2.48E-02	1.24E-03	1.087
K-39(n,2n)g	6	fns_5min	4.76E-03	2.85E-04	1.031
K-41(n,α)	(6)	fns_5min	2.64E-02	1.58E-03	1.095
Ca-40(n,t)g	5	fns_5min	1.28E-04	8.94E-06	1.266
Ca-44(n,p)	6	fns_5min	3.55E-02	3.20E-03	1.042
Ca-48(n,2n)	6	fns_7hour	9.43E-01	1.04E-01	0.847
Sc-45(n,2n)g	5	fns_5min	1.67E-01	8.34E-03	1.087
		fng_ScSmGd#	1.19E-01	3.81E-03	1.630
Sc-45(n,2n)m	6	fng_ScSmGd#	1.09E-01	5.11E-03	1.090
Sc-45(n,α)	6	fng_ScSmGd#	4.74E-02	4.13E-03	1.100
Ti-46(n,2n)	6	sneg_1	5.82E-02	7.57E-03	1.001
		cf252_flux_1#	9.30E-05	3.10E-05	0.136
Ti-46(n,p)	(6)	fzk_2	1.21E-01	1.32E-02	0.909
		cf252_flux_1#	1.38E-02	3.00E-04	0.976
		cf252_flux_1#	1.36E-02	1.21E-03	0.990
		cf252_flux_1#	1.24E-02	1.20E-03	1.086
		cf252_flux_1#	1.39E-02	1.21E-03	0.969
Ti-46(n,p)g	6	fns_7hour	2.18E-01	1.09E-02	0.826
Ti-47(n,p)	6	cf252_flux_1#	2.03E-02	1.10E-03	1.060
		cf252_flux_1#	1.89E-02	4.00E-04	1.139
		cf252_flux_1#	1.94E-02	9.70E-05	1.109
		cf252_flux_1#	2.20E-02	9.00E-04	0.978
		cf252_flux_1#	2.16E-02	1.18E-03	0.996
Ti-48(n,p)	6	fns_7hour	6.38E-02	3.83E-03	0.925
		fns_5min	5.11E-02	2.56E-03	1.077
		fng_heat#	8.53E-02	1.15E-02	0.666
		cf252_flux_1#	4.20E-04	1.00E-05	0.959
		cf252_flux_1#	4.17E-04	1.59E-05	0.966
		cf252_flux_1#	3.80E-04	2.00E-05	1.060
Ti-49(n,p)	6	fng_heat#	2.36E-02	4.25E-03	1.369
Ti-50(n,p)	6	fns_5min	1.40E-02	7.02E-04	0.901
		fng_heat#	1.34E-02	2.43E-03	0.985
Ti-50(n,α)	5	fng_vanad	9.19E-03	2.05E-03	0.714
V-51(n,γ)	6	fng_vanad	6.53E-02	3.98E-03	1.045
		sneg_1	1.60E-03	2.40E-04	0.376
		cf252_flux_1#	2.80E-03	3.00E-04	0.748
V-51(n,p)	6	fns_5min	2.36E-02	1.18E-03	1.136
		fng_vanad	2.01E-02	1.11E-03	1.094
		sneg_1	2.75E-02	1.92E-03	1.071
		cf252_flux_1#	7.10E-04	1.10E-04	1.000
		cf252_flux_1#	9.30E-04	1.00E-04	0.763
		cf252_flux_1#	7.13E-04	5.88E-05	0.996
V-51(n,α)	6	fns_5min	1.43E-02	7.17E-04	1.064
		fns_7hour	1.74E-02	1.04E-03	0.901
		fng_f82h	1.67E-02	4.00E-03	0.879
		sneg_1	1.70E-02	6.38E-04	1.034
		sneg_2	1.59E-02	7.39E-04	1.008
		cf252_flux_1#	3.88E-05	1.20E-06	1.015
Cr-50(n,2n)	6	fng_vanad	2.29E-02	4.29E-03	0.954

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		fng_Cr	3.01E-02	5.82E-03	0.888
Cr-50(n,t)	6	fzk_2	2.70E-04	5.40E-05	0.912
Cr-52(n,2n)	6	fns_7hour	3.42E-01	1.71E-02	1.000
		fzk_2	3.90E-02	5.85E-03	1.241
		fng_Cr	3.38E-01	3.05E-02	1.044
		fng_cucrzr#	4.62E-01	3.69E-02	0.760
		tud_cucrzr#	3.27E-01	3.53E-02	1.160
Cr-52(n,p)	6	fns_5min	7.20E-02	1.80E-03	0.740
		sneg_1	9.97E-02	4.49E-03	0.941
		fng_Cr	7.12E-02	9.92E-03	0.934
		cf252_flux_1#	1.07E-03	7.00E-05	1.218
Cr-53(n,p)	6	sneg_1	5.95E-02	5.89E-03	0.817
		cf252_flux_1#	3.06E-04	2.70E-05	1.817
Mn-55(n,2n)	6	fns_7hour	7.34E-01	3.67E-02	1.031
		cf252_flux_1#	5.80E-04	1.40E-04	0.896
		cf252_flux_1#	4.08E-04	9.00E-06	1.273
Mn-55(n,γ)	6	fns_7hour	8.58E-04	4.29E-05	0.950
		fns_5min	3.99E-03	2.39E-04	1.006
Mn-55(n,p)	6	fns_5min	2.66E-02	1.33E-03	1.177
Mn-55(n,α)	6	fns_5min	1.95E-02	9.77E-04	1.081
Fe-54(n,2n)	(6)	sneg_1	9.23E-03	2.58E-03	1.124
Fe-54(n,p)	6	fns_7hour	3.31E-01	3.31E-03	0.926
		sneg_1	3.09E-01	1.54E-02	0.918
		sneg_2	3.43E-01	1.71E-02	0.959
		fzk_2	2.87E-01	4.30E-02	0.992
		fng_f82h	2.69E-01	1.90E-02	1.027
		cf252_flux_1#	8.46E-02	2.00E-03	1.046
		cf252_flux_1#	9.25E-02	5.00E-03	0.956
		cf252_flux_1#	8.78E-02	8.78E-04	1.007
		cf252_flux_1#	8.76E-02	4.35E-03	1.010
		cf252_flux_1#	7.90E-02	3.00E-03	1.120
Fe-54(n,t)	(5)	fzk_2	9.00E-05	1.80E-05	0.850
Fe-54(n,α)	6	fng_SiC	8.22E-02	4.11E-03	0.923
Fe-56(n,p)	6	fns_5min	9.14E-02	2.64E-03	1.039
		fns_7hour	1.07E-01	5.36E-03	0.971
		fng_f82h	9.31E-02	6.58E-03	0.996
		fng_SiC	9.58E-02	4.79E-03	0.973
		fng_vanad	9.16E-02	1.45E-02	0.848
		sneg_1	1.07E-01	3.27E-03	0.959
		sneg_2	1.10E-01	4.59E-03	1.014
		cf252_flux_1#	2.07E-02	1.01E-03	0.070
		cf252_flux_1#	1.15E-03	8.00E-05	1.259
		cf252_flux_1#	1.45E-03	6.00E-05	0.998
		cf252_flux_1#	1.45E-03	3.50E-05	0.998
		cf252_flux_1#	1.18E-03	8.00E-05	1.227
		cf252_flux_1#	1.40E-03	1.68E-05	1.034
Fe-57(n,p)	6	sneg_1	7.12E-02	9.26E-03	1.110
Fe-58(n,γ)	6	fng_SiC	1.26E-03	6.30E-05	1.145
		fng_eurofer	2.48E-02	4.27E-03	0.776
Co-59(n,2n)	(6)	fns_7hour	7.08E-01	3.54E-02	0.956
		cf252_flux_1#	5.70E-04	3.00E-05	0.709
Co-59(n,2n)m	5	fns_7hour	3.33E-01	1.66E-02	1.389
Co-59(n,γ)m	5	fns_5min	7.76E-03	3.88E-04	1.205
Co-59(n,γ)	(6)	cf252_flux_1#	6.97E-03	3.40E-04	0.685
Co-59(n,p)	6	cf252_flux_1#	1.96E-03	1.00E-05	0.869
Co-59(n,α)	6	fns_5min	2.53E-02	1.26E-03	1.099

