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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PREPARATION OF PROCESSED NUCLEAR DATA LIBRARIES FOR THERMAL, FAST AND FUSION RESEARCH AND POWER REACTOR APPLICATIONS

Summary Report of the IAEA Consultants' Meeting
organized by the International Atomic Energy Agency
and held at the IAEA Headquarters, Vienna, Austria,
8 to 10 December 1993

Prepared
by

S. Ganesan
IAEA Nuclear Data Section
Vienna, Austria

March 1994

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Abstract

An Consultants Meeting on "Preparation of Processed Nuclear Data Libraries for Thermal, Fast and Fusion Research and Power Reactor Applications" was convened by the International Atomic Energy Agency and held during December 13-16, 1993 December 8-10, 1993 at the IAEA Headquarters, Vienna. The detailed agenda, the complete list of participants and the recommendations are presented in this report.

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1. Introduction

An IAEA Consultants Meeting on "Preparation of processed nuclear data libraries for thermal, fast and fusion research and power reactor applications" was held during December 8-10, 1993 at the IAEA Headquarters, Vienna.

The main purpose of the meeting was to review the current status of work in the subject of interfacing nuclear data banks to application calculations of thermal, fast and fusion research and power reactors, and, to assist the Agency in identifying appropriate IAEA activities related to nuclear data processing.

The evaluated nuclear data files such as ENDF/B-VI, JENDL-3.1, BROND-2 and CENDL-2 distributed by the Nuclear Data Centres are not directly used as input to neutronics or other applied calculations such as radiation safety and shielding, but are first converted to pre-processed files which are post-processed into multigroup files which are then cast into specially formatted libraries that are compatible with neutronic codes.

Both the developed and developing countries are finding it difficult to sustain and fund adequately the processing activities. The processing tasks demand specialized expertise using computer resources committed over a long period of time (several years) to execute the tasks. There has been no active common forum to bring the scientists, in particular in developing countries working in this area together. The field of study of nuclear data processing and preparation of processed nuclear data libraries form the connecting bridge between basic evaluated nuclear data files and application calculations.

Although a lot of sophisticated developments have taken place in the creation of processing codes such as NJOY, AMPX, GRUCON, REX1 etc., as a result of the IAEA code verification project, numerical inconsistencies discovered in the processing codes were rectified. Not all problems have been completely solved. The urgent need to provide a consistent and correct multigroup data for core physics and shielding applications for thermal, fast and fusion research and power reactor applications derived from the recently released basic evaluated data files remain to be fulfilled.

The meeting provided the first opportunity at the Agency to share the experiences on cross section data processing methods and validation procedures for specific applications.

2. Organization of the Consultants' Meeting and Meeting Proceedings

The main focus in this Consultants Meeting was on the following:

1. Developments in the NJOY code system, sharing of past experiences and future plans
2. Verification of accuracy of nuclear data processing and discussion; Sharing of experiences and future plans of the processing methods for the following:
3. WIMS Library Update Project
4. Review of current and future needs of multigroup libraries and the plans for future, including plans for compilation and distribution of multigroup libraries for integral checking and validation purposes.
5. To assess the need, if any, to initiate a Coordinated Research Programme on this topic

The agenda which consisted of detailed presentations and discussions of working groups is presented in Appendix A. The conclusions and recommendations are presented in Appendix B. The complete list of participants and their affiliations are provided in attachment C.

The meeting was subdivided into two parts. As shown in Appendix A, presentations were given by 14 participants from 10 member states on a wide range of topics during the first half of the meeting. A summary of the presentations will be given as part of the proceedings of the meeting and will not be covered in this report. The latter half of the sessions was spent identifying the critical problematic issues related to cross section processing and drafting a set of recommendations to IAEA to help guide Agency efforts in providing nuclear data services to member states. Session 1 was chaired by Dr. Budi Santoso, Session 2 by Ir. P. F. A. de Leege and Session 3 and Session 4 by Dr. E. Menapace. Dr. J.E. White served as the co-chairman of the meeting and, in addition, as Secretary of the Working Group drafted the conclusions and recommendations which are reproduced in Appendix B of this document.

