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Summary Report from

First Research Coordination Meeting on

Nuclear Data Libraries for Advance Systems - Fusion Devices (FENDL - 3)

International Atomic Energy Agency (IAEA)
Vienna, Austria

2 - 5 December 2008

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March 2009

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Abstract

The first Research Co-ordination Meeting of the Nuclear Data Libraries for Advance Systems - Fusion Devices (FENDL - 3) was held at the IAEA Headquarters in Vienna from 2 to 5 December 2008. A summary of the meeting is given in this report along with discussions which took place. An important outcome of the meeting was the agreement to create a new FENDL-3.0 Starter Library. Finally, a list of task assignments was prepared together with the plan for future CRP activities.

March 2009

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1. INTRODUCTION

The participants of the first Research Coordination Meeting (RCM) on Nuclear Data Libraries for Advanced Systems - Fusion Devices (FENDL-3) were welcomed by N. Ramamoorthy, DIR - NAPC who presented the history of the IAEA involvement in nuclear data activities for fusion applications.

R. Forrest was elected as the chairman of the meeting and A. Trkov as rapporteur. The proposed Agenda was discussed. With minor modifications related to the sequence of presentations the Agenda was adopted.

The Coordination Research Project (CRP) officer, A. Mengoni, introduced the background, the objectives, the envisaged scope and the timeline of the FENDL-3 project. The list of relevant nuclides and possible data sources from recent evaluations was listed, mentioning ENDF/B-VII, JEFF-3.1, JENDL/HE and the TENDL-2008 library. The latter is a comprehensive library covering an extensive list of isotopes, incident particles and libraries in ACE format and is based purely on default nuclear model calculations with TALYS. The meeting continued with the presentations as follows.

2. BACKGROUND INFORMATION ON THE FENDL-3 CRP

Based on the recognition that energy plays an increasingly prominent role in the world and the expectation that nuclear fusion can provide an abundant energy source, the IAEA is currently providing support for the exchange of scientific and technical information on fusion research through conferences, meetings and projects. The most important initiative on fusion research is presently the ITER project. All the materials to be used in ITER went through a procedure of quality assurance which utilized benchmark experiments (bulk shield experiments, streaming experiment, Silicon Carbide blocks, Tungsten blocks, Breeder blanket, etc.). These experiments are tested against simulations based on Monte Carlo or other transport methods. Here, the role of basic Nuclear Data information is fundamental. Only by using credible Nuclear Data Libraries will all of these experiments provide the necessary reliability for design and quality assurance.

The Fusion Evaluation Nuclear Data Library (FENDL) has been created under the auspices of the IAEA in the mid-1990s, and went through a procedure of validation by benchmark experiments by the Fusion nuclear data community. The first version of this library contained evaluations judged to be the best available by February 1997. The present version of FENDL (FENDL-2.1) was released in 2003, and has been extensively used for ITER material studies (ITER Project Management and Quality Programme: Quality Assurance in Neutronic Analyses).

Meanwhile, plans are underway to construct a facility to test candidate fusion reactor materials under high neutron radiation dose conditions approximating those to be found in a fusion reactor. This facility – International Fusion Materials Irradiation Facility (IFMIF) – involves accelerating high currents (up to 250 mA) of deuterons to 40 MeV and impinging them on a liquid lithium target to produce neutrons. Deuterons that strike elements of the accelerator transport system, as well as various target materials, would induce radioactivity that needs to be considered in the safe operation of this facility as well as in its eventual decommissioning. The status of energy differential deuteron cross-section data from a few MeV up to 40 MeV is considered by the IFMIF development community to be inadequate for the purposes of assessing the facility with respect to operational safety and licensing issues. In

particular, the FENDL library does not contain data for incident charged particles (e.g. protons and deuteron), while the maximum energy for incident neutrons is limited to 20 MeV.