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		cf252_flux_1#	2.00E-04	1.00E-05	1.118
		cf252_flux_1#	2.17E-04	1.40E-05	1.031
		cf252_flux_1#	2.22E-04	4.00E-06	1.008
		cf252_flux_1#	2.00E-04	1.00E-05	1.118
Ni-58(n,2n)	6	fns_7hour	3.25E-02	7.27E-04	1.012
		fng_f82h	3.65E-02	1.01E-02	0.891
		fzk_2	5.42E-03	5.42E-04	0.964
		sneg_1	4.37E-02	3.06E-03	0.964
		sneg_2	3.27E-02	2.29E-03	0.958
		cf252_flux_1#	8.95E-06	2.80E-07	1.074
Ni-58(n,n'p)	6	fns_7hour	6.43E-01	2.27E-02	0.920
		fng_vanad	5.29E-01	1.07E-01	0.886
		fzk_2	1.07E-01	1.07E-02	0.812
		sneg_1	7.20E-01	5.04E-02	0.915
		sneg_2	6.43E-01	3.86E-02	0.945
		fng_f82h	5.08E-01	4.79E-02	1.085
		fng_eurofer	4.76E-01	1.38E-01	1.056
Ni-58(n,p)	(6)	fns_7hour	3.08E-01	6.88E-03	0.998
		fzk_2	4.37E-01	4.37E-02	0.772
		fng_vanad	2.72E-01	4.09E-02	0.882
		sneg_1	2.98E-01	2.09E-02	0.914
		cf252_flux_1#	9.50E-02	4.50E-03	1.237
		cf252_flux_1#	1.05E-01	5.00E-03	1.119
		cf252_flux_1#	1.13E-01	4.80E-03	1.036
		cf252_flux_1#	1.19E-01	6.00E-03	0.987
		cf252_flux_1#	1.18E-01	3.00E-03	0.996
		cf252_flux_1#	1.18E-01	3.56E-04	0.996
		cf252_flux_1#	1.19E-01	4.78E-03	0.992
		cf252_flux_1#	1.21E-01	2.00E-03	0.971
Ni-58(n,t)	5	fzk_2	4.40E-05	1.10E-05	0.406
Ni-60(n,p)	(6)	fzk_2	5.52E-02	5.52E-03	0.771
		sneg_1	1.51E-01	1.20E-02	0.857
		sneg_2	1.62E-01	1.29E-02	0.902
Ni-60(n,p)m	6	fns_5min	8.01E-02	3.40E-03	0.790
		fng_heat#	6.45E-02	8.39E-03	0.999
Ni-62(n,p)g	6	fns_5min	1.71E-02	1.02E-03	1.042
		fng_heat#	2.22E-02	2.99E-03	0.832
Ni-62(n,p)m	6	fns_5min	1.50E-02	6.38E-04	1.075
		fng_heat#	1.85E-02	2.50E-03	0.911
Ni-62(n,α)	6	fzk_2	4.60E-03	4.60E-04	0.959
Cu-63(n,2n)	6	fns_5min	4.59E-01	2.30E-02	1.075
		tud_cucrzr#	4.91E-01	5.55E-02	1.090
		cf252_flux_1#	3.00E-04	2.70E-05	0.718
		cf252_flux_1#	1.83E-04	7.00E-06	1.177
Cu-63(n,γ)	5	cf252_flux_1#	1.76E-02	1.40E-03	0.591
Cu-63(n,α)	(6)	fns_7hour	4.39E-02	3.95E-03	0.867
		fng_SiC	1.99E-02	9.94E-04	1.712
		fzk_2	1.50E-02	1.50E-03	0.778
		fng_cucrzr#	3.51E-02	3.16E-03	0.994
		tud_cucrzr#	3.44E-02	3.34E-03	1.120
		cf252_flux_1#	6.71E-04	1.80E-05	1.026
		cf252_flux_1#	7.09E-04	1.70E-05	0.971
Cu-65(n,2n)	6	fns_7hour	8.47E-01	5.08E-02	0.900
		fng_SiC	9.40E-01	1.88E-02	0.856
		fzk_2	1.57E-01	1.57E-02	1.053
		fng_cucrzr#	9.79E-01	6.86E-02	0.876
		tud_cucrzr#	8.16E-01	2.84E-01	1.151

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		cf252_flux_1#	6.65E-04	2.30E-05	1.088
Cu-65(n,γ)	6	cf252_flux_1#	8.00E-03	1.20E-03	0.863
Cu-65(n,α)m	6	fng_cucrzr#	5.80E-03	8.71E-04	1.161
		tud_cucrzr#	4.83E-03	5.50E-04	1.530
		fzk_2	1.21E-03	1.94E-04	0.996
Cu-65(n,nα)	6	fng_SiC	1.25E-03	1.25E-04	1.439
		fzk_2	7.10E-04	1.42E-04	1.092
		fng_cucrzr#	2.27E-03	2.27E-04	0.783
		tud_cucrzr#	1.50E-03	1.36E-04	1.090
Cu-65(n,p)	6	fng_SiC	2.12E-02	1.06E-03	0.935
		fzk_2	7.40E-03	7.40E-04	0.909
		fng_cucrzr#	2.16E-02	1.30E-03	0.933
		tud_cucrzr#	1.85E-02	1.37E-03	1.190
Zn-64(n,2n)	6	fns_5min	1.53E-01	7.64E-03	1.010
Zn-64(n,p)	6	cf252_flux_1#	4.11E-02	1.30E-03	1.074
		cf252_flux_1#	3.82E-02	1.50E-03	1.155
		cf252_flux_1#	4.64E-02	2.30E-03	0.951
		cf252_flux_1#	3.94E-02	1.00E-03	1.120
		cf252_flux_1#	4.18E-02	1.75E-03	1.055
		cf252_flux_1#	4.13E-02	2.82E-03	1.068
Zn-66(n,p)	6	fns_5min	6.28E-02	3.14E-03	1.045
Zn-68(n,γ)m	5	cf252_flux_1#	1.85E-03	1.20E-04	0.246
Ga-69(n,2n)	6	fns_5min	7.82E-01	3.91E-02	1.099
Ga-71(n,2n)	6	fns_5min	8.99E-01	4.50E-02	1.088
Ge-74(n,p)	(6)	fns_5min	9.98E-03	5.99E-04	0.961
Ge-76(n,2n)	(6)	fns_5min	1.04E+0	7.26E-02	1.100
Ge-76(n,2n)m	6	fns_5min	9.27E-01	6.49E-02	0.884
As-75(n,p)	(6)	fns_5min	1.89E-02	1.14E-03	1.158
As-75(n,p)m	6	fns_5min	1.25E-02	9.96E-04	0.838
Se-78(n,2n)m	6	fns_5min	6.29E-01	6.29E-02	1.087
Se-80(n,2n)m	6	fns_5min	1.70E-01	1.87E-02	0.884
Se-80(n,p)	6	fns_5min	1.51E-02	1.81E-03	0.934
Se-82(n,2n)	(5)	fns_5min	1.00E+0	7.02E-02	1.306
Br-79(n,2n)	6	fns_5min	8.26E-01	9.09E-02	0.990
Br-81(n,2n)g	6	fns_5min	3.71E-01	4.08E-02	1.069
Rb-85(n,2n)m	6	fns_5min	4.15E-01	2.08E-02	1.020
Rb-87(n,2n)m	6	fns_5min	4.49E-01	2.24E-02	1.074
Sr-84(n,2n)	(6)	fns_7hour	6.37E-01	3.18E-02	1.010
Sr-84(n,γ)m	5	cf252_flux_1#	2.42E-01	2.70E-02	0.192
		cf252_flux_1#	3.54E-02	2.34E-03	1.312
Sr-86(n,2n)	(6)	fns_7hour	9.45E-01	6.61E-02	1.020
Sr-86(n,γ)m	5	cf252_flux_1#	1.82E-01	2.20E-02	0.093
Sr-88(n,2n)m	6	fns_7hour	2.53E-01	1.27E-02	0.882
		fns_5min	2.26E-01	1.13E-02	0.980
Sr-88(n,p)	6	fns_5min	1.49E-02	7.45E-04	0.909
Y-89(n,n′)m	6	fns_5min	3.71E-01	2.23E-02	0.971
Y-89(n,2n)	6	fns_7hour	1.09E+0	6.52E-02	0.862
		fns_5min	8.25E-01	1.65E-01	1.111
Y-89(n,α)m	6	fns_5min	1.90E-03	9.49E-05	1.002
Zr-90(n,2n)	6	fns_7hour	7.07E-01	4.24E-02	0.971
		fzk_1	1.37E-02	1.37E-03	6.901
		fng_cucrzr#	9.24E-01	6.47E-02	0.750
		tud_cucrzr#	6.71E-01	6.91E-02	1.120
		cf252_flux_1#	2.67E-04	1.50E-05	0.815
		cf252_flux_1#	2.21E-04	6.00E-06	0.985
Zr-90(n,2n)m	6	fns_5min	1.16E-01	5.81E-03	1.220

