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I N D C INTERNATIONAL NUCLEAR DATA COMMITTEE

Extension and Improvement of the FENDL Library for Fusion Applications

Summary Report of an IAEA Consultants' Meeting

Fiziko-Energeticheskij Institut
Obninsk, Russia
22 – 24 June 1999

Prepared by
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November 1999

IAEA NUCLEAR DATA SECTION, WAGRAMER STRASSE 5, A-1400 VIENNA

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Abstract

The discussions and conclusions of the meeting on "Extension and Improvement of the FENDL Library" are summarized in this report. It is shown that the FENDL-2.0 activation sublibrary was validated successfully. However, a number of deficiencies was identified. Possible improvements are proposed which should lead to the release of the FENDL-2.1 version of the library early in 2001.

November 1999

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Introduction

The IAEA Nuclear Data Section (NDS), in co-operation with several nuclear data projects, has created the International 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 coordinator for the assembling, processing, and testing of the FENDL library and has organized a series of international meetings.

FENDL library is a collection of selected nuclear data from the various national libraries and contains: activation cross sections, decay data, dosimetry data, fusion reaction cross sections, and the general purpose basic evaluations (pointwise and processed) to be used for transport calculations. In the present version (2.0) of FENDL these 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 the multigroup structure
FENDL/MC-2.0	general-purpose evaluations processed into the structure suitable for Monte Carlo calculations.

The first four sublibraries of FENDL-2.0 were released on 14 March 1997 upon the approval of the Advisory Group Meeting held in Vienna from 3 to 7 March 1997. It should be noted that due to their completeness (13,006 reactions in FENDL/A-2.0 and 1867 nuclides in FENDL/D-2.0) the actual utilisation of the first three sublibraries is very general and not limited to fusion applications.

Objectives

The objectives of the present Meeting were:

- review recent testing, validation and applications of the FENDL/A-2.0 sublibrary,
- identify needs for sublibrary improvements and extensions,
- discuss and establish procedures for updating/revisions of the current evaluations,
- review Web-access tools for FENDL-2.0 and other dissemination issues.

The Meeting decided to extend these objectives onto decay and dosimetry sublibraries (FENDL/D-2.0 and FENDL/DS-2.0) since both are closely related to FENDL/A-2.0 and there is no other forum to review these two sublibraries.

Organisation and attendance

The Meeting was held at the IPPE in Obninsk (Russia) from 22 to 24 June 1999. It was attended by four internationally recognized experts from four countries, an IAEA representative and 7 observers (Russia) (see Appendix 2).

Proceeding and results

The Meeting was opened by A. Pashchenko (IPPE, Obninsk) and by M. Herman (IAEA) who made a remark on the current IAEA policy toward FENDL library. M. Herman informed the participants that IAEA-NDS is committed to continue support of the FENDL activities concentrating in the near term on maintenance of the FENDL library. No new Advisory Group Meetings are planned in the near future, but the NDS expects to organize periodic Consultants' Meetings to stimulate and monitor validation of the library and to keep it up to date with the most recent evaluations.

R. Forrest (Culham, UK) was elected as Chairman and the Agenda of the Meeting (see Appendix 1) was adopted.

Discussions during the Meeting concentrated on three main topics (validation, applications and status of evaluation activities) aiming toward assessment of FENDL/A-2.0 and indication of needs for improvements. Observed deficiencies are summarised in the next section of this Report.

Validation

Integral experiments are a rich source of information with which a wide range of validation and comparison exercises can be made in the activation data field. Materials samples have been irradiated in a wide range of simulated D-T neutron fields at three European laboratories and at JAERI-FNS. The latter experiment is unique because decay heat rather than activity was measured. Some results from that experiment were reported during the Meeting.

Maekawa described the decay heat experiment performed at the JAERI Fusion Neutronics Source (FNS) facility in 1996 using the Whole Energy Absorption Spectrometer (WEAS). A comprehensive data base of decay heat (conveyed by both β- and γ-rays) has been obtained for 32 fusion reactor relevant materials in a wide range of cooling times from 1 min to 400 days. The experiment was analysed by the ACT4 code using several activation cross section libraries including FENDL/A-2.0. It was found that in most cases the FENDL/A-2.0 sublibrary predicts adequately the decay heat power, indicating high precision of cross sections and completeness of the data. In particular, good agreement was found for SS316, F82H and Zr using FENDL/A-2.0.

