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Processing and validation of JEFF3.1 library in ACE format at 10 different temperatures

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Abstract. In July 2006 the NEA/Data Bank made available upon request the JEFF-3.1 library in ACE format (NEA-1768 ZZ-MCJEFF3.1NEA). This library contains continuous energy neutron cross section data files for use in the Monte Carlo program MCNP. The nuclides processed are all the evaluations of the General Purpose Library and Thermal Scattering JEFF-3.1 Library, including the important light nuclei, structural materials, fission products, control rod materials and burnable poisons, all major and minor actinides. This library was generated with the NJOY-99.90 nuclear data processing system plus some specific updates required for correct processing. The library has undergone strict Q&A procedures. All inputs used for processing JEFF3.1 with NJOY99.90 and the documented derived version are provided. The validations made, using benchmark experiments for criticality (ICSBEP) and shielding (SINBAD) are documented in the report.

1 Introduction

The evaluated nuclear data library JEFF-3.1 [1] was released in May 2005. The neutron General Purpose library contains incident neutron data for 381 materials from ^{1}H to ^{255}Fm (isotopes in isomeric state ^{58M}Co, ^{110M}Ag, ^{115M}Cd, ^{127M}Te, ^{129M}Te, ^{148M}Pm, ^{242M}Am, ^{244M}Am) and the Scattering Thermal library (STL) covers 9 materials.

The code system used for the processing was NJOY99 [2] and, in particular, the ACER module. For the correct processing of the JEFF3.1 library, various patches to the code NJOY99.90 are needed. The patches have been provided by several authors and are supplied together with the library and its documentation. All inputs used for processing and the documented derived version are provided in NEA-1768.

In order to cover a large number of applications, the library has been processed at a wide range of temperatures: 300, 400, 500, 600, 700, 800, 900, 1000, 1200 and 1800 Kelvin degrees (the NEA package is separated as separate entity for each temperature to facilitate handling). The library at 300 K has been verified: visually (no discontinuities, correct processing in all range) and by comparison with other libraries available for the same purposes (ENDF/B-VI.8, JEF2.2, JENDL3.3...). A Quality Assurance procedure has been also established to ensure the quality of the processed file.

Various criticality and shielding benchmarks (*International Handbook of Evaluated Criticality Safety Benchmark Experiments from the OECD-NEA project* (ICSBEP) [3], *Shielding Integral Benchmark and Database* (SINBAD) [4]) have been performed to validate the processed library. Results from the Quality Assurance procedure used are documented in a complete report distributed together with the files.

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2 Processing evaluated nuclear data to ACE format

NJOY is a modular computer code used for converting evaluated nuclear data in the ENDF format into different type of libraries useful for criticality and shielding applications. The JEFF-3.1 evaluated nuclear data file has been processed using NJOY-99.90 with some additional updates. The patch up90 was not able to process the whole JEFF-3.1 library.

The processing sequence for generating ACE-formatted library suitable for use by the MCNP [5] code is shown below in figure 1.

The library contains continuous energy neutron cross section data files for use in the Monte Carlo code MCNP. Also, Probability Tables (PT) have been generated for those materials containing unresolved resonance data. In addition, several STLs have been processed for [6]: Hydrogen bound in polyethylene, water and ZrH; Graphite, D bound in D2O, Be and Be in BeO.

3 Quality Assurance procedure

We have performed a Q&A procedure for each nuclide of the JEFF3.1 library processed.

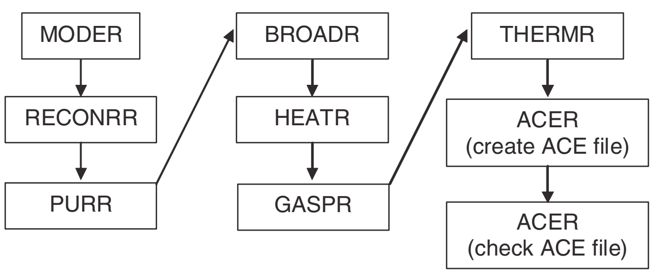

Fig. 1. NJOY processing sequence for ACE-format neutron library.

