THE JEFF-3.0 NUCLEAR DATA LIBRARY

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ABSTRACT

The JEFF-3 nuclear data file project is briefly presented. The JEFF-3.0 General Purpose library, which was released in April 2002, is described in some detail. This library contains neutron cross section evaluated files for 340 nuclides in standard ENDF-6 format. It is intended to be used for various neutron transport applications in the 0 to 20 MeV energy range. The main differences with respect to JEF-2.2, the previous library produced by the JEF project, are outlined. The improvements to be expected from this new JEFF-3.0 library are discussed. Finally, information regarding the preparation and future release of the JEFF-3 Special Purpose files is provided.

1. INTRODUCTION

The Joint Evaluated File (JEF) project was initiated in the early eighties by member countries of the OECD Nuclear Energy Agency (NEA) Data Bank. The aim of this project was to produce the best possible evaluated nuclear data files to meet the needs of fission reactor technology applications. The latest revision of the JEF files is the JEF-2.2 library [1] which was released in 1992.

In the mid-nineties, the decision was taken to start work on a new library, called JEFF-3 [2], representing a major upgrade with respect to JEF-2.2. The goal of this new library was not only to achieve improved performance for existing nuclear reactors but also to produce a more extensive set of files applicable to a wide range of applications, including future nuclear power plants, advanced fuel cycles, nuclear waste transmutation systems, etc. The European Fusion File (EFF) project and the associated European Activation File (EAF) project, sponsored by the European Community Fusion Technology Programme, agreed to contribute to this new initiative which was therefore named the Joint Evaluated Fission and Fusion (JEFF) file project.

The JEFF Scientific Co-ordination Group (SCG), whose members are nominated by the Nuclear Science Committee Executive Group, has responsibility for the overall management of the project. As for the past JEF libraries, the Secretariat is the NEA Data Bank which provides general information and maintains a list of actions relative to the JEFF project. The NEA Data Bank also provides support

for assembling, QA testing, maintaining, and distributing the libraries and the associated documentation, as well as for collecting user feedback and requests.

This paper provides a description of the JEFF-3.0 General Purpose library [3] which was officially released on April 26, 2002 (Section 2 and 3). The expected improvements over JEF-2.2 are indicated (Section 4). The status of the JEFF-3.0 Special Purpose files is also discussed (Section 5).

2. FROM JEF-2.2 TO JEFF-3.0

Over the past ten years or so, the latest versions of the JEF-2 and EFF-2 files have been extensively tested, benchmarked and used for a wide range of applications including thermal reactors, fast reactors, criticality and shielding calculations. A number of JEF-2.2-based libraries are currently used by the nuclear industry as inputs to large production code systems.

Considerable evidence has been accumulated from this extensive use, demonstrating that the overall quality of the files was reasonably good [1]. However, it has also been found that cross section improvements were desirable for many materials: U-235 (epithermal capture), plutonium isotopes, in particular Pu-240, Th-232, sodium, lead, structural materials, Li-7 and Be-9, neutron absorbers such as Er and Hf isotopes, and for several important fission products [4,5]. In addition, it has long been recognized that JEF-2.2 fission yield and radioactive decay data are in need of a major revision.

The objective of the JEFF-3 file project is to address these needs.

The development of the JEFF-3.0 library has followed a stepwise approach as resources available for carrying out the work were (and still are) very limited. The General Purpose section, made of cross sections for neutron transport applications below 20 MeV, has been developed first. This file will be progressively complemented by other Special Purpose "annex" files.

The JEFF-3.0 evaluations are the results of a careful review and selection process, which started in 1996 [6] and took into account the results of the JEF-2.2 extensive benchmarking, as well as the results of checks and tests on preliminary JEFF-3T test versions of the file. Some of the JEFF-3T evaluations were adopted, either totally or in part, from the EFF, JENDL3.2, ENDF/B-VI, BROND-2.2 and CENDL-2 files [7], as all these files have adopted the same ENDF-6 format. However, as a general rule, it was decided to give preference to the available JEF or EFF data whenever no other data could be proven to be of better quality.

The JEFF-3.0 library is subdivided into different sections:

(1) General Purpose files, from 0 to 20 MeV, except for Al-27 and Pu-239 for which the upper energy is 150 MeV and 30 MeV, respectively.

