Summary of JEFF Proposals to change the ENDF-6 format

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Introduction

This short paper summarises the discussion among the members of the JEFF Project in order to propose changes to the ENDF-6 format. O. Bouland, A. Nouri, A. Koning and R. Perel contributed the proposals and to the discussion on the JEFF electronic forum http://www.nea.fr/lists/jeff.html. Another proposal was contributed by P. Ribon and J-C. Sublet regarding the resonance region. This proposal is being discussed and the finalised version will be published as JEF/DOC-925.

Comments related to the procedures and to the ENDF-102 manual

Limitation of the number of points

There are restrictions in the ENDF-6 format on the number of points used to tabulate the distributions. An example is discussed below. While these restrictions were justified by the shortage of memory and the requirements of old versions of FORTRAN to have fixed dimension arrays, these justifications are not valid any more. It is thus suggested to remove these limitations.

Example: The number of incident energy points at which angular distributions might be given is restricted to 1200 points. This limit is usually not sufficient to correctly represent the scattering anisotropy when the resonance range is in the MeV range (e.g. structural materials like Cr-52). In principle, the Blatt-Biedenharn can be used to derive the angular distributions from resonance parameters. However, none of the existing processing codes implements this option. The ENDF-6 format does not recommend the procedure either. This limit might also be exceeded with the extension of the evaluated files to 200 MeV.

Summary of the ENDF rules

Appendix F of the ENDF-102 manual summarises the basic ENDF rules. This appendix is not up-to-date. For instance, it is quoted (page F-3): “When the elastic scattering is represented by Legendre coefficients, an energy-independent transformation matrix must be given to perform a CM to laboratory conversion”. Page 4.6 of the manual gives a more reasonable recommendation “A transformation matrix may be given in File 4 for elastic scattering. In general, this matrix is no longer required in ENDF/B because it is no longer needed in data processing codes”.

Proposals for format changes

Including stable isotopes in the Decay data file

Motivation: A decay data library is composed with radio-isotopes described in (MF=8/MT=457). If a nuclide is not included in the radioactive decay data file it is not clear whether that nuclide is not evaluated or that the nuclide is stable. Furthermore, the basic information described in (MF=8/MT=457) are of interest (e.g. mass, isomeric level designation, spin, parity) and it would be helpful to have this nuclear structure information for all nuclides, including the stable ones. Therefore, it is desirable to allow the description of stable nuclides in this section. The structure of the section is:

[MAT, 8,457/ ZA, AWR, LIS, LISO, 0, NSP] HEAD
[MAT, 8,457/ T1/2, ΔT1/2, 0, 0, 2*NC, 0/ (E-ΔE,ΔE) 3 / LIST
[MAT, 8,457/ SPI, PAR, 0, 0, 0, 0/
RTYP1, RFS1, Q1, ΔQ1, BR1, ΔBR1,
-----------------------------------------------
RTYPNDK, RFSNDK, QNDK, ΔQNDK, BRNDK, ΔBRNDK] LIST
<Subsection for Spectrum1>
<Subsection for Spectrum2>
-----------------------------------------------
<Subsection for SpectrumNSP>
[MAT, 0, 0/ 0.0, 0.0, 0, 0, 0, 0] SEND

Where NSP is the number of radiation types (NSP might be equal to zero).and NC the number of average energies given. A proposal was made by J.E. Hoogenboom (JEF/DOC-535) to adapt this section to include stable isotopes. The proposal was discussed at the previous CSEWG meeting and it was felt that a better solution might be possible. In the following, we will provide a proposal that

Introduce a new flag (NST) to describe whether the nuclide is stable or radioactive.

[MAT, 8,457/ ZA, AWR, LIS, LISO, NST, NSP] HEAD

if NST = 1 (stable isotope), the section would be:

[MAT, 8,457/ ZA, AWR, LIS, LISO, 1, 0] HEAD
[MAT, 8,457/ 0.,0., 0, 0, 0, 6, 0] 
[MAT, 8,457/ 0.0, 0.0, 0, 0., 0 0.0, 0.0, 0.0, 0.0] 
[MAT, 8,457/ SPI, PAR, 0, 0, 0, 0]

Otherwise if NST = 0 (the default option which suits all the existing files) the structure remains unchanged.

If this proposal is accepted, it would be fairly straightforward to update the manual to reflect this change.

Extending MAT numbers

Materials in the ENDF format are identified by a four-digit integer called the MAT number. This number is used by the processing codes to locate the desired material in an
ENDF file or tape. However, the restriction to 4 digits has many inconvenience that will be described here.