Recognizing these difficulties in March 2006, the International Nuclear Data Committee (INDC) recommended the extension of the FENDL library to cover the nuclear data needs of the IFMIF community. A Technical Meeting aiming at identifying possible detailed objectives for a CRP was held at IAEA, Vienna, on 31 October – 2 November 2007. The CRP has arisen as a consequence of the discussions at this Technical Meeting. The CRP was approved by IAEA Research Program Advisory Committee on December 2007.

3. PRESENTATIONS

T. KAWANO - Los Alamos National Laboratory, Los Alamos, NM, USA

T. Kawano presented updates to the ENDF/B-VII library for structural materials. The updates include removal of errors and improvement of gas production data based on new measurements at the LANSCE facility, Los Alamos. New evaluations are planned or in progress for Ti, V, Fe and Ni isotopes. Improved nuclear models are needed to reproduce the most recent measurements for multi-particle emission reactions. Kawano will send the new Ti files to J-C. Sublet to check the effects of self-shielding.

M. SAWAN - University of Wisconsin, Madison, WI, USA

M. Sawan presented the possible impact of replacing the FENDL-2.1 evaluations originating from the ENDF/B-VI.8 library with ENDF/B-VII data. Nuclides to focus on are the isotopes of S and K, ^3H (inertial fusion), ^6Li , ^9Be , ^{10}B , ^{16}O , ^{19}F , $^{35,37}\text{Cl}$, ^{197}Au (inertial fusion) and ^{208}Pb . The calculations for the simple ITER-like benchmark case showed relatively small impact on the neutron and gamma fluxes, but large differences in heating calculations. Some of the differences were traced to a bug in data processing which will be resolved in the new updates to the NJOY processing system. Significant changes to tritium breeding in the Inertial Confinement Concept were observed.

J.C. SUBLET - Commissariat a l'Energie Atomique (CEA), DEN, St. Paul lez Durance, France

J-C. Sublet indicated the need to include absorbers like Ag, In, Cd, Hf, Gd, thermal scattering data and photonuclear reactions into nuclear data libraries for fusion devices. The Be and Cu evaluations from JEFF-3.1 perform better in benchmark analysis and should be considered for FENDL-3. The importance of the energy grid and the interpolation for emitted particle spectra was shown to have a large influence on the calculated spectra. Subtle differences in the elastic scattering angular distributions of important nuclides (such as ^2H) may lead to large differences in integral parameters like k-eff, as demonstrated for some HEU solutions in heavy water from ICSBEP. Various features of the activation library EAF-2007 and its predecessors were described.

S. KUNIEDA - Japan Atomic Energy Agency (JAEA), Tokai-mura, Japan

S. Kunieda described the JENDL/HE-2007 file, which contains cross-sections for incident neutrons and protons with energies up to 3 GeV. The nuclear model calculation scheme was outlined, including some novel approaches that smoothly join the methods applicable at high energies. Selected examples of differences between major libraries were shown for illustration. The TIARA benchmark calculations show marked improvement compared to the LA150 library, although the differences could also originate from normalization or a hidden

data processing problem. The JENDL/HE evaluations can be considered candidates for FENDL-3, but contain no covariance data. The timeframe for the development and release of the JENDL-4 library was presented, and is scheduled for release end of 2009. The library extends up to 20 MeV.

P. BATISTONI - ENEA, Frascati, Italy

P. Batistoni presented the experimental programme at ENEA-Frascati that could be used to validate the FENDL-3 library. Most of the experiments are included in the SINBAD database available from the NEA Data Bank. SiC is not predicted well with FENDL-2.1 data.

F. TARKANYI - Hungarian Academy of Sciences, Debrecen, Hungary

F. Tarkanyi addressed the topic of measurements and evaluation of charged particle induced activation cross-sections. Current status of the data, participating institutions, facilities and evaluation methods were described. Possible contributions to FENDL-3 include proposals for new measurements, evaluation of experimental data, recommendations on the quality of the available data and validation through integral measurements.

