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# Progress report on the Fusion Evaluated Nuclear Data Library (FENDL)

M. Herman and D.W. Muir
International Atomic Energy Agency, Nuclear Data Section,
A-1400 Vienna, Austria

Presentation at the NEANSC Working Party on
International Evaluation Cooperation (WPEC)
Brookhaven, New York, USA, 19-21 April 1999

**ABSTRACT**

With the completion of the FENDL-2.0 library, the main emphasis of the FENDL project has changed from library production to validation and maintenance. In support of this more modest goal, the IAEA plans to hold small Consultants' Meetings annually to stimulate and monitor data testing activities and to permit the incorporation of improved evaluations. The first meeting in this new series was held in Vienna on 12-14 October 1998 to review recent testing and validation of the basic and derived transport-data sublibraries in FENDL-2.0. Findings and conclusions of this Meeting are reported below.

## INTRODUCTION

The IAEA Nuclear Data Section (NDS), in co-operation with several major nuclear data projects, has created the Fusion Evaluated Nuclear Data Library (FENDL). The goal of the effort is to provide a comprehensive and high quality data library in support of design of the International Thermonuclear Experimental Facility (ITER) project and other fusion-related developments. Within the scope of this activity IAEA has served as a co-ordinator for the assembling, processing, and testing of the FENDL library and has organized a series of international meetings in the 1987-1999 time frame.

FENDL is a collection of nuclear data selected from various national libraries and contains: activation cross sections, decay data, dosimetry data, fusion reaction cross sections, and general purpose data evaluations calculations (in basic and processed forms) for transport. In Version 2.0 of FENDL, the data are collected in the following sublibraries:

- FENDL/A-2.0 - activation cross sections
- FENDL/D-2.0 - decay data
- FENDL/DS-2.0 - dosimetry data
- FENDL/C-2.0 - fusion reaction cross sections
- FENDL/E-2.0 - general purpose basic evaluations

- FENDL/MG-2.0 - general purpose evaluations processed into multigroup form
- FENDL/MC-2.0 - general purpose evaluations processed into the form of input for Monte Carlo calculations.

The first four sublibraries of FENDL-2.0 were released on 14 March 1997 following approval by the Advisory Group Meeting held in Vienna 3 - 7 March 1997. The general purpose (transport) sublibraries were released on 15 May 1998, both as basic evaluated data and in processed form.

The IAEA Nuclear Data Section remains committed to the support of the fusion design activities through the FENDL project. However, with the completion of the FENDL-2.0 library, the main emphasis of the FENDL project has changed from library production to validation and maintenance. In support of this more modest goal, small Consultants' Meetings will be organized approximately annually to stimulate and monitor data testing activities and to permit the incorporation of improved evaluations as they become available.

The first of this new series of Consultants' Meetings was held in Vienna on 12-14 October 1998 to review recent testing and validation of the basic and derived transport-data sublibraries in FENDL-2.0. (See the report INDC(NDS)-395, Vienna, March 1999). Findings and conclusions of this Meeting are reported below. (The second such meeting will be held in Obninsk, Russia, in June 1999 and will be devoted to the testing and validation of the FENDL/A-2.0 activation sublibrary.)

## STATUS OF THE FENDL-2.0 TRANSPORT SUBLIBRARIES

Following recommendations of the FENDL Advisory Group Meeting (AGM) in March 1997, evaluations for $^{3}$He, $^{4}$He, $^{197}$Au (from ENDF/B-VI), and Ti (from JENDL-3) were included in the FENDL-2.0 library. All new selected evaluations were checked at the NDS using CHECKER, FIZCON and PSYCHE codes that revealed a number of minor deficiencies. Typical problems included:

- energies out of order
- width deviates too much from the average (typical for light nuclei)
- maximum energy of secondary energy distribution incorrect
- distribution negative (but negligible)
- average energy exceeds available energy
- different energy ranges for different isotopes in natural material evaluations
- abundance of an isotope incorrect
- Q-value for an isotope incorrect
- normalization different from unity
- incorrect mass.

Authors were asked to correct the evaluations and most of these inconsistencies were removed. The remaining ones are judged to have no impact on practical calculations. This round of corrections resulted in the replacement of the evaluations for the following materials: $^{16}$O, $^{28,29,30}$Si, $^{51}$V, Ga, Zr, Mo, W, and $^{197}$Au.

All new entries were reprocessed by the authors according to the uniform specifications (see Appendix 3 of INDC(NDS)-395), the library was assembled, and the quality assurance tests were performed by J. White. The RADE code detected no serious problems. Larger discrepancies (above 10%) were observed only between very small cross sections and scattering arrays, which have little if any practical impact. Consequently, transport sublibraries FENDL/E-2.0 -/MC-2.0, and -/MG-2.0 were officially released on 15 May 1998.

It should be noted that FENDL-2.0 files for $^{56}$Fe ***do not*** contain double counting of $\gamma$'s, in contrast to the version present in the EFF-3.0.