Independent analysis of the same experiment was reported by **Forrest**. About 130 reactions of FENDL/A-2.0 were validated by the JAERI decay heat measurements and European integral measurements. It turned out that about 50% of the calculated values are in excellent agreement (better than 10%) with the experiments. Additional 15% are in good (better than 20%) agreement. Some cross section data needing improvements were identified. In several cases this validation led to the replacement of original data by more accurate evaluations.

Follow-up experiments at FNS facility were discussed by **Maekawa**. Sample materials for *all* the elements, except for noble gases and some light elements, will be irradiated by 14-MeV neutrons and total decay energy produced in the samples will be measured by WEAS. The experimental data will be taken in the three irradiations and measurement scenarios shown in Table 1.

Table 1.

	Irradiation	Cooling
1	5 min	0.5 – 60 min
2	10 hours	0.2 – several hundreds days
3	1 month	1 month – several years

The first experiment has already been conducted in June 1999. Due to the suitable features of WEAS, i.e., the high sensitivity and the capability for high counting rates, all the irradiations will be completed by the end of March 2000. Experimental data for the 5 minutes irradiation will be available by the end of 1999. The experimental data can be utilised for validation of FENDL/A, FENDL/D and other activation and decay data libraries for almost all elements that can be included in low-activation materials for fusion reactors.

Maekawa also reported on the results of another integral experiment that was conducted by using a 19-MeV deuteron and beryllium neutron source available at FZK, Karlsruhe, Germany, under the JAERI-FZK collaboration. Since the white neutron spectrum in the d-Be neutron field is considerably different from the d-t neutron spectrum, activation cross section data for energies other than 14 MeV and up to 20 MeV can be tested. The neutron flux spectrum at the irradiation position was determined by the multi-foil activation method with many dosimetry reactions. Two steel samples, stainless steel 316LN ITER-grade (SS-316LN-IG) and low activation ferrite steel (F82H), were irradiated at the d-Be neutron field. Radioactivities induced in the samples were measured at several cooling times by the HP-Ge detector. Analyses were performed with the ACT4 and FISPACT codes using the FENDL/A-2.0, JENDL Activation File and EAF-4.1 cross section library. As a result, all major radioactivities were predicted adequately while some minor radioactivities indicate necessity of cross section modifications.

It should be noted that above mentioned integral measurements do not test low energy reactions (e.g., neutron capture).

Blokhin reported on the measurements of activity in Vanadium and V-Ti-Cr alloys that are considered as a material for the advanced breeding blanket of ITER. Irradiations were performed in the BR-10 fast reactor. After extracting the specimens form the reactor, activities of isotopes ^{46}Sc, ^{54}Mn, ^{58}Co, ^{60}Co, ^{94}Nb, and ^{182}Ta have been measured for 3 years. The results were compared against calculations performed with the code FISPACT-3.0(5) using FENADL/A-1 sublibrary. The agreement for the V-Ti-Cr alloys was rather poor but performance of the FENDL/A-2.0 sublibrary remains to be tested. It was shown that V, Ti, and Cr do not produce long-lived activities except for ^{46}Sc which is produced in decay of Ti. Major sources of long-lived activities were technological impurities Ni, Nb, W, Re, Co, Fe, Mn, Cu, and Mo.

Filatenkov reported an extensive series of differential measurements performed at Khlopin Institute (St. Petersburg, Russia). 116 reactions and 16 isomeric ratios were measured in the energy range between 13.4 and 14.9 MeV. Experimental errors vary between 1.2 and 30% but in most cases they are better than 5%. The results were compared against FENDL/A-2.0 sublibrary. In 72 cases the new experiments agree with FENDL/A-2.0 within experimental errors. Strong deviations were observed in 10 cases out of which the 5 most serious are listed in the next section (Deficiencies). It was noted that in many discrepant cases ADL-3 library performs better than FENDL/A-2.0.

Manokhin reported on testing FENDL/A-2.0 against recent measurements and empirical systematics. Several examples of inconsistencies were found for threshold reactions (see Section on deficiencies).

Applications

Utilisation of FENDL/A-2.0 in DCHAIN-SP code system for spallation neutronics analyses was presented by **Maekawa** on behalf of H. Takada and K. Kosako. For analysing the decay and build-up characteristics of spallation products, the DCHAIN-SP code has been developed on the basis of the DCHAIN-2 code by revising the decay data and implementing the neutron cross section data. The decay data were newly processed from the data libraries of EAF-3.1, FENDL/D-1 and ENSDF. The neutron cross section data taken from FENDL/A-2.0

sublibrary were also prepared to account for the time evolution of nuclides by the neutron field at the produced position. The DCHAIN-SP code solves the time evolution of decay and build-up of nuclides in every decay chain by the Beteman method. The code can estimate the following physical quantities of produced nuclides: inventory, activity, decay heat by the emission of α, β and γ-ray, and γ-ray energy spectrum, where the nuclide production rate estimated by the nucleon-meson transport code such as NMTC/JAERI is used as an input data.

