

# Formats and Processing Committee Report

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Committee Chairman

## Introduction

The Formats and Processing session had too many items to cover in the allotted 8:30 am—12:30 pm time slot. The session was not initiated until 9:30 am, because the previous committee session needed an hour to complete their reports. At 12:30, the Formats and Processing session was halted for lunch, and resumed at 1:30 pm. Reports were continued until 3:00 pm, at which time the session was halted, in order to allow the next committee to begin their session. In the wrap-up session on Thursday morning, it was pointed out that the Formats and Processing session still had several items that weren't properly addressed. At this point it was decided to allow this committee session to resume after the wrap-up session, and at 9:30 am, the session was resumed. The items relating to formats for Version VII were revisited, and discussions on them were completed by 10:00 am, at which time a new topic was initiated related to formats for Versions beyond VII. The chairman left a little before 10:30 am, and the session apparently continued until around 11:30 am.

## Formats Manual

V. McLane (NNDC): A brief report was made regarding the ENDF-102 Formats Manual, that noted the manual was in good shape. Several minor modifications were made over the previous year to make downloading the manual easier and more efficient.

Several action items had been introduced in the previous year's Formats Manual topic discussion. Most of them have been successfully addressed.

- 1) A request by A. Trkov for a description of how to properly use "unit-base" transform interpolation resulted in a write-up that was posted on the BNL Format Proposals web site. This is included on pages 165-167.
- 2) A posting regarding the definition of a parameter previously designated as the energy of the CM in the laboratory system was also made. This is included on page 169.
- 3) A request that versions of Reich-Moore equations be made available that avoid numerical problems associated with using the equations published in ENDF-102 was satisfied by the publication<sup>1</sup> by M. Dunn of these equations in the September 2002 issue of Nuclear Science and Engineering.
- 4) The action item related to including one of more real examples of how to interpret and use the Kalbach-Mann procedures was not completed. After realizing the difficulty of making many modifications on things like equation numbers in ENDF-102, M. Greene decided that the item could be more easily addressed by

including the material in the AMPX-2000 User's Guide, and providing a copy of the material for posting on the BNL web site. This will be completed before the next CSEWG meeting.

### **Utility Codes**

C. Dunford (NNDC): All programs must be compiled with a FORTRAN-95 compiler. Extensive modifications have been made to take advantage of the new features of FORTRAN-95. Versions of CHECKR, FIZCON, PSYCHE, STANEF and INTER have graphical interfaces for use with Windows and Unix operating systems. At last year's meeting, M. Greene agreed to canvass users of the checking code suite to determine if there was sufficient interest to justify converting LISTEF, PLOTEF, and GETMAT to FORTRAN-95. The results of the survey were that these codes could be retired, and they will not be maintained for Version 7. Dunford's notes are given on page 171.

### **Processing Codes**

R. MacFarlane (LANL): NJOY99 has been fairly stable during the last year. A few new features had been added and some bugs have been repaired. A new FORTRAN 95 version called NJOY2000 is still under development and is being tested. The NJOY report is included on page 173.

R. McKnight (ANL): The majority of the ANL activities related to formats and processing were related to the needs of the VIM code.

D. McNabb (LLNL): LLNL has initiated a young, but very broad set of activities related to cross-section evaluation and processing. New evaluations have been completed for Br, Kr, and Se isotopes. The evaluations are based on a wide range of sophisticated models and techniques. An upgrade to process ENDF/B-VI has required 3 years and the processed results are being tested. Processing includes both Monte Carlo and deterministic applications. McNabb offered several new items for consideration in ENDF/B formats beyond version VII. Also included in his notes (pages 117-128) is a discussion of the advantages and disadvantages of using XML as a data transmittal vehicle.

M. Dunn (ORNL): AMPX-2000 has been used to process 305 ENDF/B-V and 340 ENDF/B-VI evaluations and the results are being tested. Point data are produced for Monte Carlo and resonance self-shielding applications and multigroup data for Monte Carlo and deterministic code applications. A prototypic continuous energy Monte Carlo code is under development. New modules for converting point kinematics data to probability distributions needed for the Monte Carlo code and also for adjoining the kinematics data file have been developed. Dunn's notes are included on pages 175-176.

### **ENDF-7 Format Proposals**

M. Greene gave the initial presentation in this section, which was a summary of the conclusions of a three-party (R. MacFarlane, D. Cullen and M. Greene) intensive exchange of observations and ideas regarding the impacts of various possible methods for extending ENDF-6 to accommodate ENDF/B-VII. A write-up of these findings was intended to be distributed to the standard CSEWG mailing list, but, unfortunately, the list that was “lifted” from an e-mail did not include all participants, such that, unfortunately, some of the attendees did not have the chance to review the material before the meeting. The write-up is included on pages 177-180. Basically, the study (which involved an exchange of more than 200 e-mails) noted that

- a) the present format could be easily searched using the ZA, and LISO parameters (instead of MAT/MF/MT),
- b) the current structure and data field lengths accommodate all situations that were thought to need more precision, etc.,
- c) it was felt that it is very desirable to maintain backwards-compatibility,
- d) ENDF-6 can be modified to meet foreseeable needs.