(2) Special Purpose thermal scattering data. These consist simply of five thermal scattering data sets, carried over from JEF-2.2, corresponding to H_2O, D_2O, graphite, beryllium and polyethylene in $S(\alpha, \beta)$ form.

(3) Special Purpose activation files.

(4) Special Purpose fission yield data.

(5) Special Purpose radioactive decay data.

A detailed presentation of the General Purpose files is provided in the next section. For convenience, the isotopes have been grouped in six "classical" categories: light materials, structural materials, fission products, heavy materials, major actinides and minor actinides.

3. JEFF-3.0 GENERAL PURPOSE FILES

The JEFF-3.0 General Purpose library is made of 340 evaluated files (as opposed to 312 for JEF-2.2). Out of these 340 files, approximately half are files carried over from JEF-2.2, mostly fission products.

3.1 LIGHT MATERIALS

This group includes all isotopes or elements up to $Z = 21$ (vanadium).

There are 34 such light isotopes or elements in JEFF-3.0, as in JEF-2.2. However, in the new JEFF-3.0 file, most JEF-2.2 files have been replaced by improved evaluations adopted from other, more recent libraries. The only exceptions are O-16, O-17, Na-22, Na-23, Cl-nat and the Ar isotopes which are kept from JEF-2.2.

Beryllium is taken from the recent (2000) EFF-3.0 evaluation, a completely new file.

Hydrogen, Li-6 and B-10 are all from ENDF/B-VI.3 (consistent with ENDF/VI standards), and so are deuterium, B-11, C-nat, and nitrogen.

Na-23 in JEFF-3.0 is actually a modified version of JEF-2.2 in which S. Kopecky's 1997 accurate re-evaluation above the inelastic scattering threshold (450 keV) was introduced, up to 2 MeV. Above 2 MeV and in order to match Kopecky's data at 2 MeV, the JEF-2.2 inelastic scattering cross section was lowered by 30% while the elastic cross section was increased by 30%.

Al-27 is a very recent evaluation kindly made available to the JEFF-3 project by ORNL. It contains new resolved resonance parameters over an extended energy range (0 to 850 keV). This evaluation is based on high-resolution transmission and capture measurements by Guber (1999) and Rohr (1994) at ORELA.

In the case of silicon, the JEF-2.2 Si-nat evaluation was replaced by isotopic data for Si-28, Si-29, and Si-30. Conversely, natural sulphur from JENDL-3.2 was selected to replace S-32, S-33, S-34 and S-36 from JEF-2.2.

Sc-45 was not present in JEF-2.2. The ENDF/B-VI.3 file was adopted for JEFF-3.0.

As in JEF-2.2, there is no evaluation for neon ($Z = 10$).

3.2 STRUCTURAL MATERIALS

This group is made of the following elements: Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Zr, Nb, Mo.

The JEFF-3.0 General Purpose library contains 38 nuclides belonging to this group. New evaluations have been produced for the most important ones: Cr-52, Fe-56, Ni-58 and Ni-60, while ENDF-B/VI.3 or JENDL-3.2 evaluations have been adopted for most of the others.

Cr-52 in JEFF-3.0 is a considerably improved evaluation with respect to JEF-2.2. It includes contributions by S. Tagesen, H. Vonach, A. Trkov, and O. Bouland. The latter produced Reich-Moore resonance parameters for computing the total, elastic and capture cross sections from 0 to 1.2-MeV [8]. The other chromium isotopes are from ENDF/B-VI.3.

Fe-56 is the EFF-3.1 file produced in 2001 by the EFF Project. This evaluation is the product of a European collaboration involving F. Fröhner, V. Pronyaev, S. Tagesen, A. Köning, A. Trkov and others. It contains resolved resonance parameters re-evaluated by Fröhner from 0 to 850 keV, the energy of the first inelastic threshold. The total cross section between 850 keV and 10 MeV was revised on the basis of measurements performed at IRMM Geel. The inelastic scattering cross section was also revised. The other JEFF-3.0 iron isotopes are from JEF-2.2 (Fe-57 and Fe-58) and from ENDF/B-VI.3 (Fe-54).