3. Meeting Attendance

The meeting was attended by 18 scientists from 11 Member States (India, Indonesia, Italy, Japan, Korea, Netherlands, Russia, Slovenia, Switzerland, United Kingdom, and the U.S.A) including two staff members (S.Ganesan and K.M. Akhtar) from the Agency. In all, 5 experts were awarded by the Agency limited financial

support in the form of lump sum grant to defray partially the travel and subsistence expenses. The complete list of participants and their affiliations are presented in Appendix C.

4. Results of the Meeting:

The meeting participants reviewed the current status of work in the subject of interfacing nuclear data banks to application calculations of thermal, fast and fusion research and power reactors, and prepared a summary report to assist the Agency in identifying appropriate IAEA activities related to nuclear data processing.

The meeting participants strongly recommended the initiation of an IAEA Co-ordinated Research Programme on physics of nuclear data processing with a goal to help the production of consistent working nuclear data libraries for various application calculations.

The complete set of recommendations to the Agency are given in Appendix B to help guide Agency efforts in providing nuclear data services to member states.

The participants from developing countries endorsed the IAEA WIMS-D4 Library Update Project (WLUP) which was presented and discussed at the meeting. As illustrated in the document "UPDATE OF THE WIMS-D4 NUCLEAR DATA LIBRARY, Status Report of the IAEA WIMS Library Update project", compiled by S. Ganesan, INDC(NDS)-290, presented at the meeting, considerable progress has been achieved in this project. The WLUP is being carried out by correspondence and at no cost to the Agency. Over 23 laboratories from 18 countries have participated in Stage I and Stage II of WLUP. The project is expected to be completed by 1996. The results of this project will be well validated multigroup nuclear data libraries in WIMS-D4 format with quality assurance for use in developing countries around the world.

APPENDIX A

International Atomic Energy Agency

IAEA Consultants' Meeting

on

"Preparation of Processed Nuclear Data Libraries for Thermal, Fast and Fusion Research and Power Reactor Applications"

IAEA Headquarters, Vienna, Austria

8 to 10 December 1993

AGENDA

Wednesday, 8 December

08:30 a.m.-10:00 a.m. Formalities, Registration

10:00 a.m. Opening of the Consultants' Meeting
C.L. Dunford, Head-Nuclear Data Section, IAEA

Technical Remarks by the Scientific Secretary
S. Ganesan, IAEA

Election of Chairman
Adoption of the Agenda

10:30 a.m. Coffee Break

10:45 a.m.-12:00 a.m. Session 1.

(1) K. Devan, Kalpakkam, India: "The role of IAEA in fulfilling nuclear data needs."

(2) B. Santoso, Jakarta, Indonesia: "Establishment of computer code system for nuclear reactor design analysis (in Indonesia)."

(3) T. Zidi, Ain-Oussera, Algeria: "Nuclear data from experience to application." (Presented by S. Ganesan).

(4) P. de Leege, Delft, the Netherlands: "NSLINK, preparing AMPXMASTER (SCALE) library from NJOY output."

(5) H. Maekawa, JAERI, Japan:
"Cross section libraries based on JENDL-3.1 and JENDL-3.2."

(6) J.E. White, Oak Ridge, U.S.A.:
"Module for checking and validating. Processed multigroup cross sections."

Discussions

12:00 a.m.-02:00 p.m. Lunch Break

02:00 p.m.-05:30 p.m. Session 2.

(6) (continued)
J.E. White, Oak Ridge, U.S.A.:
"Module for checking and validating. Processed multigroup cross sections."

(7) C.J. Dean, Dorset, United Kingdom:
"Production of application libraries for WIMS."