R. FORREST - UK Atomic Energy Authority, Abingdon, UK

R. Forrest outlined the status of the EAF-2007 library and plans for the release of EAF-2009. Contents (i.e. energy range, reactions, incident particles, uncertainties, etc.) and validation methods were described. Special features of the user interface include importance diagrams and "cooling curves" and of SAFEPAQ-II such as statistical analysis of the cross-section database were described. The latter can help to identify dominant nuclides, important reactions and hence the reactions that require re-measurement or evaluation.

R. CAPOTE NOY - IAEA, Vienna, Austria

R. Capote-Noy gave an overview of the NDS activities in relevant Coordinated Research Projects and Data Development Projects, namely RIPL-3, W-evaluation, radioisotope production cross-section projects, extension to IRDF-2002, etc. The links to the relevant web-pages were given.

M. LAUGHLIN - ITER, Cadarache, France

M. Laughlin gave a presentation on the status of ITER, focusing on the design details which might impact nuclear data needs, particularly the shielding of electronics and diagnostic equipment, kerma for electronic materials and activation data for real materials. M. Laughlin was asked to prepare a list of candidate materials of possible interest to ITER that are not included in FENDL-2.1.

U. FISCHER - Forschungszentrum Karlsruhe, Karlsruhe, Germany

U. Fischer described the activities of FZK and possible contributions to FENDL-3. Evaluations in progress are $^{182,183,184,186}\text{W}$, ^{181}Ta , ^{55}Mn and $^{50,52,53}\text{Cr}$. A model of the $d^{6,7}\text{Li}$ source for IFMIF is also under development. Methodology for data evaluation and validation was described through examples.

P. PERESLAVSTEV - Forschungszentrum Karlsruhe, Karlsruhe, Germany

P. Pereslavstev presented the details of the evaluation and validation of nuclear data for the tungsten isotopes. He pointed out the differences between evaluations, including some formatting defects in the new IAEA evaluation. He defended the exclusion of the Vonach prescription for correcting the Frehaut measurements on the $(n,2n)$ cross-section, but there

remained differences of opinion. A similar discussion arose in connection with the measured elastic angular distribution data and the contribution from the inelastic channels.

A. TRKOV - Jozef Stefan Institute, Ljubljana, Slovenia

A. Trkov re-iterated the important aspects that the updated FENDL library should include, like the extension above 20 MeV, inclusion of incident charged particle data, covariances and benchmarking. He listed recently available candidate libraries and databases that could serve as a data source. He stressed the need to prepare working application data libraries to enable benchmark testing. He listed some of his current activities and responded to the comments by Pereslavtsev, who identified a few problems with the IAEA tungsten evaluations; most of them were relatively simple formatting issues that do not affect benchmark calculations.

H. KIM - Korea Atomic Energy Research Institute (KAERI), Daejeon, Korea

H. Kim described the activities on nuclear data evaluation and benchmarking at KAERI. Empire-II and TALYS nuclear model codes are used. Several fusion-related benchmarks were analysed. Evaluations of the neutron-induced reactions for the tungsten isotopes were shown. Charged-particle induced reactions on ^{27}Al were also evaluated. Plans for the future include charged-particle evaluations for Si, and other relevant isotopes.

A. IGNATYUK - Institute of Physics and Power Engineering (IPPE), Obninsk, Russian Federation

A. Ignatyuk discussed various aspects of nuclear data evaluations for incident charged particles, showing the differences and limitations of various nuclear model codes. Typically, nuclear models overpredict the (d,2n) reaction channel. It seems that blind calculations of deuteron-induced reactions can not be predicted well at present. A considerable amount of experimental data are available, which can form the basis for the improvements of nuclear models.