EFF evaluations for Ni-58 (EFF-2.4) and Ni-60 (EFF-3.0) were adopted in JEFF-3.0. The EFF-3.0 evaluation for Ni-60 was distributed in 2000. It is based on ENDF/B-VI.1 and contains updated data above 450 keV. Ni-59 is from JEF-2.2, while the other nickel isotopes are from ENDF/B-VI.3.

The isotopes of manganese, zirconium and molybdenum are from JENDL-3.2, except Zr-93, Zr-95 and Mo-99, which are from JEF-2.2.

The JEF-2.2 Cu-nat file is replaced by Cu-63 and Cu-65 files from ENDF/B-VI.

Zn-nat from BROND-2.2 replaces Zn-64, the only zinc isotope present in JEF-2.2.

3.3 FISSION PRODUCTS

This category includes all nuclides having atomic numbers ranging from $Z = 32$ to 39 and from $Z = 43$ to 65. Note that the Zr ($Z = 40$), Nb ($Z = 41$), and Mo ($Z = 42$) isotopes are not part of this group but are in the structural materials group.

The JEFF-3.0 library contains a total of 175 such fission products. Most of them are evaluations carried over from JEF-2.2, with a few additions: Ge-70 (JENDL-3.2), Se-79 (JENDL-3.2), Ba-130 (EFF-2.4), plus four stable isotopes which were not present in JEF-2.2: Cd-108 (ENDF/B-VI.4), Ba-132, La-138 and Gd-152 (all JENDL-3.2). Note that a few stable isotopes, already missing in JEF-2.2, are still missing in JEFF-3.0: Pd-109, Ce-136, Ce-138.

Several fission products important for light water reactor applications were revised to reflect some of the trends derived from the JEF-2.2 benchmarking [4, 5]:

- Cs-133: the recent ENDF/B-VI.7 evaluation containing new resonance parameters was adopted;

- Nd-143: the JEF-2.2 evaluation was modified. The neutron width of the bound level was increased by 4%;

- Sm-149: the ENDF/B-VI.4 evaluation was adopted, but with the neutron width of the first resonance (0.097 eV) increased by 3%;

- Eu-154 and Eu-155: both were taken from ENDF/B-VI.7, which contains revised resonance parameters and thermal cross sections.

The main other changes with respect to JEF-2.2 are for Tc-99 (JENDL-3.2), Cd (ENDF/B-VI.4), In (JENDL-3.2), Sn (EFF-2.4) and Ba (JENDL-3.2).

3.4 HEAVY MATERIALS

Heavy materials are characterized by $Z = 66$ to 83.

There are 39 such materials in JEFF-3.0. The main changes with respect to JEF-2.2 are:

- Erbium isotopes from BROND-2.2, including Er-162, Er-164, Er-168 and Er-170 which were not present in JEF-2.2;

- Hafnium isotopes from JENDL-3.2;

- Tungsten isotopes from JENDL-3.2;

- Gold from ENDF/B-VI.4;

- Pb-nat replaced by lead isotopes from JENDL-3.2;

- Bismuth taken from ENDF/B-VI.4.

In addition, evaluated files for Os-nat, Ir-nat, Pt-nat, Hg-nat, Tl-nat, none of which were available in JEF-2.2, have been included in JEFF-3.0.

3.5 MAJOR ACTINIDES

The major actinides are those actinides which can be present in sufficiently large quantities to influence the neutron spectrum. They are: Th-232, U-233, U-235, U-236, U-238, Np-237, Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, Am-241, Am-243. Good scattering cross sections, as well as resolved and unresolved resonance data, are needed for these 13 nuclides.

JEFF-3.0 contains new evaluations for all these major actinides, except Am-241 and Am-243 which are JEF-2.2 files with fission energies from ENDF/B-VI.

The Th-232 evaluation, which had not been updated since JEF-1 (= ENDF/B-IV), has been replaced by the JENDL-3.2 file. The (MLBW) resolved resonance range goes from 0 to 3.5 keV, while the unresolved range extends from 3.5 to 50 keV.

JENDL-3.2 was also chosen for U-233. This evaluation contains (Reich-Moore) resonance parameters calculated by H. Derrien. The resolved resonance range extends from 1 eV to 150 eV and the unresolved range from 0.15 to 30 keV.

The U-235 evaluation adopted in JEFF-3 is that of Leal-Derrien-Larson-Wright [9] in which the resolved resonance range (0 to 2.25 keV) has been entirely revised, resulting in a larger capture resonance integral, consistently with the JEF-2.2 benchmarking conclusions.

