ENDF Formats and Procedures

WPEC Subgroup B Report

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Background

At the last CSEWG Meeting in November 2001 an announcement was made that the ENDF/B-VI Rev.8 library is frozen and that the next library released will be ENDF/B-VII. Initiation for comments and suggestions for the new format was made. Corrections to the ENDF-6 formats manual and urgently needed extensions to the formats will still be considered, if necessary.

A document prepared by M. Greene was circulated by e-mail. A discussion on the subject is expected at the JEFF Meeting in Aix on 24-26 April 2002. Several comments and suggestions had been exchanged via e-mail, which are listed below.

The sections below represent a compilation that lists different proposals. The details are described by the authors in separate presentations. In this paper only the title and the proposer for extension/modification are stated, followed by comments where clarification or discussion is needed to reach a consensus.

Required clarifications and identified errors in the ENDF manual

Transformation matrix in MF 4 (O. Bouland)

The text in Appendix F is obsolete and should be corrected.

Requirements for format changes and extensions

Limits on the number of points (A.Nouri, A. Koning)

The limit on the number of points for cross section representation should be increased or abolished.

The limit on the number of incident particle energy points to describe angular distributions should be raised or abolished.
Representation of \((n,\gamma+n)\) reaction (A. Koning)

Is there a need for a new MT number or could the reaction be lumped into MT 5?

Isomeric cross sections (A. Koning)

Is it really necessary to go into details to describe energy/angle correlated distributions for isomers in MF 6? To uniquely identify excitation functions for nuclide production see next section.

ZA designation in MF 9, 10 (EAF99/A.Trkov)

In the EAF99 library the L1 parameter of the TAB1 record in MF 10 is used to store the product nucleus ZA designation. This is proposed to be ENDF standard.

Using this convention the excitation function for any product nucleus resulting from lumped reactions in MT 5 can be uniquely described.

It might be worth adding a requirement to the procedures that partial cross sections in MF 10 are redundant if the corresponding sections in MF3 are present. If only partial cross sections are given then they should form a complete set (i.e. their sum equals the complete reaction cross section that would appear in MF3). In this way cross sections in MF 3 and MF 10 could co-exist in the same file. At present, MF10 cross sections are not included in the cross section summation (?)

Note that a new module ACTIVATE of the Pre-Pro-2000 codes is available that converts MF3+MF9 data into MF10. The GROUPIE code can also process the MF 10 data.

More MT numbers (J.C. Sublet)

Some additional MT numbers can probably be accommodated easily, but one should check for possible solutions via MF 10, as discussed in the previous paragraph.

Avoiding redundant MF files (A. Koning, A. Plompen)

MF 9 was introduced to avoid the need for repetitive pointwise representation of resonance reactions since equivalent MF10 data cannot be accommodated in the resonance parameters. Abandoning the use of MF9 is not practical.

Counter-arguments were presented by R.L. Perel against abandoning MF 4, 5.

Extension of Kalbach representation (A. Koning)

The proposal was favourably consider by the JENDL Compilation Group.
Quality or completeness flag per isotope (A. Koning)

If adopted, careful consideration should be given to the criteria. Partial evaluations intended for dosimetry purposes were mentioned. On the other hand, there exist fission product evaluations, which are “complete”, but only the capture cross section was really evaluated. Although “complete” for neutron transport calculations, the quality of other reactions is questionable. If one wishes to use such a file for coupled neutron/photon transport, the evaluation is also incomplete.

Would the following categorisation be sufficient: activation, dosimetry, neutron transport, neutron transport with full particle emission data?

Stable isotopes in the Decay data file (A.Nouri, A.Koning)

A refinement of the old proposal is presented.

Material MAT numbers (A.Nouri, A.Koning)

It is argued that the existing MAT conventions are inadequate. Adoption of MacFarlane’s proposal is suggested. This would force changes to all processing codes. A softer option would be to make the MAT numbers again arbitrary (some national projects do not adhere to the rules anyway) and to modify codes to search the files by ZA/LIS0. The option to search for the required material by ZA is already implemented in the PrePro codes and it would not be too difficult to implement it in NJOY. This would also simplify inputs, since ZA numbers are easier to interpret than the MAT numbers.

Resonance region methods (P.Ribon, J.C. Sublet)

A detailed proposal and justification for format improvement was prepared.