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		fng_heat#	1.17E-01	3.52E-03	1.273
Zr-90(n,p)m	5	fng_heat#	9.83E-03	7.87E-04	1.170
		cf252_flux_1#	4.50E-05	6.00E-06	1.346
Zr-90(n,n′p)m	5	fns_5min	2.29E-02	1.15E-03	0.923
Zr-94(n,γ)	6	cf252_flux_1#	8.75E-03	6.50E-04	0.663
Zr-94(n,p)	6	fns_5min	6.50E-03	3.25E-04	1.099
Zr-96(n,2n)	6	fns_7hour	1.54E+0	7.68E-02	0.943
Zr-96(n,γ)	5	cf252_flux_1#	4.17E-03	2.10E-04	3.447
Nb-93(n,2n)m	6	fns_7hour	4.72E-01	2.36E-02	0.952
		fng_SiC	3.93E-01	1.18E-02	1.059
		fzk_2	2.76E-01	4.14E-02	0.294
Nb-93(n,n′α)m	6	fns_5min	2.75E-03	1.93E-04	1.010
Nb-93(n,γ)m	5	fns_5min	5.47E-03	3.28E-04	0.885
		fng_heat#	1.24E-02	2.10E-03	0.199
Nb-93(n,α)g	5	fng_heat#	4.46E-02	7.58E-03	0.157
Nb-93(n,α)m	6	fns_5min	5.16E-03	2.58E-04	1.052
		fng_SiC	4.76E-03	2.86E-04	1.128
Mo-92(n,2n)	(6)	fns_5min	2.19E-01	1.10E-02	0.980
		fng_heat#	2.14E-01	2.35E-02	1.053
Mo-92(n,n′p)m	6	fns_7hour	1.49E-01	1.04E-02	0.951
Mo-92(n,p)m	6	fns_7hour	6.19E-02	3.09E-03	0.952
Mo-92(n,p)	(5)	cf252_flux_1#	1.68E-02	7.00E-04	0.723
Mo-92(n,α)	(5)	sneg_1	2.27E-02	2.04E-03	1.285
		cf252_flux_1#	4.20E-04	2.00E-05	0.508
Mo-95(n,p)g	6	fns_7hour	3.24E-02	1.62E-03	1.028
Mo-95(n,p)m	5	cf252_flux_1#	1.44E-04	1.44E-04	0.569
Mo-95(n,p)	5	cf252_flux_1#	2.20E-02	2.00E-03	0.015
Mo-96(n,p)	6	sneg_1	2.08E-02	2.08E-03	1.174
Mo-98(n,γ)	6	cf252_flux_1#	2.63E-02	1.30E-03	1.045
Mo-98(n,p)m	6	fng_heat#	6.18E-03	6.80E-04	0.898
Mo-98(n,α)	6	fns_7hour	7.21E-03	5.04E-04	0.878
Mo-100(n,2n)	6	fns_7hour	1.50E+0	7.50E-02	0.952
		sneg_1	1.53E+0	1.22E-01	0.990
		sneg_2	1.51E+0	1.21E-01	0.989
		fng_vanad	1.12E+0	3.63E-01	0.987
Mo-100(n,γ)	6	cf252_flux_1#	1.48E-02	1.11E-03	0.956
Ru-96(n,2n)	6	fns_5min	5.29E-01	2.65E-02	1.010
Ru-102(n,p)m	6	fns_5min	8.06E-03	4.03E-04	0.854
Rh-103(n,n′)m	5	fns_5min	1.31E-01	3.40E-02	2.222
Rh-103(n,γ)g	5	fns_5min	2.30E-02	1.84E-03	2.671
Rh-103(n,γ)m	5	fns_5min	1.58E-03	1.26E-04	3.571
Pd-106(n,p)m	6	fns_5min	7.84E-03	4.70E-04	1.042
Pd-108(n,2n)m	6	fns_5min	3.44E-01	1.72E-02	1.251
Pd-108(n,p)g	6	fns_5min	4.86E-03	2.92E-04	0.971
Pd-110(n,2n)m	6	fns_5min	4.17E-01	2.50E-02	1.112
Ag-107(n,2n)g	6	fns_5min	6.87E-01	3.44E-02	0.909
		fng_heat#	7.45E-01	8.19E-02	0.870
Ag-109(n,2n)g	6	fns_5min	6.23E-01	3.74E-02	1.067
		fng_heat#	7.57E-01	8.32E-02	0.909
Cd-110(n,γ)	(5)	cf252_flux_1#	2.04E-01	7.00E-03	0.194
Cd-112(n,2n)m	6	fns_5min	5.15E-01	2.58E-02	1.073
		fng_heat#	6.89E-01	2.07E-02	0.835
Cd-116(n,γ)	(5)	cf252_flux_1#	3.80E-02	1.40E-02	0.261
In-113(n,2n)	(5)	cf252_flux_1#	9.50E-03	4.75E-03	0.150
In-113(n,2n)m	5	cf252_flux_1#	3.75E-03	1.85E-03	0.307
In-115(n,2n)g	5	fns_5min	2.01E-01	1.00E-02	1.192