J. KOPECKY - JUKO Research, Alkmaar, Netherlands

J. Kopecky outlined the historical developments of the European Activation Files (EAF) and the uncertainty information contained therein. The results of the recent TENDL library will be used to improve the uncertainty estimates (including more refined energy dependence) in the EAF file. The presentation complements the one by R. Forrest.

M. AVRIGEANU - National Institute of Physics and Nuclear Engineering, Magurele, Romania

M. Avrigeanu talked about the nuclear data needs for the IFMIF facility. The status and prospects for global optical model parameters for incident deuterons was presented. Semi-microscopic and phenomenological OMP analysis for ^{27}Al was done. In the second step of the deuteron induced reactions analysis, all contributing reaction mechanisms: elastic-scattering, breakup, stripping, pre-equilibrium and statistical emissions to the deuterons interaction with ^{27}Al , for energies from 3 to 60 MeV have been considered. The results imply that deuteron-induced activation cross-sections based on model calculations should be updated using improved models. The work is related to the IAEA RIPL-3 project, which many of the state-of-the-art nuclear model codes use as the source of information.

Y. WATANABE - Kyushu University, Fukuoka, Japan

Y. Watanabe presented the activities on ITER- and IFMIF-related data in Japan. These include measurements of thick target yields and neutron-emission cross-sections as a function

of outgoing particle energy for incident-deuterons of 25 and 40 MeV, as well as the analysis of the data by model calculations. Measurements and analysis of data for incident neutrons at intermediate energies in collaboration with foreign partners were also described. The double differential proton production data from 175 MeV quasi monoenergetic neutrons on carbon were well reproduced by the JENDL/HE evaluation. Measurements for incident neutrons of 90-110 MeV on Al and 140-160 MeV on Fe were also reported. Proton-induced double differential cross-sections include measurements on several targets and incident particle energies. Neutronics experiments for Japanese ITER test blanket module and benchmark analysis were listed.

4. DISCUSSION

An extensive discussion took place after the presentations. The main objectives of the CRP have been reviewed and an action plan established in order to meet the final goals. In summary, it was decided to create a starter library for neutrons. This library will be created with the rules defined below and will contain the most recent updates of all the materials already present in FENDL-2.1.

For charged particles, several issues need to be solved before a proper library for fusion applications can be created. An action list aiming at solving these issues has been agreed. The activation library for Fusion applications which will be part of the FENDL-3 package will be mostly based on EAF-2007 (European Activation File, 2007). Additional details have been discussed and are reported here below.

Finally, for the inclusion of covariance files (uncertainties), it has been decided to create a “shadow” library, which could be based on model calculations (see the recent release of the TENDL databases). This approach has been suggested and adopted in order to maintain the consistency between evaluation of data (e.g. cross sections) and of their related uncertainty which, at present, can only be performed consistently on the basis of model calculations.

5. FENDL-3.0 STARTER LIBRARY

After an extensive discussion, it was proposed to create a “Starter Library” (FENDL-3/SLIB), with all possible “trivial” updates of the various files present in the FENDL-2.1 library. The FENDL-3/SLIB, should also be used to test application library tools. FENDL-3/SLIB will be a neutron-induced library only.

The following rules for creation of FENDL-3/SLIB have been agreed by the participants.

Rules of Creation

1. Replace the present evaluation with updates
ENDF/B-VI.8 to ENDF/B-VII.0
JENDL-3.x to JENDL/HE-2007
JEFF-3.x to JEFF-3.1.1 (available from NEA)
BROND-2.1 to BROND-3.0
replace element MATs with isotopic evaluations where available
2. Adopt evaluations from libraries that contains standards
(example: H-1 from ENDF/B-VII in place of JENDL-3.3)