Two recommendations of the 1997 FENDL Advisory Group Meeting are pending:

- Thinning of the total and inelastic scattering cross sections in the $^{56}$Fe evaluation was not performed - however, the new EFF-3.1 evaluation, which will be considered as an update for the next FENDL release, has been thinned by A. Trkov.
- Replacement of nat-Zr, nat-Mo, nat-Sn, and nat-W evaluations with isotopic ones - no candidates for replacement were submitted to NDS.

Release of the transport sublibraries on 15 May 1998 coincided with the publication on the NDS WWW-server (www-nds.ieae.or.at) of the newly designed WWW-pages for the whole FENDL-2.0 library. All files can be downloaded directly through the Web browser. In order to decrease transfer time most of the files (the large ones) are compressed with GNU gzip. The compression code gzip is available free of charge for most of the operating systems including UNIX, VMS, and MS Windows. Since September 1998, the full documentation of FENDL-2.0 library is also available from the FENDL WWW-site.

FENDL-2.0 can still be downloaded with the classic FTP protocol from the NDS FTP-server: iaeand.iaea.or.at (username: FENDL2), or obtained on CD-ROM (see next paragraph).

Following the recommendations of the last Consultants' Meeting two obvious errors in the basic and derived files for $^{29}$Si and $^{56}$Fe were corrected (see section "User Feedback ..."). After replacement of the erroneous files, the FENDL-2.0 library has been frozen and is referred as "FENDL-2.0, Version January 14, 1999". This version is available on-line from the NDS server and off-line as a CD-ROM (IAEA-NDS-CD-06).

## VALIDATION AND BENCHMARKING

Comprehensive benchmarking of FENDL-2.0 candidate evaluations was reported previously (INDC(NDS)-356, 1996). The most remarkable achievement of the first experiments on ***bulk shield*** is that the uncertainty imposed on the calculations by nuclear data uncertainties (FENDL-1, EFF-2/3) has been shown to be within ± **30%** for all relevant nuclear responses in the shield blanket and in the vacuum vessel up to the toroidal field coils.

The derived FENDL/E-2.0 sublibraries issued 15 May 1998 have been benchmarked using the following integral experiments:

- FNS/JAERI clean benchmarks for V and V-alloy (V-4Ti-4Cr), Fe.
- FNS/JAERI TOF experiments on Be, Fe.
- OKTAVIAN/Osaka University spherical shell experiments on Be, Al, Si.

- KANT/FZK spherical shell experiment on Be.
- TUD/Dresden iron slab experiment.
- FNG/ENEA bulk shield experiment with SS-316 and water.
- FNG/ENEA streaming experiment in a SS-316/water shield.
- FNS/JAERI duct streaming experiment in an iron shield.

All of the mentioned experiments were calculated with the MC data files except the FNS/JAERI clean experiment on Fe which was also calculated with the MG data.

In addition to the mentioned elements, the FENDL-2.0 evaluations included in these benchmark calculations comprise the following materials: SS-316 (Fe, Cr, Ni, Mn, Mo, Si), air (N, O), water, and water equivalent material (H, C, O), concrete (H, B, Na, Mg, Fe, Al, Si, K, Ca), Cu and V-alloy (V, Cr, Ti).

In the benchmark validation, most of the important materials were considered and, in general, improvements have been observed with respect to the FENDL-1 results. Further testing is needed to cover *all* of the evaluations contained in FENDL-2.0. The Consultants' Meeting, therefore, recommended performing additional benchmark analyses. Recognizing the lack of integral data for some important materials like Sn, Nb, Al, Si, Ti and Zr, integral experiments on these materials were strongly recommended.

Five participants of the last Consultants' Meeting presented the results of their benchmark calculations for $^{56}$Fe. Four of them included in their intercomparison also the most recent iron evaluation - EFF-3.1. The results show that the new evaluation is superior to the one included in FENDL-2.0 and therefore should be considered as a possible replacement evaluation for the future FENDL release.

## USER FEEDBACK REGARDING THE DERIVED SUBLIBRARIES

The following problems, related to the use of the derived FENDL/MG-2.0 and FENDL/MC-2.0 sublibraries were reported:

1. TRANSX-2 cannot properly post-process MATXS files when some components of a mixture have thermal scattering matrices and some do not.

2. The array size is insufficient when calculating the self-shielding correction in TRANSX-2. This affects calculation of light nuclei like $^{12}$C using FENDL/MG-2.0.

   **ACTION:** These two problems were solved with patches to the TRANSX-2 code prepared by Kazuaki Kosako and provided to NDS by F. Maekawa. They are available from the FENDL Web-site at NDS. Users should download both patches and apply them to TRANSX-2 code before running calculations.

3. Unphysically large γ-ray production cross sections are given in the FENDL/MG-2.0 for $^{29}$Si due to the inconsistency of the "NK" key for MT=102 in MF=12 and 14 in the basic FENDL/E-2.0 evaluation for $^{29}$Si.

   **ACTION:** The $^{29}$Si files were corrected by J. White and are available in the 14 January 1999 version of FENDL-2.0.