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
In-115(n,γ)m	5	cf252_flux_1#	1.24E-01	3.60E-03	0.385
		cf252_flux_1#	1.39E-01	6.00E-02	0.343
In-115(n,γ)	(5)	fns_5min	5.03E-02	2.52E-03	3.368
Sn-112(n,2n)	5	fng_heat#	1.67E+0	2.25E-01	0.666
Sn-118(n,2n)m	6	fns_7hour	9.65E-01	1.06E-01	0.787
Sn-118(n,p)m	6	fns_5min	6.48E-03	3.89E-04	0.937
Sn-120(n,2n)m	5	fns_7hour	4.89E-01	3.23E-01	1.608
Sn-120(n,p)m	6	fns_5min	3.50E-03	2.10E-04	0.952
Sn-124(n,2n)g	6	fns_7hour	8.76E-01	1.23E-01	0.980
Sn-124(n,2n)m	6	fns_5min	4.29E-01	2.58E-02	1.112
Sb-121(n,2n)g	6	fns_5min	7.79E-01	3.89E-02	1.205
Te-130(n,2n)g	6	fns_5min	5.58E-01	4.46E-02	1.053
I-127(n,2n)	6	cf252_flux_1#	2.07E-03	7.00E-05	1.085
I-127(n,γ)	5	fns_5min	1.96E-02	1.18E-03	1.666
Cs-133(n,2n)	6	fns_5min	1.10E+0	8.77E-02	1.190
Ba-132(n,2n)	(6)	fns_7hour	1.33E+0	6.79E-01	1.042
Ba-134(n,2n)m	6	fns_7hour	6.98E-01	9.78E-02	1.099
Ba-134(n,γ)	(5)	cf252_flux_1#	2.55E-01	2.80E-02	0.197
Ba-136(n,2n)m	6	fns_7hour	9.06E-01	1.27E-01	1.076
Ba-136(n,γ)	(5)	cf252_flux_1#	2.93E-01	2.90E-02	0.049
Ba-138(n,2n)m	6	fns_5min	6.72E-01	5.38E-02	1.200
Ba-138(n,γ)	5	cf252_flux_1#	3.80E-03	4.00E-04	0.416
		cf252_flux_1#	1.30E-03	2.60E-04	1.216
Ba-138(n,p)	(6)	fns_5min	2.67E-03	2.67E-04	1.112
La-139(n,p)	6	fns_5min	2.87E-03	1.52E-03	1.483
Ce-140(n,2n)m	6	fns_5min	6.86E-01	4.11E-02	1.099
Ce-140(n,α)m	6	fns_5min	2.67E-03	1.60E-04	1.107
Ce-142(n,p)	5	fns_5min	1.96E-03	1.84E-03	2.581
Pr-141(n,2n)	5	fns_5min	1.02E+0	8.13E-02	1.384
Nd-142(n,2n)m	5	fns_5min	4.22E-01	5.07E-02	1.333
Nd-150(n,2n)	5	fns_5min	8.15E-01	1.14E-01	1.812
Sm-144(n,2n)	(6)	fns_5min	1.04E+0	1.15E-01	1.148
Sm-144(n,2n)m	6	fns_5min	5.32E-01	6.38E-02	0.984
Sm-150(n,p)	6	fng_ScSmGd#	6.05E-03	7.26E-04	1.245
Sm-152(n,α)	6	fng_ScSmGd#	2.55E-03	3.06E-04	0.810
Sm-154(n,2n)	5	fng_ScSmGd#	1.84E+0	6.42E-02	0.939
		fns_5min	2.01E+0	5.23E-03	0.808
Eu-151(n,γ)m	5	fns_5min	1.33E-01	1.87E-02	2.609
Gd-158(n,p)	6	fng_ScSmGd#	3.17E-03	1.46E-04	1.170
Gd-158(n,α)	5	fng_ScSmGd#	1.11E-03	6.67E-05	2.000
Gd-160(n,2n)	5	fns_5min	1.20E+0	2.27E-01	1.209
		fng_ScSmGd#	1.96E+0	6.08E-02	0.779
Gd-160(n,γ)	6	fns_5min	3.81E-03	6.10E-04	1.563
Gd-160(n,p)	5	fns_5min	2.11E-03	5.27E-04	0.942
Tb-159(n,2n)m	5	fns_5min	1.91E+0	4.39E-01	0.262
Tb-159(n,p)	5	fns_5min	4.47E-02	3.71E-02	0.109
Dy-156(n,2n)	6	fng_Dy#	1.53E+0	8.09E-02	1.120
Dy-158(n,2n)	6	fng_Dy#	1.92E+0	7.28E-02	0.969
Dy-162(n,p)	5	fns_5min	2.62E-03	2.88E-04	1.482
		fng_Dy#	4.08E-03	1.92E-04	1.000
Dy-163(n,p)	6	fng_Dy#	3.33E-03	1.37E-04	0.957
Dy-164(n,γ)	(5)	fns_5min	6.93E-02	1.52E-02	2.767
Dy-164(n,γ)g	5	fng_Dy#	2.97E-02	1.34E-03	1.98
Dy-164(n,γ)m	6	fns_5min	1.41E-01	2.40E-02	0.852
Dy-164(n,p)	5	fns_5min	1.74E-03	2.26E-04	1.432
Ho-165(n,2n)	(5)	fns_5min	3.24E+0	4.53E-01	0.485

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
Ho-165(n,2n)m	5	fns_5min	1.91E+0	2.68E-01	0.485
Er-166(n,2n)	6	fns_5min	1.37E+0	1.78E-01	1.267
Er-168(n,p)	6	fns_5min	2.49E-03	2.49E-04	1.010
Tm-169(n,2n)	6	fns_5min	2.00E+0	4.99E-01	0.893
Yb-168(n,2n)	6	fns_5min	1.38E+0	5.10E-01	1.219
Yb-174(n,p)	5	fns_5min	1.99E-03	3.19E-04	1.375
Yb-176(n,n′)m	5	fns_5min	1.05E+0	1.79E-01	0.016
Lu-175(n,γ)m	6	fns_5min	5.08E-02	1.12E-02	1.203
Hf-174(n,2n)	6	fng_hafnium	1.86E+0	3.73E-01	1.000
Hf-176(n,2n)	6	fng_hafnium	1.75E+0	1.96E-01	1.024
Hf-177(n,n′)n	5	fns_5min	5.67E-03	4.53E-04	1.000
		fng_heat[#]	4.42E-03	7.07E-04	1.124
Hf-178(n,p)	(6)	fng_hafnium	3.67E-03	1.18E-03	0.781
Hf-178(n,p)m	6	fng_hafnium	5.94E-04	1.08E-04	1.039
Hf-179(n,p)	5	fng_hafnium	1.08E-02	2.51E-03	0.597
Hf-180(n,n′)m	6	fng_hafnium	1.14E-02	6.65E-04	0.984
Hf-180(n,2n)m	5	fns_5min	3.33E-01	2.67E-02	1.000
		fng_heat[#]	6.29E-01	1.01E-01	0.670
Hf-180(n,γ)	5	fng_hafnium	9.28E-03	1.51E-03	0.507
Hf-180(n,p)	5	fns_5min	6.21E-04	3.73E-05	3.778
		fng_hafnium	3.87E-03	9.36E-04	0.614
		fng_heat[#]	3.85E-03	6.16E-04	0.640
Ta-181(n,2n)g	6	fns_7hour	7.91E-01	7.91E-02	1.351
		fns_5min	1.05E+0	1.36E-01	0.952
Ta-181(n,γ)	6	fng_eurofer	1.19E+0	1.79E-01	1.118
		cf252_flux_1[#]	1.20E-01	6.50E-03	0.835
		cf252_flux_1[#]	8.92E-02	1.07E-03	1.122
Ta-181(n,p)	5	fns_7hour	4.92E-03	9.34E-04	0.663
W-180(n,2n)m	6	fzk_2	8.70E-02	2.61E-02	1.117
W-180(n,3n)	5	fzk_2	1.71E-02	2.56E-03	1.003
W-182(n,2n)	6	fns_7hour	1.56E+0	2.18E-01	1.235
		fng_tung	1.37E+0	1.75E-01	1.153
		fzk_2	5.39E-01	7.24E-02	0.750
		fng_eurofer	1.44E+0	1.66E-01	1.106
W-182(n,p)	(6)	sneg_1	6.30E-03	2.02E-03	0.928
		fng_tung	3.73E-03	6.19E-04	1.157
		sneg_1	4.44E-03	3.02E-04	1.316
		sneg_2	3.87E-03	8.12E-04	1.162
W-183(n,p)	5	sneg_1	4.42E-03	3.45E-04	1.465
		sneg_2	4.75E-03	4.51E-04	1.119
W-183(n,α)m	5	fzk_2	1.80E-05	3.60E-06	0.659
W-184(n,p)	6	fns_7hour	2.40E-03	1.68E-04	1.064
		fng_tung	2.63E-03	2.28E-04	0.911
		fng_f82h	1.98E-03	2.94E-04	1.276
		sneg_1	2.78E-03	1.80E-04	1.173
W-184(n,α)	6	fng_tung	6.27E-04	5.39E-05	1.162
		fzk_2	1.66E-04	2.49E-05	0.862
		sneg_1	7.52E-04	5.64E-05	1.290
		sneg_2	5.35E-04	9.64E-05	1.540
W-186(n,2n)	(6)	fns_7hour	1.36E+0	1.90E-01	1.235
		fzk_2	4.86E-01	6.84E-02	0.872
		fng_tung	1.34E+0	1.65E-01	0.984
W-186(n,2n)m	6	fns_5min	3.30E-01	4.29E-02	1.888
		fng_tung	5.71E-01	9.30E-02	0.943
		sneg_1	7.83E-01	5.64E-02	0.880
W-186(n,n′p)	5	fng_tung	1.74E-04	2.50E-05	1.633