Discussions

Thursday, 9 December

09:30 a.m.-12:00 a.m. Session 3.

(8) P.A. Androssenko, Obninsk, Russia:
"Experience in the direct use of the library ENDF-B/VI in the Monte Carlo calculations."

(9) A. Tsiboulia, Obninsk, Russia:
"Some aspects of preparation and testing of group constants. Group constant system ABBN-90."

(10) W.-G. Hwang, Kyunggi-Do, Republic of Korea:
"Experiences with NJOY and pre-processing system on PC-486 and benchmarks of WIMS library generated from ENDF/B-VI."

(11) G.-C. Panini, Bologna, Italy:
"Nuclear data processing at ENEA: Instruments and methods."

(12) J.-D. Kim, Daejon, Republic of Korea:
"NJOY processed multigroup library for fast reactor applications and point data library for MCNP - experience and validation -."

(13) A. Trkov, Ljubljana, Slovenia: "Processing of nuclear data for applications."

(14) S. Ganesan, IAEA-Nuclear Data Section: "Information on the current IAEA activities in nuclear data *processing*."

Discussions

12:00 a.m.-02:00 p.m. Lunch

02:00 a.m.-05:30 p.m. Session 4.

Additional Papers, if any.

Summary, Conclusions and Recommendations.

05:30 p.m. WINE and CHEESE PARTY, VIC Restaurant.

Friday, 10 December 1993

09:30 a.m.-12:00 p.m. Session 4 (continued).

12:00 a.m.-02:00 p.m. Lunch

02:00 p.m.-05:30 p.m. Session 4 (continued).

Conclusion of the Meeting.

APPENDIX B

Summary Report

IAEA Consultants Meeting on
"Preparation of Processed Nuclear Data Libraries for Thermal, Fast and Fusion Research and Power Reactor Applications"

December 8-10, 1993 IAEA Headquarters

ATTENDEES: Mr. K. Devan (India),
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Mr. Jung-Do Kim (Korea),
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Dr. Anatoli Tsiboulia (Russia),
Dr. Andrej Trkov (Slovenia),
Dr. Matjaz Ravnik (Slovenia),
Dr. Sandro Pelloni (Switzerland),
Dr. Christoper J. Dean (United Kingdom),
Dr. Dermott E. Cullen (U.S.A.),
Dr. John E. White (U.S.A.),
Dr. Srinivasan Ganesan (IAEA),
Mr. Khalid Mahmud Akhtar (IAEA).

BACKGROUND

The evaluated nuclear data files are not directly used as input to neutronics or other applied calculations. First, the nuclear data is pre-processed into pointwise form which is in turn translated into a multigroup or other processed interpretation of the original reference data. Finally, the resulting data is cast into well defined formats which are compatible with neutronics codes.

The processing tasks demand specialized expertise using computer resources and manpower committed over a period of years. There is no theory of nuclear data processing and the preparation of data libraries remains an art. The subject involves the development and validation of computer software using knowledge of evaluated data formats and procedures, knowledge of the accuracy of various computer platforms, checking the quality assurance of processed results including benchmark data testing, and an understanding of the use of the processed data. Also, the subject requires knowledge of the physics governing the interaction of neutrons and gamma-rays with materials including Doppler broadening effects, thermalization effects, calculation of pointwise cross sections from resonance parameters, calculation of damage

and kerma cross sections, self-shielding of resonances in both the resolved and unresolved energy ranges, calculation of group-to-group transfer matrices for neutron, neutron-to-gamma, and photon processes.

The primary aim of the meeting was to share experiences on cross section data processing methods and validation procedures for specific applications. The objective was to assist the Agency in identifying appropriate IAEA/NDS activities related to nuclear data processing. The technical specifications for cross section processing are dependent on the nuclear system (e.g. thermal, fast, fusion, research, and power reactor systems) and may change with improved calculational methods and data. It was noted that a single processed library cannot satisfy the needs of all applications. Reactor physics, criticality, and radiation shielding have different cross section requirements.