3.1 Checking NJOY output messages for each nuclide

The total number of messages from the NJOY processing were compiled. All messages were understood, most of them were related to incomplete evaluations [7]. The reason to run the ACER module twice is to evaluate the consistency of the ACE format, we checked and corrected problems that might be detected with the second run. However, ACER does not include the capability to check the proper processing of the unresolved resonance probability tables [8, 9]. The PT method was implemented in MCNP to account statistically for the average resonance parameters specified in the unresolved resonance range. In PT method, the average parameters are used to generate ladders of representative resonances. Cross sections from these ladders are then used to create cross-section probability distribution functions, from which a cross sections table (total, elastic, fission, and radiative capture) is prepared as function of probability.

Originally, evaluators decided to drop plans to include data for any isotope with a large number of negative cross sections in the PT data. The problems were traced to negative background cross sections in ENDF libraries [10]. So the negative cross section problems in the PT are related with the evaluation and it is not a problem with the PURR module of NJOY (the method of calculating the probability table as implemented in NJOY should not lead negative values by itself [11]).

To summarize, there are a number of possible problems or abnormalities with the PTs that can be directly noticed for some isotopes. Three different situations with three approaches were investigated: i) Probability bins with a probability of 0, these bins will not be sampled so *it can be accepted*; ii) zero cross section values (either for the entire bin or for specific reactions), can occur either in the lower bins because the cross section becomes very small or when the particular row has a fractional probability of zero (in this case, the row will never be sampled) so *zero cross section can be allowed*; and iii) negative cross section values that *cannot be allowed* (and the library file has to be recalculated without probability tables), unless they appear in a row with zero fractional probability (in which case the PTs will not be used).

The procedure in this work has been to simply omit the PT from ACE file whenever negative values are found. The list of isotopes that had negative PT values is listed as follows: ^{22}Na, ^{36}Ar, ^{101}Ru, ^{104,106,107,108,110}Pd, ^{109}Ag, ^{139}La, ^{141}Pr, ^{147}Pm, ^{144,145,146,148}Nd, ^{238}Np, ^{252}Cf, ^{253}Es.

3.2 Q&A with ACELST code

Here, we have maintained that "*the human eye will be used as a wonderfully complex tool, able to spot inconsistency and error with amazing precision*" [11]: looking for unexpected discontinuities in cross sections, examine secondary distributions, threshold regions and resonance regions.

We have applied the Q&A procedure developed in ref. [12]. For checking the contents of all the ACE-formatted files, we have converted back to ENDF6 format using the code ACELST [13]. These ENDF6 files were compared with the original evaluation using both NJOY and PREPRO-2004 code [14] system (LINEAR + RECENT + SIGMA1). Warnings and messages from PREPRO-2004 codes are useful to complete an additional check.

We can conclude that the processed data were judged to be acceptable. However, some differences between NJOY and PREPRO-2004 should be investigated: Tl-nat capture cross section (inconsistency found at low neutron thermal energy due to the type of interpolation law used at low energy), the total cross sections (NJOY calculates the total cross section summing the partial cross sections and PREPRO-2004 processes directly the total cross section) and different resonance treatment. Also inconsistency data for ^{58}Co resonance capture cross section was found in JEFF-3.1.

4 NJOY updates to process ACE library

Several *Research Centres* have developed specific NJOY99.90 updates to be used in nuclear data processing. An intensive work has been performed to compile the most recent NJOY updates to process the JEFF-3.1 library.

Firstly, the following patches were compiled for the correct processing of the full file: D. Leichtle, I. Schmuck (FZK) to correctly process ^{9}Be(n,2n), D.L. Aldama (NDS/IAEA) patch included in the IAEA/ADS-lib/V1.0, A. Hogenbirk (NRG) for ACER-processing of delayed neutron data after the extension in JEFF3.1 to 8 groups, M. Mattes (IKE) for thermal scattering cross sections. Other updates have been provided by O. Cabellos (NEA Data Bank), M. Pescarini (ENEA), Kazuaki Kosako (Shimizu Corporation), J.C. Sublet (CEA), A. Trkov (IAEA) IAEA-FENDL and WLUP. We have collected these updates, and we have obtained a unique update to be used in this work. To reach this objective an extensive work has been performed: checking consistency between different updates and correcting small mistakes.

Finally, a comparison with the most recent NJOY updates [15] shown that most of the previous updates were included except for the delayed neutron, the ^{9}Be(n,2n) reaction and some specific updates for JEFF-3.1.