JENDL-3.2 was chosen for U-236.

The U-238 evaluation was slightly modified at high energies in the following way. Starting from the JEF-2.2 file, the JENDL-3.2 inelastic cross section, energy and angular distributions were inserted. In addition, the ENDF/B-VI.7 (n,2n) and (n,3n) cross sections were also introduced. The elastic cross section was then recalculated at high energies so as to preserve the JEF-2.2 total cross section. The resonance and low energy ranges were left unchanged.

The Np-237 evaluation was taken from ENDF/B-VI.4, with the (n,2n) and (n,3n) cross sections from JEF-2.2.

The Pu-238 evaluated file in JEFF-3.0 is based on JENDL-3.2 with the addition of unresolved resonance parameters from BROND-2.2.

The JEFF-3.0 Pu-239 evaluation differs significantly from JEF-2.2. The resolved resonance region extends up to 2.5 keV (instead of 1 keV in JEF-2.2), and the unresolved range up to 30 keV. The resonance parameters are those of H. Derrien and T. Nakagawa. The evaluation above 30 keV and up to 30 MeV is from CEA Bruyères-le-Châtel. It is the result of a detailed theoretical analysis based on the available experimental data and microscopic level densities. The analysis involved coupled channel optical model calculations followed by Hauser-Feshbach statistical/preequilibrium calculations [10].

The JEFF-3.0 Pu-239 file contains new values for the prompt, delayed and total neutron yields. Moreover, following O. Serot's suggestion [11], the components of the energy released by Pu-239 and Pu-238 fission (MT = 458) have been updated and the fission *Q*-values revised accordingly.

The JEFF-3.0 Pu-240 and Pu-241 evaluations were constructed from the corresponding JENDL-3.2 files.

For Pu-240, the following resonance parameters were incorporated:

- H. Derrien and O. Bouland [12], in the 0 to 5.7 keV resolved range,
- O. Bouland [13] in the 5.7 to 40 keV unresolved resonance range.

For Pu-241, the use of the revised resonance parameters recently produced by H. Derrien [14] up to 20 eV results in an increase of the 0.3 eV resonance capture cross section, which is consistent with integral experiments. These parameters were therefore included in the JEFF-3.0 file.

The JEFF-3.0 Pu-242 evaluation is the JENDL-3.2 file with modifications by A. Ventura. The resolved resonance range (MLBW) extends up to 1.15 keV and the unresolved range up to 40 keV.

3.6 MINOR ACTINIDES

There is a total of 41 minor actinides in the JEF-3.0 General Purpose library. Twenty-nine of those were already present in JEF-2.2. The additional evaluations are for Th-227, Th-228, Th-229, Th-233,

Th-234, Np-236, Am-244, Am-244m, Cm-249, Cm-250, Bk-250, Cf-254, Es-254, Es-255. All of them are from JENDL-3.2.

The main changes concern the curium isotopes, the other files being carried over from JEF-2.2 with minor or no modifications. JENDL-3.2 evaluations were adopted for Cm-242, Cm-243, Cm-245, Cm-247 and Cm-248. For Cm-242 and Cm-243, however, the JEF-2.2 data were kept above the unresolved resonance range (40 keV). Cm-246 is a recent evaluation by V. Maslov.

The ENDF/B-VI.2 evaluation was chosen for Am-242. Indeed, measurements performed at ILL Grenoble have shown that the JEF-2.2 thermal capture and fission cross sections for this nuclide were largely overestimated.

As in the case of Pu-238 and Pu-239, the components of the energy released by fission (MT = 458) have been updated for the following actinides, with the fission *Q*-values revised accordingly: Th-230, Pa-233, Pu-236, Pu-237, Am-242m, Cm-241, Cm-242, Cm-243, Cm-244 [11].

4. JEFF-3.0 CONSISTENCY CHECKS AND EXPECTED PERFORMANCE

Before its release, the JEFF-3.0 General Purpose file underwent thorough testing by the NEA Data Bank according to recently-developed Quality Assurance procedures which included running the BNL format and physics checking codes (CHECKR, FIZCON, PSYCHE) on every evaluated data set. As part of the tests, the file was also processed with NJOY 97.107, 97.108 and 99.05. These tests helped identify and correct a few inconsistencies which had not been detected by the QA checks. In addition, checks were also performed by comparisons with JEF-2.2 using the JANIS [15] portable software which was developed for convenient tabular and graphical viewing of ENDF-6 formatted files.