ORGANIZATION OF MEETING

The meeting was subdivided into two parts. Presentations were given by 14 participants from 10 member states on a wide range of topics during the first half of the meeting. A summary of the presentations will be given as part of the proceedings of the meeting and will not be covered in this report. The latter half of the sessions were spent identifying the critical problematic issues related to cross section processing and drafting a set of recommendations to IAEA to help guide Agency efforts in providing nuclear data services to member states.

SUMMARY/CONCLUSIONS

Within the time allowed, this summary attempts to capture the central views and concerns of the participants. The information is organized into the broad categories of evaluations, processing procedures, self-consistency/internal checking, data testing, documentation, alternatives to NJOY91, and interfacing routines for post-processing. The comprehensive nature of the NJOY cross section processing system combined with the capability of NJOY to process ENDF-6 formatted data has resulted in its worldwide use. The comments that were collected from the participants contain citations to NJOY which is used to mean cross section processing.

EVALUATIONS:

Future evaluated nuclear data files should adhere to a standard format. It is the recommendation of this group that organizers of evaluated files adopt the ENDF-6 format. It is recognized that many evaluations use ENDF-5 format and this group encourages some movement towards a single standard format. Furthermore, the group recognizes the general purpose evaluated files (BROND, CENDL, ENDF, ENDL, JEF, JENDL), special purpose evaluated files (EAF, EFF, JENDL-DF, JENDL-FF, and REACT), and the composite fusion evaluated file FENDL/E which is guided by the engineering design

needs of the ITER project and other fusion projects. Help from the International Evaluation Cooperation effort is needed to identify the best evaluated data for specific applications. Associated with each of the major evaluated files are special purpose libraries such as the sublibraries of FENDL.[1]

All evaluated files should be executed with the checking codes by the data center with responsibility to distribute the evaluated data.

Many presenters discussed problems in reconstructing pointwise data from resonance parameters. The group discussed the feasibility of working with evaluations containing no resonance parameters; however, resonance parameters are still needed for the purpose of resonance self-shielding (especially in the unresolved resonance range). The compactness of the files resulting from the use of resonance parameters is still viewed as a benefit. It is suggested that the reference evaluated files should be run through a sequence of checking codes to detect flaws that would hinder future production processing. There was agreement that the sequence RECONR/BROADR/THERMR/HEATR/UNRESR from NJOY91 should be used as well as the ENDF checking codes CHECKR/FIZCON/PSYCHE. Also, a parallel sequence for resonance reconstruction using the IAEA preprocessing package (PRE-PRO) was recognized as useful for providing independent results for comparison. Also, PRE-PRO contains modules (FIXUP/LEGEND) that test the physics enbodied in the evaluation. Problems in the unresolved resonance range do occur during processing and some evaluations contain parameters that are not acceptable from a physics point of view. The problem arises when one tries to calculate the unresolved cross section at low values for background dilution. Evaluations should include covariance files for at least the structural materials. The processing of covariance data with NJOY91 appears adequate at the present time. There is an alternative to NJOY91 for covariance processing which was developed by the French at Saclay.

PROCESSING PROCEDURES:

There is a need to reconstruct resonances to 0.1% accuracy. This requires at least 9 significant figures (software/hardware requirements).

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[1]FENDL/E - General Purpose Evaluation Library
FENDL/A - Activation Library
FENDL/DS - Dosimetry Library
FENDL/D - Decay Data Library
FENDL/C - Incident Charged-Particle Library
FENDL/MC - Processed Monte Carlo Library
FENDL/MG - Processed Multigroup Library
FENDL/U - Processed Uncertainty Library

It may not be very significant for thermal reactors; however, it is important for the high energy resolved resonances in fast systems. In addition, 9 significant digits are important both for major actinides and structural materials to describe the sharp and very narrow resonances.