5 Validation

5.1 Criticality validation

An extensive criticality validation suite could be used by the *International Handbook of Evaluated Criticality Safety Benchmark Experiments from the OECD-NEA project* (ICSBEP) [3]. Two suites of calculations to assess the reactivity impact of changes to associated nuclear data libraries taken from ICSBEP were performed: i) a validation suite proposed in ref. [16], ii) and an additional validation, also included in ICSBEP for: Np237, heavy-Water solutions, very thermal Pu solution, unmoderated ZEUS benchmark. Other references have been used to compare these calculations [9, 17]. Table 1 summarizes the cases in the criticality validation suite.

Table 1. MCNP criticality validation suite.

		Description	Benchmark	ENDF/B-VII R.D.Mosteller [16]	NEA JEFF-3.1
PU	Fast	Jezebel	1.00000 (200)	0.99980 (30)	1.00038 (26)
		Jezebel-240	1.00000 (200)	1.00030 (30)	1.00337 (27)
		Pu Buttons	1.00000 (300)	0.99840 (30)	0.99698 (30)
		Flattop-Pu	1.00000 (300)	1.00040 (30)	1.00277 (31)
		THOR	1.00000 (60)	1.00790 (30)	1.00271 (27)
		Pu-MF-11	1.00000 (100)	0.99920 (40)	0.99722 (34)
	Interm	HISS/HPG	1.00000 (1100)	1.01060 (20)	1.00654 (42)
	Thermal	PNL-33	1.00240 (210)	1.00630 (30)	-
		PNL-2	1.00000 (650)	1.00290 (50)	1.00504 (43)
		PU-SOL-THERM-009	1.00030 (330)	1.01910 (20)	1.01515 (49)
U233	Fast	Jezebel-233	1.00000 (100)	0.99970 (30)	1.00379 (24)
		Flattop-23	1.00000 (140)	0.99940 (30)	1.00612 (30)
		U233-MF-05_case2	1.00000 (300)	0.99790 (30)	1.00010 (30)
	Interm	Falstaff_case1	1.00000 (830)	0.99050 (50)	0.98416 (48)
	Therm	SB_2.5	1.00000 (240)	0.99880 (40)	0.99700 (44)
		ORNL-11	1.00060 (290)	1.00410 (20)	0.99723 (17)
HEU	Fast	Godiva	1.00000 (100)	0.99940 (30)	0.99696 (27)
		Tinkertoy-2	1.00000 (380)	1.00040 (30)	-
		Flattop-25	1.00000 (300)	1.00290 (30)	1.00220 (28)
		Godiver	0.99850 (110)	0.99780 (40)	0.99444 (32)
		HEU-MET-FAST-73	1.00120 (150)	1.00800 (30)	1.00849 (26)
	Intermediate	Zeus-2	1.00010 (80)	0.99580 (40)	0.99490 (35)
		UH3	1.00000 (470)	0.99520 (40)	-
	Thermal	SB-5	1.00150 (280)	0.99570 (50)	0.99797 (50)
		ORNL-10	1.00150 (260)	0.99890 (20)	0.99874 (17)
		HEU-SOL-THERM4_c1	1.00000 (330)	0.98390 (40)	0.98438 (38)
IEU	Fast	IEU-MF-03	1.00000 (170)	1.00270 (30)	0.99897 (27)
		BIG-TEN	0.99480 (130)	0.99520 (20)	0.99774 (23)
		IEU-MF-04	1.00000 (300)	1.00720 (30)	1.00379 (28)
	Intermediate	Zebra-8H	1.03000 (250)	1.01980 (20)	1.01579 (23)
	Thermal	IEU-CT-02_c3	1.00170 (440)	1.00080 (30)	1.00081 (33)
		STACY-36	0.99880 (130)	0.99940 (30)	0.99860 (20)
LEU	Thermal	BaW XI_2	1.00070 (120)	1.00000 (30)	0.99984 (30)
		LEU-ST-02_c2	1.00240 (370)	0.99610 (30)	0.99630 (28)
SPEC	Thermal	*SPEC-MET-FAST-08*	1.00190 (360)	0.99240 (30)	0.99177 (24)

* Cases with differences more than 2*σ are marked in red.