The ENDF rules for MAT number allocation are:

\[
\text{MAT} = 100 \times Z + \text{NN} \quad \text{where NN is a two-digit integer}
\]

Rule 1) First stable isotope: NN = 25

Rule 2) NN(A+1,G) - NN(A,G) = 3 (leave the room for two isomeric states between two successive stable isotopes)

Rule 3) NN(A, ST1) - NN(A, ST2) = 1

It is always a problem to infer the nuclide from a MAT number. Examples are: 9228 for U-235, 9237 for U-238. Furthermore, the rules described above are usually not easy satisfy in the case of a comprehensive decay data library. Rule 1 is not applicable if there are more than 9 isotopes before the first stable nuclide. Rule 2 does not leave the room for more than two isomeric states. Rule 2 is not applicable if:

\[
(\text{Number of isotopes} - 1) \times 3 + (\text{number of states} - \text{number of isotopes}) < 99
\]

The proposed new structure of the ENDF file made by B. MacFarlane at the last CSEWG meeting solves this problem.

Storage of (n, gamma n) cross sections

There is no special MT-section for (n, gamma n) reactions in the present ENDF-6 format. It should be made clear in the manual how to store these cross sections. The (n, gamma n) cross section is a continuum cross section. The associated reaction mechanism is that a neutron is captured, a gamma is emitted and and next a neutron is emitted, back to the ground state or to an excited state. The cross section is typically 5-10 millibarn in the few MeV region. I have not seen an example of (n, gamma n) so far in any of the libraries, though it could be that it is sometimes erroneously buried in some MT-section. It can not be stored in MT91 (continuum inelastic cross section), since the checking and the processing codes expect that the Q-value of MT91 is equal to that of the last discrete level. A new MT-number is however not necessary. The procedure I am using now is to store the total (n, gamma z) cross section (being equal to the sum of (n, gamma n), (n, gamma p)…(n, gamma alpha)) in MF3/MT5, and to use MF6/MT5 to split it into (n, gamma n), etc. cross sections using the yields. The energy angle-distributions can be given as usual.

Avoid redundant MF files

It should be recommended to use only MF1,2,3,6,8 and 10 in NEW evaluations. Moreover, in the mass range 20 < A < 209 (fission and light nuclides being a different
matter), there is no reason why the structure of one evaluation should differ from the next, with the exception of the resonance range. This raises a few issues:

- The elastic angular distribution MF4/MT2 presently seems to be the only data that needs to be stored in MF4, see e.g. 35Cl of ENDF-B/V1.8. Can this be moved to MF6/MT2 (NJOY)? An advantage is that all checking and processing codes could bypass subroutines that handle MF4. All future coding effort could be put in MF6.

- MF12,13 and 15 are redundant. All photon production can be stored in MF6. For discrete photons, this can even be done in a more exclusive way than in MF12,13,15.

- In Maurice Greene's write-up it is stated that the info of MF5 can be moved to MF6. Is this also true for fissile nuclides (fission neutron spectra)? Maybe MF5 should only appear for fission spectra.

- There is no reason why the isomeric cross sections should not be stored in an ENDF-6 transport file. This would make an evaluation truly complete. Presently, there are independent activation libraries (like EAF) which contain activation cross sections only. A long-term goal (well, short-term for some of us) would be to have only complete data files based on MF1,2,3,6,8,10 out of which derived activation libraries can be processed at any temperature.

- If this proposed "unification" is feasible, it may be an idea to print the relevant parts of the ENDF-6 manual in boldface or, somewhat less drastic, to put some recommendation sign in the margin. Users would not be bothered with redundant or non-recommended parts.

Isomers at high energies

A procedure should be defined to store isomeric cross sections at high incident energies in MF6/MT5. The residual production cross section could be split into a cross section for the ground state and a cross section for the isomer(s). It could be that this is possible already in ENDF-6 (through the LIP flag), but I don't know whether NJOY is prepared for this.

Extension of Kalbach representation

It could be helpful to have a small extension of the Kalbach representation. To explain this, I will make the distinction between the Kalbach representation and the Kalbach systematics. The Kalbach representation, i.e. the formula (6.4) of the ENDF manual, is very powerful. The Kalbach systematics, i.e. the phenomenological formula for the a-coefficient below Eq. (6.5) is only reasonably powerful. It is based on many experimental angular distributions from all over the periodic table and thus not a perfect way to represent the cross sections for an individual isotope, if one has experimental data. Obviously, if one has perfect fits for an individual isotope, tabulated angular distributions
could be used, but this will result in much larger datafiles. By including the possibility to
give the a-coefficient, for example by enabling NA=2 with LANG=2, one can get a better
angular representation for each energy point while keeping the size of MF6 within
reasonable bounds.

**Quality or completeness flag per isotope**

One could for example give an A,B or C grade to an evaluation based on its
completeness. I realise that the judgement of this may be rather subjective. Nevertheless,
some quality statement for each isotope would be helpful. Some of the modern
evaluations of ENDF-B/VI are almost complete in terms of described reaction channels
(usually the Los Alamos evaluations, such as 35,37Cl or the Pd isotopes), whereas others
(24Mg, 40Ar, 98Mo to name a few) are virtually empty. The danger is that a user might
not realise this, but instead simply observe that the isotope is in the library so that it can
be safely used.