For large production projects, input decks should be prepared and tested for selected nuclides. Standard processing sequences are encourged to reduce human error. The same set of error tolerances should be used for all nuclides. (It is recognized that this might be overkill for some materials.)

When using NJOY, the following suggestions were made:

The practice of processing one material at a time is the best recipe. A large library (about 50 nuclides) has been run successfully with NJOY(GAMINR).

Dividing the processing task into two parts (pointwise generation and group averaging) can help simplify the error checking process and can save both valuable time and costs.

Never use sigma zero equal to zero; use instead 1.E-6.

In NJOY(RECONR), do not use a number of significant digits that exceeds the limits on the representation of real numbers on the adopted computer platform.

In the case of wrong Kerma, the upper kinematic limits (MT=443) should be adopted. To see whether Kerma is correct use printing option 2 in NJOY(HEATR) and be sure Kerma factors are within their proper physical range.

Care should be taken to ensure consistency of processed data with cross section definitions assumed in the codes that will ultimately use the processed data.

SELF-CONSISTENCY/INTERNAL CHECKING:

The evaluated nuclear data files should have already passed the ENDF checking routines. A summary of the CHECKR/FIZCON findings should be distributed with the data.

In general, the pointwise files will be consistent after resonance reconstruction. There is a need to check for non-physical values (e.g. negative or zero cross section values) and understand why they appear.

At the group level, it is valuable to include checks on the GENDF data to expose processing methods deficiencies or problems with the evaluated data. One also gains insights as to whether the processed data is consistent with the definitions expected in the transport codes.

DATA TESTING:

The INTER code can also be used to generate overall parameters (e.g. fission spectrum averaged cross sections, resonance integrals, thermal maxwellian averaged cross sections, 2200 m/s cross sections). These quantities can also be generated from product libraries.

Visualization of the groupwise data is more useful than scanning printed output and should be encouraged.

Both neutron and gamma-ray benchmark data testing are very important to help establish information on the performance of the processed library. Benchmarks do provide information on the weaknesses of the evaluated data.

For the purpose of data testing it is recommended to create an international library of evaluated integral and macroscopic experiments (for example, an extension to document ENDF-202 would be very useful and timely).

Benchmark data testers should use standard benchmarks from this database but may also like to study the experimental reports and improve the benchmarks as well. This is necessary because results will be compared with experiment. The models in the CSEWG benchmark specification document refer to current methods. As methods improve, it will be possible to model the experiment in better detail and may make the recommended calculational models and methods obsolete.

The CSEWG documentation should move to an electronic format.

Data testing can be performed by comparing calculated integral parameters with measured values. Routine calculations can be done using deterministic codes. Validity of results can be assessed on specific examples using more refined techniques such as Monte Carlo methods which make direct use of evaluated data (like Monte Carlo program system BRAND).

Documentation should include adequate experiment description as well as inputs to selected codes which are used in the analysis.

DOCUMENTATION:

Processing code

The NJOY documentation is improving and the use of postscript files can accelerate the information exchange problem for some users. In general, the need for complete and up-to-date documentation in hardcopy form is essential for any code used to process cross sections.

It is important to continue the practice of providing comments in the fortran describing the current function and input specification (e.g. NJOY and PRE-PRO).

Final Processed Library Package

Formal specification of the version of the processing code and basic data should be noted. Details of any local enhancements should be documented. (These should be sent to the author of the processing code).

The primary application of the library and any known limitations on the use of the library should be noted.

Details of the library generation process should be included.

Sample problems designed to demostrate how to use the data and the associated post-processing tools.

Sample listings of NJOY input data should be included. References to all benchmark data testing should be cited.

Each processed library should include in the data file itself relevant information about source of the basic data and the calculational procedure used to obtain the processed data.