4. Not all the files contained in FENDL/MG-2.0 and FENDL/MC-2.0 were produced according to the same processing specifications. Only new FENDL/E-2.0 entries follow processing specifications provided in the IAEA INDC(NDS)-373 report issued in July 1997. Some of the MC and MG files produced before that date (all evaluations taken over from FENDL-1.0) do not fulfill these specifications. In particular, gas production cross sections are missing for some materials.

   **ACTION:** The Nuclear Data Section will consider the possibilities of reprocessing all evaluations that do not follow agreed uniform specifications.

5. The smallest $\sigma_0$ value for Cu data in FENDL/MG-2.0 is 10. Since the pure copper would be used in a fusion reactor, $\sigma_0$ values of the order of 1 or 0.1 might be needed.

   **ACTION:** The Nuclear Data Section will consider the possibilities of reprocessing Cu evaluation with the above mentioned $\sigma_0$ values.

6. The *nnc* number used in FENDL/MC-2.0 is not fixed. To select a desired library for MCNP calculations, one specifies the "nnc" part of t07he ZAID numbers defined as *"zzaaa.nnc"* where *"zz"* and *"aaa"* are atomic and mass numbers of a material, respectively. In FENDL/MC-1.0 *nnc*=00c is used for all materials, while three numbers (00c, 07c, and 40c) are used in FENDL/MC-2.0. Unique *nnc* numbers would be better.

   **ACTION:** In order to avoid confusion it was decided to keep the current notation. Users are advised to download XDIR files, which automatically take care of proper addressing. The unified notation will be introduced in the next release of the library.

7. Imprecise values of the KERMA coefficients in the FENDL/MC-2.0 sublibrary were reported by F. Maekawa. The KERMA data were recently investigated in the FNS direct nuclear heating experiment. Considered materials were Be, C, Al, Si, SiC, Ti, V, Cr, Fe, Ni, SS-316, Cu, Zr, Nb, Mo and W. In some cases, especially for the heavier nuclei, the nuclear heating rates calculated with MCNP differ from the experimental data by as much as 20%. These discrepancies can be attributed to the invalid neutron KERMA coefficients used in calculations. In the MCNP libraries, KERMA coefficients are calculated using the energy-balance method, which is not as accurate as the direct one. It is recommended that the latter method be used to produce FENDL/MC sublibrary. A modification of the NJOY code is needed for this purpose.

8. The EFF-3.0 multigroup data files for $^{56}$Fe contain double counting due to the fact that processing was performed using NJOY/UNRESR module, while the unresolved parameters are left in the evaluation for historical reasons.

   **ACTION:** The FE056EFF3.M and FE056EFF3.G files were processed without NJOY/UNRESR module and replaced in the 14 January 1999 version of the FENDL-2.0 library.

## FURTHER UPDATES AND IMPROVEMENTS OF THE FENDL-2.0 LIBRARY

Due to limited financial support, which does not allow for further large Advisory Group Meetings, the following formal procedure has been adopted for new and/or revised evaluations to be incorporated in future revisions of FENDL:

1. A proposal for a new or revised evaluation can be made to the FENDL co-ordinator at IAEA/NDS by regional projects (e. g., ENDF, EFF, BROND, JENDL, CENDL).

2. The FENDL co-ordinator then requests from the proposing regional project the following:

   - the evaluated (E) data file,
   - the derived MG and MC files. When preparing the derived files, the specifications set up for FENDL-2.0 have to be applied as much as possible,
   - a review kit for the new evaluations or an updated one for revised evaluations.

3. The FENDL task co-ordinator submits the review kit to the other regional project co-ordinators asking for independent reviews of the new/revised evaluation.

4. Based on the outcome of the reviews the FENDL co-ordinator makes a decision and informs the project co-ordinators.

5. An accepted evaluation is considered as an up-date to the existing FENDL-2.0 library and is then placed on a list of "pending evaluations". The corresponding E, MG and MC data files will be made available on the Web server in addition to the reference FENDL-2.0 files.

6. The "pending evaluations" will be included into a new release of FENDL after approval by a suitable Consultants' Meeting.

Following this procedure, the approval of the new release of FENDL is expected to take place at the next Consultants' Meeting on the general-purpose sublibrary.

The following new or revised evaluations have been forwarded as candidates for the next update of FENDL-2.0:

- N-15 from BROND
- Fe-56 from EFF-3.1
- Na, Mg, Ta from JENDL-3.2
- Ca, Ti, Mn, Bi from JENDL-FF.

Once these evaluations are formally submitted to the Nuclear Data Section, they will be considered according to the agreed procedure.

## CONCLUSIONS AND RECOMMENDATIONS

FENDL-2.0 has been extensively benchmarked and frozen. The Consultants' Meeting has concluded that it is currently the best and most comprehensive nuclear data library available for fusion applications. Therefore, it should be adopted as a reference library in fusion reactor design calculations and related applications. New integral experiments are recommended for important materials like Sn, Nb, Al, Si, Ti and Zr.