The study concluded that the format for Version VII should be ENDF-6, and that this should serve as the platform for the next release.

During the presentation, the salient features of other proposals were noted and discussed, such that a vote regarding what should be chosen for the next format was taken, and it was agreed that ENDF-6 would be used.

A proposal requiring some fairly minor modifications to the present formats to accommodate “Stable Isotopes” in the decay data files was made by A. Nouri. His proposal was accepted. (Details are presented on pages 181-185, which also includes other observations from the JEF community).

A proposal to activate an unused parameter in the records at the beginning of File 1 for specifying whether or not an evaluation was complete or not was made by V. McLane. After some discussion, it was decided that the NLIB parameter in File 1 already gave a safer way of doing this.

The proposal for a way of specifying energy-dependent delayed neutron time constant data was tabled by R. MacFarlane.

A format for a generalized method for using Reich-Moore data to treat situations such as charged particle channels was made by N. Larson. After some discussion, it was decided that Larson would interact with several interested parties regarding this new capability to develop a new format proposal. This new proposal will combine the simplicity of Larson’s format proposal with some of the generality allowed by the quite complicated LRF=5 (General R-Matrix) format and will be proposed at the next CSEWG meeting.

A proposal for a new format for specifying covariance data for resolved resonances was made by N. Larson. This format was tabled pending more study. An alternate proposal will probably be presented at the next CSEWG meeting.

In a discussion on increasing limits on array sizes imposed in the present file, it was voted to allow up to 20,000 energy points for specifying the angular distribution data in Files 4 and 6.

It was suggested by C. Lubitz that we would reduce some confusion by simply referring to both the version of a data collection and the format associated with that collection by simply using Arabic numerals. It was noted that the data collections in the rest of the world used this convention. After discussion that considered all of the places that documentation would have to be changed, and also noting that the other data collections all used the same ENDF formats, such that the differentiation was not a problem for them, it was decided to continue to use the present procedure of referring to the data with Roman numerals and the formats with Arabic numerals.

A posting had been made by C. Dunford regarding the fact that the present formats contained redundant and unnecessary parameters for specifying that distributions are isotropic. He also noted that the transformation matrix for converting between angular distributions in the CM and the laboratory systems were not used and were unnecessary. The group voted to eliminate the redundant flag and to drop the provision for the transformation matrix.

A proposal to move all multiplicity data to File 6 was tabled by C. Dunford.

During the first day's Formats and Processing sessions, the WPEC format proposals were passed over, because they had been delivered too late to be included in the postings, and because of severe time constraints. In the auxiliary session that was held on the last day of the meeting, each of these proposals was heard and acted on. Several of the 19 items included in the list are not format proposals *per se*, but are items regarding corrections to ENDF-102, etc. (The listing of the items in detail is given on pages 187-194.) The items are:

- 1) Obsolete text in Appendix F—this item pointed out some places where corrections on array limits, etc. are needed in ENDF-102.
- 2) Increase limit on number of cross-section values. This item suggested that the present limit of 50,000 was adequate.
- 3) Increase number of energy points allow in angular distribution data. It noted that the present limit of 1500 was inadequate and suggested 5000. (An earlier action had already raised the limit to 20,000 points.)
- 4) Representation of (n,gamma+n) reaction. It was noted that MT=5 could already handle this.
- 5) Add ZAP designation in Line 1 of the TAB1 record of MF 9,10. No action needed, since approval was made at previous CSEWG meeting.