3. Add the following materials:
 - absorbers : Ag, In, Cd, Hf, Gd (task co-ordinator: J-C Sublet)
 - additional for IFMIF : tbd by U Fischer
 - additional for ITER : tbd by P Batistoni (in conjunction with M Loughlin)
 - additional for others : tbd by H Sawan
- 3.1 sub-rule: each material added need to have a three-line (at least) justification
4. Evaluate results from experimental benchmarks and point out critical points. The starter library will contain a "warning" flag to report the finding.
task co-ordinators: C Konno, P Batistoni
5. If a material does not have HE data, the JENDL-HE file (HE part) will be adopted and merged into the evaluation. A cut at 150 MeV needs to be done.
task co-ordinators: Y Watanabe, S Kunieda
6. If JENDL/HE is not available for a given material, (examples: P, S, Sn) embed TENDL-200x when available.
task co-ordinator: S Kunieda
7. For the following light elements: H-3, He-3, He-4, Li-6, Li-7, Be-9, B-10, B-11, N-15 nothing needs to be done.

Task Assignments, Actions & Deadlines

1. Replace the present evaluation with updates
on: IAEA/NDS
deadline: March 2009
2. Replace the present evaluation with those containing standards
on: IAEA/NDS
deadline: March 2009
3. To provide a table with information on FENDL-2.1 updates, origin, and changes
on: IAEA/NDS
deadline: March 2009
4. The JENDL-HE file (HE part) will be adopted and merged into the evaluation. A cut at 150 MeV needs to be done.
on: Y Watanabe, S Kunieda
deadline: March 2009
5. Provide a group structure to produce application libraries
on: U Fischer
deadline: February 2009
6. Produce application library (ACE) for n-induced reaction, based on the starter library
on: A Trkov
deadline: four months after release of the starter lib
7. Produce application library (TRIPOLI PENDF) for n-induced reaction, based on the starter library

on: J-C Sublet
deadline: four months after release of the starter lib

Additional Actions List

- M. Laughlin: - to prepare a list of candidate materials of possible interest to ITER not included in FENDL-2.1. Distinguish between materials for particle transport and activation.
- M. Sawan: - to repeat the analysis of the impact of substituting FENDL-2.1 data originating from JEFF with the most recent JEFF-3.1 evaluations.
- to repeat the analysis of the impact of substituting FENDL-2.1 data originating from JENDL with the most recent JENDL-3.3 evaluations.
- J-C. Sublet: - to provide brief justification with references for the justification of replacing Be and Cu data in FENDL-2.1 with JEFF-3.1 evaluations for FENDL-3.

General Deadlines

Deadline for feedback from task co-ord. : end February 2009
Deadline for definition : mid March 2009
Deadline for creation : end March 2009

6. FENDL-3 for charged particles

Task assignments, actions and deadlines are given in the following.

1. p-induced reaction library

- assess available files from recently released libraries
- select the most important materials
- make proposal for adoption of files for each mats (for what available)
- report at the next meeting on results of the above

Team: T Kawano, Y Watanabe, R Capote, F Tarkanyi, HI Kim, U Fischer

Deadline: RCM-2

2. d-induced reaction library

- assess presently available files for most important materials (H-1, H-2, He-3, Li-6, Li-7)
- select the most important additional materials
- assess available files from recently released libraries for additional materials
- evaluated quality of purely model-derived libraries
- report at the next meeting the results of the above

Team: A Ignatyuk, U Fischer, M Avrigeanu, C Walker Kalbach, F Tarkanyi

Deadline: RCM-2

3. application libraries & processing

- evaluate the possibility to process and use general purpose files for p- and d-induced reactions

Team: J-C Sublet, U Fischer, A Trkov

Deadline: RCM-2

7. FENDL-3 Activation Library

Task assignments, actions and deadlines are given in the following.