Miscellaneous requirements for special purpose derived files (A. Trkov)

For convenience (e.g. to simplify input/output operations or use available software for operating on the data like plotting, group-averaging, etc.) it is often convenient to store miscellaneous data in ENDF format. For example, in the new dosimetry file IRDF-2002 it would be convenient to store standard neutron spectra; for activation analysis self-shielded cross sections would be required; etc. It is not necessary to define such extensions in the ENDF manual but merely allow for them to avoid conflicting situations.

- **Reserved MT numbers**: A block of MT numbers could be reserved for special application files (MT 260 – 269 say) to avoid conflicting extensions with other uses of the ENDF files. MT 261 is proposed to store the spectra.
Self-shielded cross sections: The only requirement is to accommodate storage of
the dilution parameter on the file. The second entry of the fourth record in MF1,
MT451 (next to the temperature) is a convenient place to store the dilution
parameter. For backward compatibility it would contain $1/\sigma_0$, i.e. the reciprocal of
the Bondarenko background cross section.

Multi-temperature/dilution ENDF files: The convention is already used
informally in NJOY. The purpose of the proposal is to formalize the approach for
derived files and allow the whole file to be repeated for different temperatures and
dilutions. The implication for checking codes is to skip checking for duplicate and
non-monotonic MAT numbers.

Alternative proposals for ENDF-7 and beyond

Summary of CSEWG Meeting (A. Nouri)
ENDF/B-VII is indeed scheduled for 2004-05. The objectives are much broader than
the format itself. The standards is one feature, but there are others including
photonuclear data, new evaluations for major actinides and fission products.

As far as the format is concerned, an ad hoc committee was created at the last meeting
"to define the ENDF-7 format and to look into possible future revolutionary format
development". The target date being the November 2002 meeting of CSEWG.

A Strawman Structure for ENDF-7 (R. E. MacFarlane)
(Prepared for the Codes and Formats Committee, Cross Section Evaluation Working
Group, Brookhaven National Laboratory, 6-7 Nov 2001).

The Europeans have requested that the ENDF format be extended to allow
more than 100 isotope/isomer combinations for one Z value. There have been a
number of needs expressed for numbers with more than the current 7 digits of
precision. People have often wanted to add more MT numbers than can be handled
easily. More values are needed for discrete levels than the current 40 or 50 (one
example being elemental evaluations with 40 levels per isotope, if we ever do that
again).

All these needs could be accommodated by giving up the tradition of repeating
the MAT, MF, and MT number on each line of the file and abandoning sequence
numbers. MAT could go to 8 or 9 digits (e.g., ZZZAAASSS for Z, A, and state). MT
could go to 4 digits, using 1001 for MT=51, 1999 for MT=91, 2000 for MT=600, etc.,
for up to 999 levels per discrete reaction. We would go to 6 fields of 13 on each line
(for up to 9 digits of precision) and use a character in column 1 to flag the
MAT, MF, MT card. For example:

```
* 92235000 3 16
  9.22350100+4 2.33025000+2 0 0 ...
-5.29778100+6-5.29778100+6 0 0 ...
   54 2
  5.32052100+6 0.00000000+0 5.50000000+6 5.59171300-3 ...
  6.00000000+6 1.40325000-1 6.25000000+6 2.32199700-1 ...
```

* 92235000 3 0
This structure converts easily into the binary ENDF formats, especially the blocked-binary format used in NJOY. It preserves all the normal ENDF record structures. It should be fairly easy to convert existing codes, such as NJOY. The most difficult part would be to handle the changes to the MT numbers. Existing evaluations would be easy to convert with a simple code.

**Abandon line-sequence number** (Reuven L. Perel)

This comment is relevant to both, Bob MacFarlane’s and Vicky McLane’s proposals regarding the digit numbers for MAT, MT, and real numbers.

**Energy-dependent decay constant** (JENDL Compilation Group)

Proposal refers to MF 1/ MT 455.

**Charged particle elastic scattering** (JENDL Compilation Group)

Proposal refers to MF 6/ MT 2.

**Covariance data in the resonance region** (JENDL Compilation Group)

Proposal refers to MF 32.

**Conclusions**

WPEC is the right forum to discuss various proposals. Tasks are to be assigned to prepare specific documentation for implementing changes into the ENDF manual in order to present a co-ordinated proposal to CSEWG.