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
		fzk_2	3.38E-04	1.01E-04	0.768
W-186(n,n′α)m	5	fzk_2	2.00E-06	8.00E-07	1.067
W-186(n,γ)	6	fns_5min	3.05E-02	5.49E-03	2.083
		fng_f82h	3.48E-01	2.46E-02	0.926
		fng_tung	1.29E+0	8.29E-02	1.011
		sneg_1	4.34E-03	3.90E-04	0.931
W-186(n,p)	6	fns_5min	1.24E-03	1.24E-04	1.639
		fng_tung	1.84E-03	2.75E-04	0.990
		fzk_2	5.44E-04	8.16E-05	0.858
		sneg_1	2.29E-03	3.66E-04	1.100
W-186(n,α)	6	fng_tung	5.33E-04	8.43E-05	0.895
		fzk_2	1.27E-04	1.90E-05	0.796
		sneg_1	7.18E-04	1.08E-04	0.890
Re-185(n,2n)g	5	fns_7hour	1.69E+0	8.44E-02	0.833
		fng_heat#	2.19E+0	3.28E-01	0.625
Re-185(n,2n)m	6	fns_7hour	3.74E-01	2.25E-02	0.901
Re-185(n,p)m	5	fns_5min	2.13E-03	2.56E-04	1.074
		fng_heat#	4.79E-03	7.18E-04	0.500
Re-187(n,2n)g	6	fns_7hour	1.65E+0	1.49E-01	1.129
		fns_5min	1.41E+0	1.13E-01	1.228
		fng_heat#	2.00E+0	2.59E-01	0.893
Re-187(n,γ)m	5	fng_heat#	3.64E-03	5.46E-04	0.500
Os-190(n,n′)m	5	fns_5min	8.47E-03	4.24E-04	2.272
Ir-191(n,2n)n	6	fns_5min	9.84E-02	4.92E-03	1.205
Ir-193(n,2n)m	5	fns_5min	1.48E-01	2.52E-02	1.000
Ir-193(n,α)	(5)	fns_5min	2.41E-04	2.89E-05	1.230
Pt-196(n,p)g	6	fns_5min	1.32E-03	9.26E-05	0.973
Pt-198(n,2n)m	6	fns_5min	7.87E-01	6.30E-02	1.178
Au-197(n,n′)m	5	fns_5min	1.97E-01	2.37E-02	1.639
Au-197(n,2n)m	5	fns_5min	6.67E-02	8.01E-03	1.670
Au-197(n,2n)n	5	fns_5min	9.06E-02	4.53E-03	1.437
Au-197(n,2n)	(6)	cf252_flux_1#	4.30E-03	5.00E-04	1.335
		cf252_flux_1#	5.27E-03	2.26E-04	1.090
		cf252_flux_1#	5.25E-03	3.10E-04	1.093
		cf252_flux_1#	5.80E-03	2.90E-04	0.990
		cf252_flux_1#	5.50E-03	1.40E-04	1.044
Au-197(n,γ)	6	cf252_flux_1#	1.10E-01	5.00E-03	0.673
		cf252_flux_1#	7.70E-02	7.70E-05	0.962
		cf252_flux_1#	7.80E-02	3.00E-03	0.950
Au-197(n,3n)m	5	fns_5min	9.61E-04	1.15E-04	0.327
Hg-198(n,γ)	(5)	cf252_flux_1#	1.68E-01	6.00E-03	0.143
Hg-200(n,2n)m	6	fns_5min	8.20E-01	6.56E-02	0.870
Tl-203(n,2n)	6	fns_5min	1.40E+0	1.97E-01	1.209
Tl-205(n,γ)	(6)	fns_5min	2.11E-03	1.05E-04	0.954
Tl-205(n,p)	6	fns_5min	1.50E-03	7.51E-05	1.010
Tl-205(n,α)	6	fns_5min	7.36E-04	1.03E-04	1.043
Pb-204(n,n′)m	6	fns_5min	4.83E-02	1.79E-02	1.154
		fng_heat#	5.62E-02	4.49E-03	0.940
Pb-204(n,2n)	(6)	fns_7hour	2.22E+0	1.11E-01	0.938
		fng_heat#	2.41E+0	1.69E-01	0.845
Pb-204(n,2n)m	5	fns_5min	1.74E+0	8.70E-02	0.679
Pb-206(n,p)	5	fng_heat#	1.11E-02	2.89E-03	0.143
Pb-208(n,p)	5	fns_5min	1.10E-03	5.51E-05	0.735
		fng_heat#	2.56E-03	4.61E-04	0.333
Bi-209(n,α)g	6	fns_5min	7.03E-04	8.44E-05	1.118
Bi-209(n,α)m	5	fns_5min	2.56E-06	3.33E-07	3.646

Table 4.1: Summary of reactions with integral data (*continued*)

Reaction	QS	Spectrum	σ (b)	Δσ (b)	C/E
Th-232(n,f)	6	cf252_flux_1#	8.94E-02	2.40E-03	0.839
		cf252_flux_1#	8.47E-02	4.90E-03	0.885
Pa-231(n,f)	6	cf252_flux_1#	9.70E-01	4.50E-02	0.872
U-233(n,f)	6	cf252_flux_1#	1.95E+0	3.12E-02	0.942
		cf252_flux_1#	1.89E+0	4.80E-02	0.969
U-234(n,f)	6	cf252_flux_1#	1.20E+0	1.40E-02	1.028
U-235(n,f)	6	cf252_flux_1#	1.27E+0	1.82E-02	0.962
		cf252_flux_1#	1.21E+0	2.20E-02	1.003
		cf252_flux_1#	1.22E+0	1.90E-02	1.002
		cf252_flux_1#	1.05E+0	3.10E-02	1.158
		cf252_flux_1#	1.23E+0	1.70E-02	0.987
U-236(n,f)	6	cf252_flux_1#	6.12E-01	8.00E-03	0.987
U-238(n,2n)	5	cf252_flux_1#	1.92E-01	1.90E-03	0.106
		cf252_flux_1#	1.22E-02	1.50E-03	1.670
U-238(n,f)	6	cf252_flux_1#	3.29E-01	1.00E-02	0.960
		cf252_flux_1#	3.24E-01	1.40E-02	0.975
		cf252_flux_1#	2.88E-01	7.00E-03	1.096
		cf252_flux_1#	3.08E-01	1.70E-02	1.025
		cf252_flux_1#	3.32E-01	5.00E-03	0.951
		cf252_flux_1#	3.11E-01	1.40E-02	1.016
Np-237(n,2n)m	5	cf252_flux_1#	4.66E-03	4.66E-04	0.621
Np-237(n,f)	6	cf252_flux_1#	1.26E+0	6.00E-02	1.044
		cf252_flux_1#	1.38E+0	1.00E-01	0.953
		cf252_flux_1#	1.37E+0	2.00E-02	0.963
		cf252_flux_1#	1.44E+0	2.29E-02	0.912
Pu-239(n,f)	6	cf252_flux_1#	1.80E+0	6.00E-02	1.003
		cf252_flux_1#	1.84E+0	2.40E-02	0.979
		cf252_flux_1#	1.86E+0	3.01E-02	0.971
		cf252_flux_1#	1.79E+0	4.10E-02	1.009
Pu-240(n,f)	6	cf252_flux_1#	1.34E+0	3.20E-02	1.025
		cf252_flux_1#	1.31E+0	3.00E-02	1.046
Pu-241(n,f)	6	cf252_flux_1#	1.62E+0	8.00E-02	1.004
		cf252_flux_1#	1.74E+0	5.40E-02	0.930
Am-243(n,f)	6	cf252_flux_1#	1.14E+0	2.30E-02	1.001

Table 4.1 covers 287 reactions and 171 are validated (QS=6 indicating that EAF data agree with both integral and differential data), while 25 summed reactions are validated. 77 discrepant reactions (QS=5 indicate that either the integral data do not agree with EAF data or no differential data exist) are found with 14 summed reactions that are discrepant. Reference [14] gives two plots for each reaction.

Figure 4.12 shows the integral data for $^{51}V(n,\alpha)^{48}Sc$, Figure 4.13 shows the differential data for the same reaction. Figure 4.12 shows that the individual error bars for each measurement overlap the error band representing the EAF library uncertainty; this overlap indicates agreement of the EAF data with the integral measurements. Figure 4.13 shows that the EAF data agree with the differential measurements; both agreements indicate that this is an example of a validated reaction.

Figures 4.14 and 4.15 show integral and differential data for the $^{160}Gd(n,2n)^{159}Gd$ reaction. In this case although there is good agreement with the differential data, of the two integral points only one has an overlap of the error bar with the error band. This is an example of a discrepant reaction.

Reference [14] covers 287 reactions which is a small number compared to the 12 617, and there are concerns as to how the remainder of the library can be tested. Such concerns

are magnified for the EAF-2007 library [103] which contains 65 565 reactions; a partial answer has been additional integral measurements (470 reactions are studied in the EASY-2007 validation report [104]) while the method of statistical analysis of cross-section (SACS) [105] is able to consider quantities such as maximum cross-section for all reactions of a type and can demonstrate that the data in a library are physically reasonable.