Neutron

1. EAF-2007 is adopted as starter library
Task: ENDF-6 formatting will be provided by J-C Sublet
Deadline: end April 2009
2. Provide improved uncertainty files
Action: R Forrest, J Kopecky
Deadline: RCM-2
3. Prepare a proposal and submit to CSEWG for format extension (new MT numbers)
Action: J-C Sublet
Deadline: October 2009

Proton

1. Provide ENDF-6 format for the EAF-2007p
Action: J-C Sublet
Deadline: RCM-2
2. EAF-2007p library and PADF (FZK) library will be validated against experimental data and IAEA medical applications library for the most important materials (Al, V, Cu, Fe, Ta, W, Ni, Cr)
Team: F Tarkanyi, U Fischer (A Konobeyev), R Capote (to provide evaluated files)
Deadline: RCM-2

Deuteron

1. Provide ENDF-6 format for EAF-2007d (action: J-C Sublet) and TENDL-200x (action: A Trkov)
Deadline: RCM-2
2. EAF-2007d library and TENDL-2008 library will be validated against experimental data and IAEA medical applications library for the most important materials (Al, V, Cu, Fe, Ta, W, Ni, Cr)
Team: F Tarkanyi, R Capote, A Ignatyuk
Deadline: RCM-2
3. M Avrigeanu will provide model calculations for Al, Cu
Deadline: July 2009
4. (d,p) reactions present in evaluated libraries will be assessed against experimental data for selected set of materials (action: A Ignatyuk, F Tarkanyi, C Walker Kalbach)
Deadline: RCM-2

8. FENDL-3 Covariances

A shadow library will be created which will contain covariances data.

1. The shadow library with covariances will be based on TENDL-2008 evaluations, for isotopes heavier than F-19. Whenever files WITH covariances are available from major libraries, those will be adopted.

Action to make this available: IAEA/NDS

Deadline: March 2009

2. For lighter nuclei, whenever files WITH covariances are available from major libraries.
3. A Trkov and U Fischer will provide a description and an example of how covariance files can be prepared for $E > 20$ MeV.
Deadline: February 2009, send outcome to A Koning.

9. CONCLUSION

A plan of the CRP activities which will lead to the creation of an updated and extended version of the Fusion Evaluated Nuclear Data Library has been elaborated. Tasks have been assigned to the participants of the CRP in order to reach the objectives. As a first step in the activity, it has been decided to create a starter library (for incident neutrons) which will be made available at the beginning of 2009 for testing.

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IAEA's
1st Research Co-ordination Meeting (RCM) on
Nuclear Data Libraries for Advanced Systems – Fusion Devices (FENDL 3.0)

IAEA Headquarters, Vienna, Austria

2 – 5 December 2008

Room F0814

AGENDA

Tuesday, 2 December

08:30 - 09:30 **Registration** (IAEA Registration desk, Gate 1)

09:30 - 10:30 **Opening Session**

- Welcoming address – N. Ramamoorthy
- Introductory remarks – A. Mengoni

10:30 – 11:30 **Break for administrative matters**

11:30 – 12:50 **Start presentations**
2 x (30 + 10 min)

12:50 - 14:00 **Lunch break**

14:00 - 17:50 **Presentations (continued)**
5 x (30 + 10 min)
(Coffee break as appropriate)

Wednesday, 3 December

9:30 - 12:40 **Presentations (continued)**
4 x (30 + 10 min)
(Coffee break as appropriate)

12:40 - 14:00 **Lunch break**

14:00 - 17:30 **Presentations (continued), start discussion**
4 x (30 + 10 min)
(Coffee break as appropriate)

19:00- **Social event: dinner at Wiener Rathauskeller**

Thursday, 4 December

9:30 - 12:30 **Discussions (continued); task assignments**
(Coffee break as appropriate)

12:30 - 14:00 **Lunch break**

14:00 - 17:30 **Discussion on agreed FENDL topics (1)**
(Coffee break as appropriate)

Friday, 5 December

9:30 - 12.30 **Discussion on agreed FENDL topics (2)**
(Coffee break as appropriate)

12:30 - 14:00 **Lunch break**

14:00 - 17:30 **Layout 1st RCM report**
(Coffee break as appropriate)

Close

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