Following these tests and prior to the JEFF-3.0 official release, it was decided to perform a limited validation of the JEFF-3.0 file by recalculating a subset of the JEF-2.2 benchmarks. This limited benchmarking, which started in early 2000 with the JEFF-3T test files, confirmed the expected improvements over JEF-2.2 [4, 16]. In particular, the following problems associated with the JEF-2.2 file appear to have been either totally or partially eliminated:

- Strong underestimation of U-236 build-up in irradiated MOX fuels;
- Reactivity over-prediction in U-235 highly-enriched thermal systems;
- Underestimation of Np-237, Pu-238 and Pu-242 build-up in UOX fuels;
- Reactivity overestimation in U-235-fuelled fast systems;
- JEZEBEL Pu metallic benchmark reactivity underestimation;
- Biases in the calculated Cs-133, Nd-143, Sm-149, Eu-155 fission product inventory;
- Calculations in disagreement with transmission measurements in blocks of iron.

However, in spite of these remarkable improvements, there were also indications that the JEFF-3.0 General Purpose library still suffers from some shortcomings:

- Slight reactivity underestimation (- 400 *pcm*) of low-enrichment uranium-fuelled PWR lattices. The reasons for this underestimation could not be immediately found. A working group has therefore been set up in the framework of the OECD/NSC Working Party on International Nuclear Data Evaluation (WPEC [7]) to tackle this problem;

- Slight overestimation of Pu-239 build-up in MOX fuels;

- Underestimation of U-233 capture in fast systems;

- Too low O-16 (n,γ) and (n,α) cross sections above 1 MeV.

In view of these shortcomings, the JEFF Scientific Co-ordination Group is considering a revision of the JEFF-3.0 General Purpose file in late 2003. This revision should contain, in addition to the necessary revisions for improving LWR reactivity calculations, covariance information for the main nuclides as well as more complete gamma-production data.

5. JEFF-3.0 SPECIAL PURPOSE FILES

The initial JEFF-3 Activation File will be made from the latest version (either EAF-2001 or EAF-2003) of the comprehensive activation file EAF produced and continuously improved by the EFF Project. Some format issues have been resolved recently. The official release of JEFF-3.0/A in ENDF-6 format is scheduled for December 2002.

The JEFF-3 Decay Data starter file assembled by the NEA Data Bank in 2001 from the UKPADD-6.1 and UKHEDD-2.2 evaluations, with complements taken from NUBASE and ENSDF data converted into ENDF-6 format, is currently under test. This file contains 3554 radioactive nuclides and 228 stable nuclides. There are new evaluations for a number of isotopes which were either missing from JEF-2.2 or in need of revision. However, considerable work is still needed on this file, both in terms of evaluation and validation, which is the reason why the official release of JEFF-3.0/DD is not scheduled before late 2003.

An updated Fission Yield starter file consistent with this JEFF-3 Decay Data starter file has been recently produced from the UKFY3 evaluations. As with the Decay Data file, work is still required on the Fission Yield file before it can be deemed ready for release.

Following discussions within the JEFF Project, the release of the JEFF-3.0 Intermediate Energy data is no longer envisaged as a separate Special Purpose file, but instead as an extension of the General Purpose file from 20 to ~ 200 MeV. Current plans are to make this release coincide with the General Purpose file update scheduled for late 2003.

6. CONCLUSIONS AND PERSPECTIVES

The JEFF-3.0 General Purpose library, officially released on April 26, 2002, has been described. The main differences and expected improvements with respect to the JEF-2.2 General Purpose file have been highlighted. Current plans are to update and complete this JEFF-3.0 cross section library by late 2003 with intermediate energy data, photon-production data and covariance information. In addition, JEFF-3.0 Special Purpose files containing new activation data, fission yields, and decay data will also be released at the same time.

Future developments of the JEFF-3 library will continue to be driven by users' needs [17]. Advanced reactors, innovative fuels and subassembly design or spallation-reaction-driven system studies are examples of current research areas which are likely to require further improvements to the JEFF-3 nuclear data files.

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