Figure 4.12: Integral data for $^{51}V(n,\alpha)^{48}Sc$, points represent the measured C/E with the associated uncertainty while the band represents the EAF library uncertainty

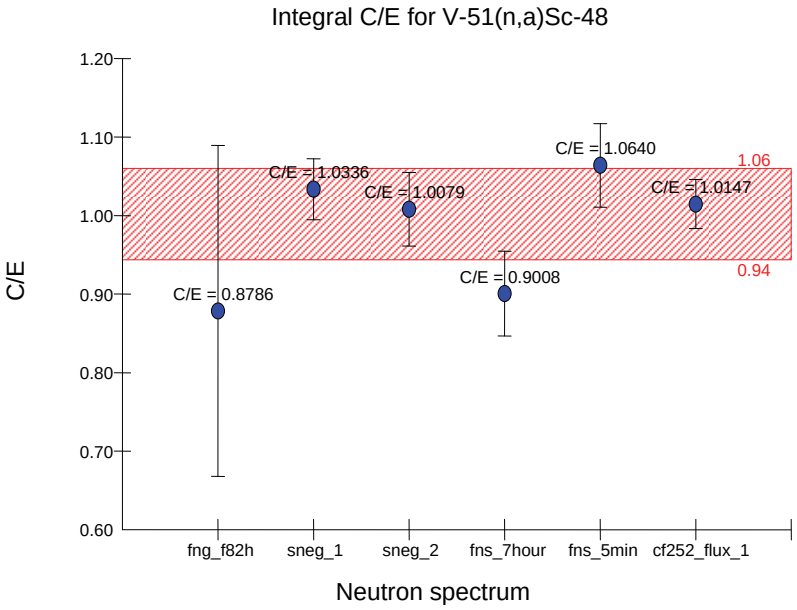


Figure 4.13: EAF-2003 values for $^{51}V(n,a)^{48}Sc$ with uncertainty shown by the dotted lines compared to experimental measurements taken from EXFOR

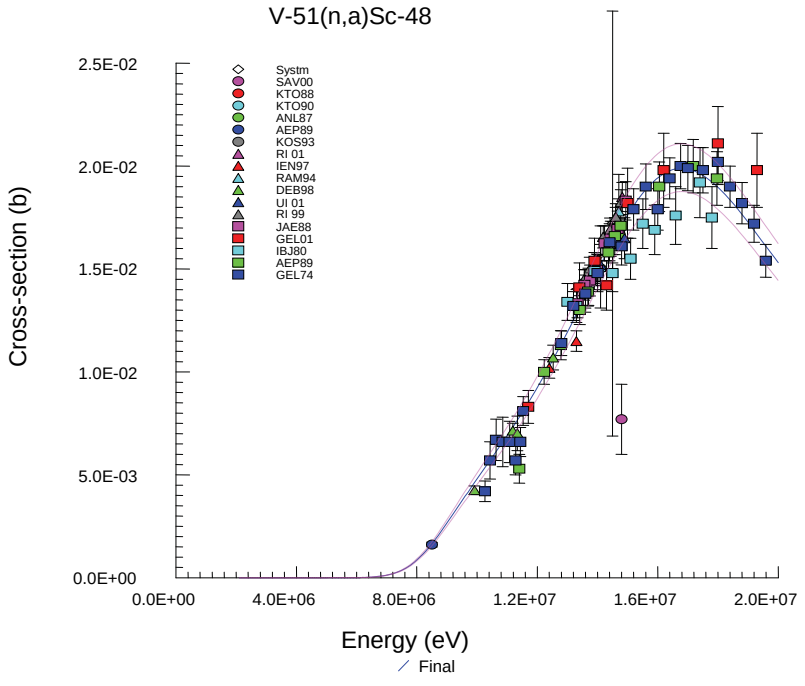


Figure 4.14: Integral data for $^{160}Gd(n,2n)^{159}Gd$, points represent the measured C/E with the associated uncertainty while the band represents the EAF library uncertainty

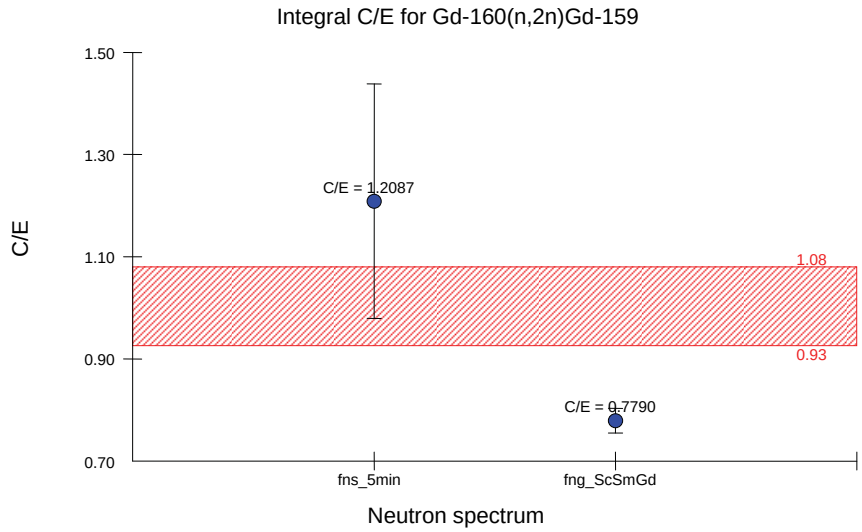
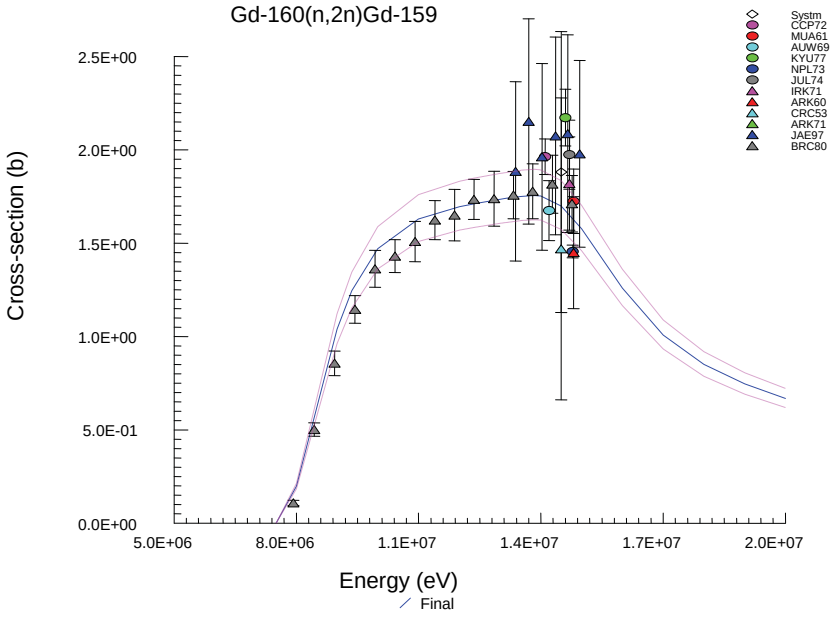


Figure 4.15: EAF-2003 values for $^{160}Gd(n,2n)^{159}Gd$ with uncertainty shown by the dotted lines compared to experimental measurements taken from EXFOR