The MCNP calculations were run with 5.000.000 active neutron histories for all but two cases in the suite (550 generations with 10.000 neutrons per generation, excluding the first 50 generations from the statistics). Only 3.000.000 active histories were used for those cases, SB-5 and Zebra-8H, because they require substantially more computer time per history than the other cases (350 generations). Nonetheless, the standard deviation for k_{eff} from those cases is comparable to those for other cases in the suite. This number of histories is sufficient to render the statistical uncertainty from the MCNP calculations essentially negligible relative to the benchmark uncertainty for most of the cases in the suite. This suite can provide a general indication of the overall performance of a nuclear data library, and is not an absolute indicator of the accuracy or reliability of a given nuclear data library.

In conclusion, we identify: i) deficiencies in fast cases (Pu, U233, HEU and IEU) and intermediate cases (HEU and IEU), ii) cross sections for Pu239 should be re-examined in the deep thermal range (PU-SOL-THERM-009), iii) fast cross sections for Cu should be reviewed (HEU-MET-FAST-73), iv) fast cross sections for Np-237 should be reviewed (SPEC-MET-FAST-08). Improvements for IEU-MF-03 (bare) and IEU-MF-04 (light reflector) and good approximation for LEU are shown.

5.2 Radiation-Shielding validation suite

A shielding validation suite taken from SINBAD Database [4] was used. Other references have been used to compare these calculations [9, 18]:

i) Ispra Iron Benchmark Experiment (study of the neutron deep penetration in homogeneous materials commonly used in the construction of advanced reactors), ii) KANT Spherical Shell Transmission Experiment on Beryllium, see figure 2 (to clarify the discrepancies in the effective neutron multiplication

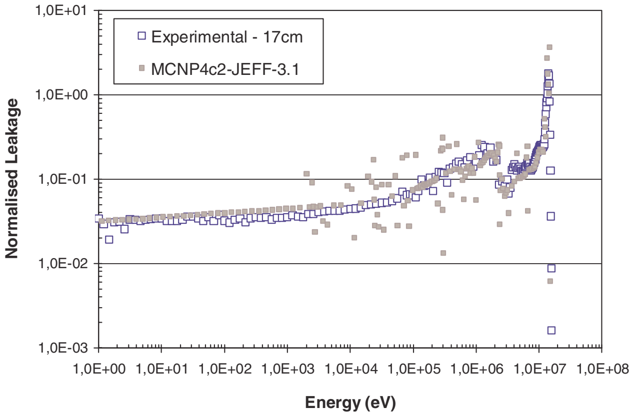

Fig. 2. KANT Experiment. Normalized leakage neutron fluency from 17 cm Be shell (an updated input has been included in SINBAD Database [4] in March 2006).

of bulk beryllium assemblies with central 14 MeV neutron sources), iii) NIST (a Cf source was placed at the centre of the experiment, and fission foils were placed at two, diametrically opposed positions, between the source and the fission foils were several combinations of shielding materials, iv) IPPE (neutron transmission benchmark experiment with 14 MeV neutrons through iron shells), v) FNS (neutron spectrum emerging from slabs of material of varying thickness from a 14 MeV D-T neutron source), vi) Oktavian (leakage current spectrum from the outer surface of a spherical pile of material is measured, at the centre of the pile a 14 MeV D-T neutron source was located.), vii) LLNL-pulsed sphere (time-of-flight measurements were performed for neutrons passing through spherical shells of varying thickness, containing different materials, the source was a 14 MeV D-T neutron source).

6 Conclusion

The JEFF3.1 library has been processed at 10 different temperatures for a wide range of MCNP applications. Quality Assurance procedures have been applied to guaranty the quality of the JEFF3.1 processed file. The processed data were judged to be acceptable according to an extensive Q&A procedure: i) checking ACE files, ii) compiling warnings and messages from NJOY and PREPRO-2004, iii) using criticality and radiation-shielding benchmarks providing a general indication of the overall performance of JEFF-3.1 nuclear data library.

Recommendations for future versions of the JEFF library have also been summarised thanks to the extensive validation carried out.

The library and the documentation associated are distributed at the NEA (request available at the NEA Data Bank website, http://www.nea.fr/abs/html/nea-1768.html). Work performed by O. Cabellos under contract with the NEA Data Bank.

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