ALTERNATIVES TO NJOY91:

NJOY is the only comprehensive code for generating data in all application areas. In response to concerns raised about distribution restrictions on NJOY, J.E. White (RSIC,USA) stated that developing countries that want NJOY should submit a request to RSIC for NJOY91 even if past denial was experienced. The changing world climate between countries might result in a favorable reply at this time.

The development of a nuclear data processing code system and/or a processed library for thermal and fast reactor applications, that will be freely available to all member countries might be a suitable topic for a Co-ordinated Research

Program of IAEA to benefit all member states.

Dermott Cullen's PRE-PRO codes have been used at the IAEA to process data for dosimetry and activation libraries. We recommend their continued use.

Valuable potential processing codes are GRUCON, AMPEX, MC^2, and the Japanese Prof GROUCH-G/B code system.

Indian development will be of interest in future with the REX series of codes.

Most codes will only process parts of the data e.g. only neutron files, or neutron and gamma interaction but not gamma source data.

AMPX77 most nearly covers the functions of NJOY but does not include production of Monte Carlo data.

The feature to process ENDF-5 format should also apply to any alternative to NJOY.

INTERFACING ROUTINES for POST-PROCESSING:

Once groupwise data is available, one is not ready to provide the needed input nuclear data required by radiation transport or other codes. There is still a need to convert the data to formats required by the end-user. Also, customized or problem-dependent data are often needed. The following interface routines are available to perform the above mentioned purposes as well as perform resonance self-shielding and temperature corrections. They are:
(TRANSX-2, AMPX77, DTFR, CCCCR, WILIT2, NSLINK, and CONSYST to name a few.)

RECOMMENDATIONS

The following summarizing remarks are intended to give guidance on the consultants thinking with respect to the future role of IAEA/NDS in the processed cross section data arena.

In developing countries, the nuclear data needs for nuclear energy programs are met with considerable dependence on International Centers. These countries find it difficult to expand their nuclear teams and provide the necessary resources to keep their technology from becoming obsolete. From the point of view of those participants with access to limited resources, IAEA/NDS provided a very useful service by creating a forum whereby specialists from both developing and developed countries were able to come together and share ideas.

The consultants group wanted to stress the following:

Currently processing codes have a problem calculating temperature dependent, self-shielded cross sections in the unresolved resonance region, for small dilutions, e.g., the cross sections can even be negative. It is recommended that the methods used to calculate this data be reviewed and a program developed to accurately calculate this data.

The IAEA should continue co-ordination of the preparation of a coupled neutron and gamma-ray library for the ITER project using ENDF-6 formatted evaluated data. (The actual production runs for the generation of the multigroup cross sections is a task that can be accomplished in a more effective manner in a major research and development environment where processing methods development and benchmark data testing co-exist. The presence of evaluation work in the same environment adds strength to the production activity.)

The calculation of improved radiation damage parameters for dosimetry applications should continue. This activity involves cross section processing without the generation of transfer matrices needed for radiation transport calculations.

IAEA/NDS should continue the WIMS/D library update project including processing the required thermal scattering law data from ENDF/B-VI.

IAEA should initiate a Co-ordinated Research program for the development of improved physics algorithms needed to interface evaluated data with applications.

The compilation and quality assurance of evaluated nuclear data files continue to be a strength of IAEA/NDS. The independent verification of pointwise data reconstructed from resonance parameters uncovered errors which provided very useful feedback to processing code developers. It is recommended that IAEA continue its activities in the verification of the accuracy of processed data for applications.

IAEA should encourage the retention of the capability to process evaluated data in ENDF-5 format. This feature is present in NJOY and AMPX77.

As a nuclear data center, IAEA/NDS should help bridge the gap between evaluators and end-users.

IAEA Consultants' Meeting on
"Preparation of Processed Nuclear Data Libraries for Thermal, Fast and Fusion Research and Power Reactor Applications"

IAEA Headquarters in Vienna, Austria

8 to 10 December 1993

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