5. Benchmarks for various applications

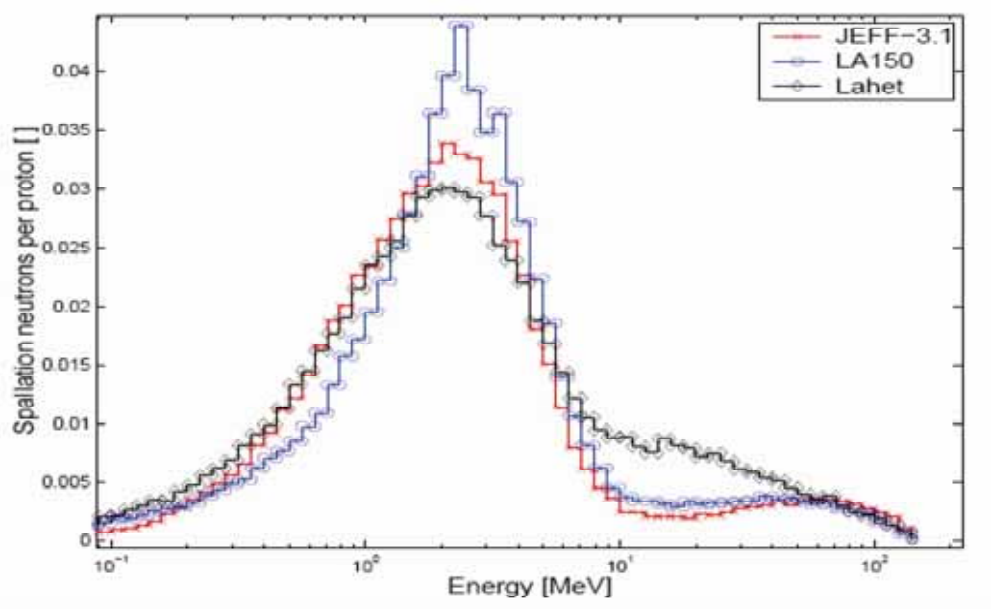
The previous chapters dealt with nuclear applications for neutron energies below 20 MeV. However, there also exist applications above 20 MeV, notably when accelerators are involved. During the development of JEFF-3.1, the accelerator-driven system (ADS) was regarded as a promising device for the solution of the waste problem. One aspect which sets ADS apart from conventional reactor systems is that the nuclear data needs extend beyond 20 MeV. Therefore, several of the JEFF-3.1 data files now contain energies up to 200 MeV. For ADS development, some validation of these higher energy data of JEFF-3.1 has taken place. We here report the results for Pb and Bi, for the target and coolant of an ADS, and Fe, for shielding.

5.1 Pb validation at intermediate energies

During the operation of an ADS, high-energy protons are directed onto a (lead/bismuth) target, in which spallation processes produce neutrons with a wide range of energies. In [106] the Monte Carlo code MCNPX25E was used to simulate a 150 MeV proton beam incident on a typical lead buffer. Figure 5.1 shows the spallation spectrum, resulting from a single interaction of a proton with a Pb nuclide. Both the proton and the neutron files of JEFF-3.1 are used in this calculation. The results are compared with those obtained with the LA150 data file [107] (= ENDF/B-VI.8) and the LAHET intranuclear cascade code. The results for both the JEFF-3.1 and the LA150 library agree reasonably well, whereas the results for the LAHET model deviate strongly especially in 10-50 MeV range. Next, the case is simulated where the spallation neutrons are transported through the lead target until they leave it. The spectrum with which the neutrons exit the target is given in Figure 5.2. Similar differences between the several libraries and models are observed as for the spallation process, but note that the spectrum calculated with the LANL library is slightly faster than the spectra obtained with both JEFF-3.1 and LAHET.

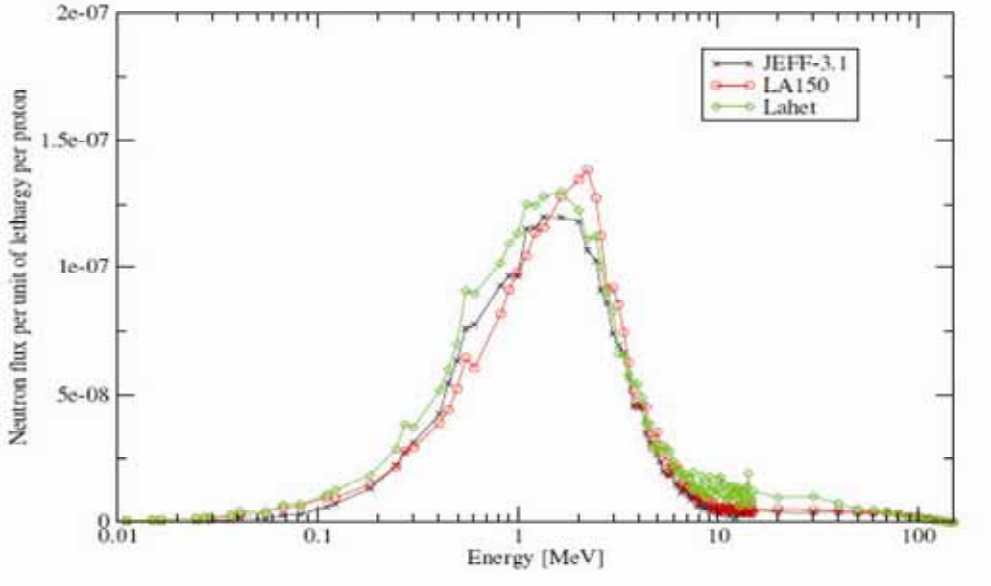
In an ADS, the source of neutrons exiting the lead target is coupled with a subcritical core in order to sustain a more or less constant neutron population. The European Fifth Framework Programme PDS-XADS [108] considered two typical lead-bismuth cooled cores: the LBE XADS design by Ansaldo [109] and the MYRRHA design by SCK-CEN [110]. Several integral parameters are calculated: the effective multiplication factor, k_{eff}, the coolant voiding coefficient and the total source multiplication, i.e. the number of fissions induced by the proton source. For both systems, there is a comparison of simulations in which these parameters are calculated using the JEFF-3.1 neutron data and the ENDF/B-VI.5 neutron data. In source-driven mode (Ms) the neutron population is sustained by an external proton source with different energies: 600 MeV for PDS-XADS and 350 MeV for MYRRHA. The void coefficient is calculated by decreasing the density of the coolant by different amounts: 10% for PDS-XADS and 5% for MYRRHA. The results shown in Table 5.1 indicate that k_{eff} is slightly decreased when using the JEFF-3.1 data, whereas the voiding coefficient is hardly affected. The several comparisons discussed above show that results using JEFF-3.1 data compare reasonably well with results from other sources. The differences are thus less significant than for the criticality benchmarks.

Figure 5.1: Spallation spectrum of a 150 MeV proton interacting with Pb, calculated with MCNPX



Comparison between new library, LA150 library and LAHET.

Figure 5.2: Neutron spectrum just outside the lead target, calculated with MCNPX



Comparison between new library, LA150 library and LAHET.

Table 5.1: Comparison of integral parameters for PDS-XADS and MYRRHA

Parameter	ENDF/B-VI.5	JEFF-3.1
PDS–XADS: k_{eff}	0.96635 (26)	0.96476 (23)
PDS–XADS: $\Delta_{void}\, k_{eff}$ [pcm/%]	-4.6 (3)	-3.2 (3)
PDS–XADS: M_S [f/s]	417	408.1
MYRRHA: k_{eff}	0.94619 (26)	0.94214 (29)
MYRRHA: $\Delta_{void}\, k_{eff}$ [pcm/%]	-155 (8)	-157 (8)
MYRRHA: M_S [f/s]	114.5	109.7

5.2 Fe validation at intermediate energies

The JEFF-3.1 Fe data files have been compared [111] with LA-150 [107] in a typical shielding benchmark by Nakashima *et al.* [112]. This provides a test for the high energy part of the JEFF-3.1 evaluation. In this experiment a 40 cm iron slab has been bombarded with a neutron beam of 68 MeV. The secondary neutron energy spectrum has been measured at the centerline and at 40 cm above this centerline. Figure 5.3 shows the experimental as well as the two calculated curves: one for JEFF-3.1 and one for LA-150. The calculations have been performed with the MCNPX code [113]. Both evaluations yield fairly similar results, which are mostly in good agreement with the measurement. Only at small outgoing energies, the JEFF-3.1 evaluation clearly underestimates neutron flux. This may very well be due to the underprediction of multi-pre-equilibrium already encountered in the (n,xp)-spectra, but most likely also present in the corresponding (n,xn)-spectra.