- 6) Abandon MF=4 and MF=5 except for MT=2 and MT=18. This proposal was listed as a recommendation for future evaluations. No action was taken.
- 7) Extend Kalbach-Mann Representation. The suggestion here was to allow specifying the a-matrix with the other Kalbach-Mann parameters, thereby, avoiding the complicated and confusing procedures required to calculate it. The suggestion was approved.
- 8) Quality of completeness flag. Earlier in the meeting, it had been noted that the NLIB parameter was available for uses such as this.
- 9) Stable isotopes in the decay data file. Earlier in the meeting, A. Nouri made a proposal that was accepted to accommodate this situation.
- 10) Assignment of MAT numbers. The restriction on how to assign these numbers was discussed earlier in the meeting, and it was agreed that we could return to the pre-ENDF/B-VI procedures wherein these were arbitrary numbers; however, in the ENDF/B-VII data collection, the present values will probably be retained, for ease of continuity. In other words, independent data collections can use their own assignments.
- 11) Resonance region representation. It was suggested that there was ambiguity in the formats and procedures descriptions in ENDF-102. Apparently, a new description is available from the JEFF community that can be considered for possible replacement.
- 12) Reserved MT numbers for derived files. Here it is suggested that MT=261-270 should not be used, if possible. No action was taken.
- 13) Add explicit description of Legendre coefficients. It was suggested that the fact that File 4 assumes that the first coefficient is unity, and that the distribution, therefore, must integrate to unity, be augmented with a procedure that allows the first coefficient to be specified. (Session Chairman's Note: I am in total agreement with this observation; however, I would rather simply see File 4 abandoned with MT=2 moved to File 6, where that is the only option allowed). No action was taken on this matter, but will very likely be re-visited at a later meeting.
- 14) Move LIS and LIS0 to the first record. No action was taken.
- 15) Nomenclature for format *versus* library. It was suggested that more material describing the procedures for assigning these numbers be included at the end of section "0.ENDF-6 Preface". No action was taken at this time.
- 16) Energy-dependent decay constant in the delayed neutron data. A proposal for doing this was supposed to be presented at this meeting, but was tabled awaiting some more work on the details. Perhaps the suggested format changes in the WPEC document can be used as presented, or extended to cover this item. In any event, a proposal is expected.
- 17) Rutherford scattering for charged particle elastic scattering. This item was approved.
- 18) Covariances of energy-dependent unresolved resonance parameters. N. Larson agreed to interact with the JENDL community regarding this item to see if an appropriate solution can be found.
- 19) Correction of equation for Kalbach-Mann systematics. A correction that is needed to ENDF-102 was noted.

- 20) Assignment of MT numbers to more reactions. It was agreed that these assignments should be made by iterating by e-mail with members of the JEFF community.

### **Beyond ENDF/B-7 Discussion**

An auxiliary task for the Formats and Processing Committee is to look at new and advanced ideas that could be used for future versions of ENDF/B regarding formats. Around 1 ½ hours of the wrap-up session on Thursday morning was devoted to discussing the possibility of using more modern data storage structures for dealing with cross-section data. In particular, XML was the topic.

As an independent exercise to explore whether or not XML could be used in place of the present formats. C. Dunford has initiated an exploratory effort to this end, and prepared material that described how ENDF/B could be stored using XML, complete with some examples of how the data would actually appear in a computer file. (This material is included on pages 195-209).

The present formats were state-of-the-art in the 60's when they were invented and have served us well. They are characterized by:

- a) fixed record lengths,
- b) fixed formats and field lengths,
- c) a very small number of record types allowed,
- d) rigid record ordering that is only decipherable by explicitly following the guidelines set forth in ENDF-102,
- e) modifications to format require corresponding modifications in many codes,
- f) no definitions of structure or record content, etc.,
- g) application specific,
- h) unreadable by eye.

In contrast, XML is characterized by:

- a) free form,
- b) can be written in a fashion that can be read,
- c) structured in a tree-based model,
- d) data attributes can be defined,
- e) not application dependent, which means that users can make use of utilities developed for other applications, such as report writing and plotting utilities,
- f) checking of data structures inherently accomplished.

This, and other, more modern approaches for storing data will continue to be investigated, as time permits. A meeting of several individuals interested in the XML and ENDF/F-B formats is planned to be held sometime in the spring of 2003, and this topic is expected to become a major item in future CSEWG meetings.

### **Procedures for Submitting Proposals for New or Revised Formats**

This procedure was included in last year's minutes, and is included to give guidelines describing the proper procedures to use in submitting format proposal.

- 1) A new format proposal should be written using ENDF/B record structures and terminology. In other words, the records should be described as HEAD, CONT, LIST, TAB1, TAB2, etc., records and should be arranged according to other structures that are now in the files. When there is obvious overlap, the terms used to describe keywords should be the same as used elsewhere in the files; e.g., AWR is the mass ratio, ABUN is the abundance, etc. The documentation that is required in a format proposal should clearly show where the new material fits into the existing document.
- 2) Revisions to existing formats should follow the same rules as described under item 1). Revisions to the existing documentation should be clearly identified.

Other guidelines regarding format proposals are:

- 1) Format proposals should be received at least one month prior to a CSEWG meeting.
- 2) NNDC will post the proposals on their web site, thereby allowing interested parties to study the proposal in advance of the meeting. This would eliminate the situation that exists now, where one is "hit" with a new proposal without having time to adequately assess its impact, or how to use it.
- 3) NNDC will post proposals that are approved at a CSEWG meeting on their web site, along with the revised pages for the documentation in ENDF-102.

### **Reference**

1. M.E. Dunn, "Computational Experiences with the Reich-Moore Resolved-Resonance Equations in the AMPX Cross-Section Processing System", *Nuc. Sci. Eng.*, **142**, 48-56 (2002).