Figure 5.3: Secondary neutron spectrum created by a 68 MeV neutron beam on a 40 cm iron slab along the centerline and at 40 cm of the axis

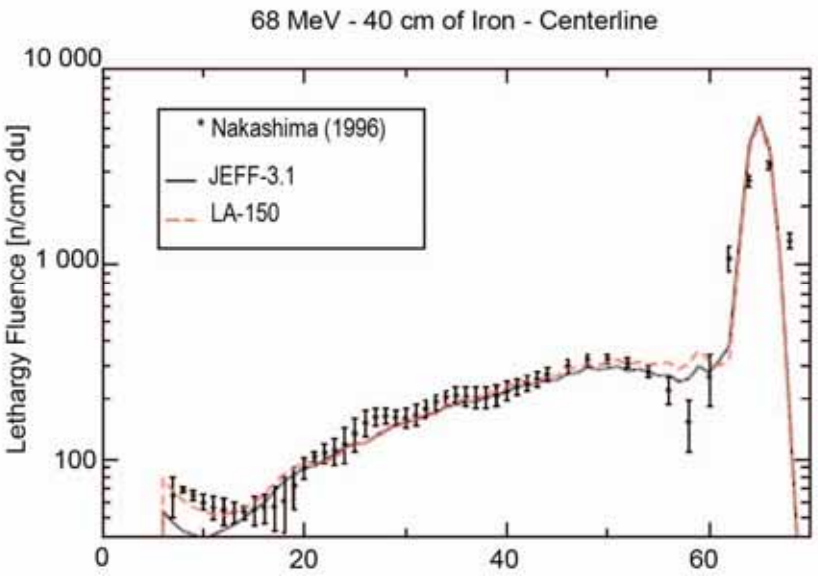
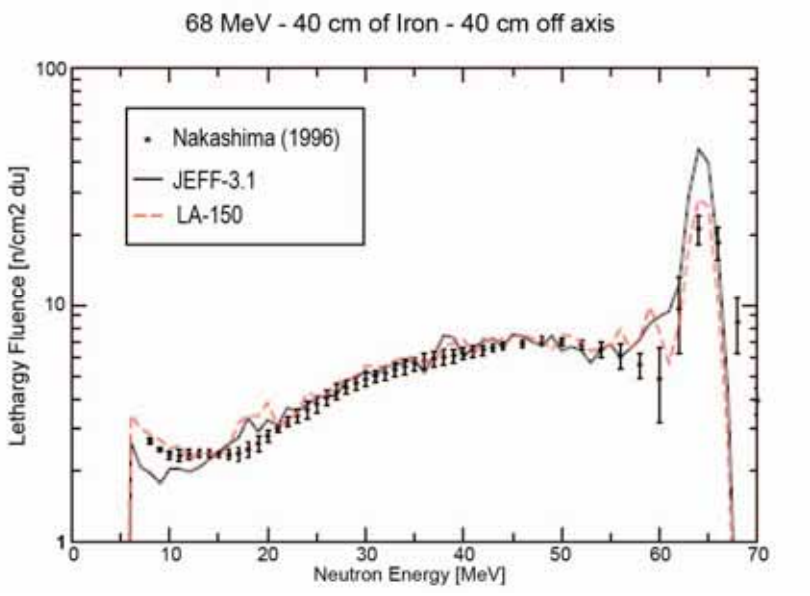


Figure 5.3: Secondary neutron spectrum created by a 68 MeV neutron beam on a 40 cm iron slab along the centerline and at 40 cm of the axis (*continued*)



Calculations have been performed with the JEFF-3.1 evaluations and with LA-150.

6. Conclusion and outlook

Over the past 20 years or so, considerable progress has been made in the nuclear data validation process. The JEFF-3.1 library has also benefited from this step forward. A key to this progress has been the continuous availability of new high-quality analytical experiments or benchmarks, typically performed in critical facilities, aimed at addressing physics effects individually. In particular, for JEFF, the most important file revisions impacting reactor applications have been motivated by the careful analysis of high-accuracy integral experiments. This is an essential point, implying that, thanks to this validation work and the corresponding feedback on the data, the performance of the JEFF-3.1 library for current reactor applications has reached a better level than what would have been achieved with differential data and nuclear models alone.

For thermal reactors, extensive, partly-automated benchmarking tests were undertaken to probe the quality of the new data library. As shown here, these studies have included Monte Carlo and deterministic criticality calculations for an unprecedented set of benchmarks. Almost all cases show improvements over the JEFF-3.0 library and, to name only one, an essential contribution to this improvement came from the international effort (WPEC Subgroup 22) to improve the ^{238}U file to correct for reactivity underestimation of LWR uranium fuelled thermal systems. For harder thermal systems the improvement is considerable with 3% high predictions reduced to less than 1%. Thermal cross-sections for many higher actinides are now within 3 standard deviations of averaged measured values; as are those for the majority of important fission products. Data for hafnium and gadolinium poisons need further attention.

The JEFF-3.1 validation of spent fuel inventory, decay heat and neutron emission calculations has been reviewed here and in JEFF Report 22, on the basis of the available benchmarks. This is based upon open publications which only include results for current thermal reactors. These results show quite good agreement for the major nuclides and decay heat, with an improvement over JEF-2.2 for PWR UOX fuel. To be useful in the development of advanced reactor systems and fuel cycles, which are predominately fast neutron systems, validation will be required on fast reactor fuels including those fuels containing high loading of minor actinides. Thus experimental activities on fast reactor fuel analyses and their benchmarking will be required to allow validation of calculations for advanced reactor fuel composition and subsequent fuel cycles and waste management.

For fusion reactors, testing of JEFF-3.1 for all materials with several existing 14 MeV shielding benchmarks (LLNL, FNS, OKTAVIAN, FNG, TUD) has been completed. In addition, a validation of the activation library against integral data has been performed by means of direct comparison with measurements of sample materials under fusion- and IFMIF relevant neutron spectra.

One important lesson learnt from the JEFF-3.1 validation study is that, in principle, if a sufficient number of well-defined, sufficiently-diverse, high-resolution and high information content experiments are available, it should be possible to produce application libraries that meet (realistic) performance targets. This suggests that (i) future integral experiments will be essential in assuring that nuclear data have the required quality for innovative fast reactor design, and that (ii) the designers' needs have to be carefully and reasonably assessed. In terms of practices, another lesson drawn from past experience is

that nuclear data evaluation and validation are most efficiently done when considered as part of an integrated approach, and involve closely-related groups of physicists.

The use of integral experiments for assessing the quality of nuclear data starts with an estimation of the impact of nuclear data uncertainty on the C/E comparisons. Depending on the value of this uncertainty, compared to the experimental uncertainty, it may be justified, under certain conditions, to use this information for attempting to improve nuclear data as part of a global statistical adjustment, for instance, as has been done with JEF-2.2 in the 1990s. This has not been repeated for JEFF-3.1. Instead, a more direct approach is being used, in which integral experiments are analysed selectively. This leads to trends in individual nuclear data, but not to adjusted nuclear data libraries. This approach has also been used for a subset of fast core experiments in order to identify the largest deficiencies of the nuclear data files. In the end, the whole process of sequential assessments and improvements has the aim of producing nuclear data libraries that meet the requests of designers of nuclear plants. With every iteration, predictions of plant characteristics will certainly improve, but might remain short of the designers' target uncertainties. It may then be necessary to use all the information available from both differential and integral experiments in a combined evaluation to try to overcome these difficulties. However, for economic and regulatory bodies, the final justification for a claim of adequate modelling accuracy of a nuclear installation will be state-of-the-art representative integral experiments.

Finally, various problems, ranging from small to significant, have been reported since the release of JEFF-3.1. Among the more important feedback for the JEFF-3.1 general purpose file is an underestimation of the thermal capture cross-section for ^{237}Np, changes of the capture and fission cross-sections up to 20 eV for ^{239}Pu, and the need to revise 7 fission product evaluations to satisfy integral fission product inventory experiments. It was decided to produce an intermediate release, JEFF-3.1.1, at the beginning of 2009 in which these and other corrections are implemented. Meanwhile, this library has been validated and has been adopted by French nuclear industry. Several experiments, such as LWR mock-up experiments, PWR and BWR chemical assays and SNF reactivity worth measurements were analysed using both TRIPOLI-4 and APOLLO-2.8 reference calculations, and the conclusion is that, for this software, JEFF-3.1 performs better than other world libraries for analyses of fuel inventory, MOX reactivity and plutonium ageing, and reactivity coefficients such as temperature coefficient and stainless steel reflectors. JEFF-3.1.1 is now used worldwide for PWR and BWR calculations, a result of the strong international effort that has been invested in the JEFF-3.1 library.

The participants to the JEFF project continuously validate, improve and complement the existing evaluated files. The next major release of the JEFF library should preserve the JEFF-3.1 performance and responds to the users' needs for both fission and fusion applications, e.g. more covariance and photon-production data, update of fission product evaluations, addition of complete proton and deuteron sub-libraries.

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