Cheng presented recent fusion blanket concepts and activation data needs in the United States. There are two main blanket concepts being developed by the U.S. systems study program (ARIES design team). One is a vanadium alloy blanket cooled by liquid lithium. The liquid lithium is also employed as the tritium breeding material. The other is a duel-structure blanket, with reduced activation ferritic steel as the main structural component, which is cooled by helium, and SiC as a containing solid material to handle the high temperature. To further enhance the efficiency and economics, the U.S. fusion technology program is also investigating the feasibility of using liquid metal or salt as the first wall material in the blanket and divertor. The innovation and technical assessment are being carried out in the APEX and ALPS technology programs. A bimetallic alloy consisting of tin and lithium has recently been considered as an attractive candidate liquid wall material due to its low vapor pressure and low melting temperature. The neutronics properties, particularly tritium breeding and activation, however, are a subject of feasibility studies. Activation data are scarce for tin isotopes. Measurements and evaluations of activation cross sections for tin isotopes are needed for the assessment of tin as a fusion blanket material.

Status of evaluation activities

Forrest reported that the European Activation File (EAF) project has been an ongoing process performed through European and world-wide co-operation that has led to the creation of succeeding EAF versions. EAF-4.1 was used in the construction of the FENDL/A-2.0 activation sublibrary. Since then versions EAF-97, EAF-97.1 and EAF-99 have been released. The latest release, EAF-99, has benefited from the results of integral experiments that have been used to adjust data. It contains 12,469 reactions on 766 targets. Many new data sources were used (e.g., JENDL/A-3.2, RDF, IRK, RNAL, LANL(Herman), Mengoni, Shibata, and Kopecky) leading to improvements especially regarding actinide data and capture reactions. An incorrect interpolation low was corrected in 353 reactions (mostly (n,γ)). Extensive comparison with EXFOR database was performed, also using plots for the Reference Neutron Activation Library (Coordinated Research Project carried out by the IAEA) and graphs prepared by D. Muir to test ECNAF-96 library. New systematics formulae for (n,p), (n,α), (n,d), (n,n'p), (n,d+n'p), and (n,t) reactions were used. In total, about 1000 reactions were modified and the pointwise file almost doubled its size (114 Mb). Improved uncertainty data were derived from EXFOR plots and/or integral experiment validation data.

Efforts to improve 1001 capture reactions contained in the EAF-99 library were reported by **Kopecky**. In the 1/v region 442 reactions were tested against experimental data. Only 2 of them differ by factor more than 2 while 32 differ by more than 30%. In the statistical region 39 evaluations were rejected on the basis of visual inspection of excitation functions against EXFOR data and replaced by new calculations with the code NGAMMA.

Next release of the EAF library, foreseen for 2001, will benefit from complete comparison with EXFOR, more integral measurements, new data sources, and will include (n,pα) reactions.

The status of other regional activation libraries was noted.

- ADL-3 updating is not foreseen, however, there is a continuing effort in dosimetry (RRDF) and gas production libraries.
- JENDL-A has not been updated since its release in 1996.
- The US activation library (REAC) has not been updated since FENDL/A-2.0 and no further work is planned.

Status of the Reference Neutron Activation Library (RNAL) developed under NDS co-ordination was reported by **Herman**. The library contains cross section data for 256 neutron-induced reactions important for a wide range of applications. The library has been assembled and the 3rd Draft of the documentation was prepared. It contains description of the library and graphical validation of cross sections against differential experimental data contained in EXFOR. It was noted that this exercise contributed to the checking of data in FENDL/A-2.0. The release of the library is foreseen for the end of 1999.

Zolotarev reported on the current efforts to produce gas production library at IPPE in Obninsk. It was noted that RNAL library benefited from this activity.

Pashchenko drew attention of the participants to the consistency between activation, dosimetry and general purpose sublibraries in FENDL and reported on the recent developments regarding Russian Dosimetry File (RRDF-98). He proposed to substitute data in both FENDL/A-2.0 and FENDL/DS-2.0 with 22 new evaluations from RRDF-98. The IAEA(NDS)-193 report could be used for justification of replacements. **Maekawa** noticed, however, that similar effort has also been completed very recently at JAERI. The new JAERI dosimetry file contains about 50 reactions. Therefore, it was proposed that both files be merged with the current FENDL/DS-2.0 to produce FENDL/DS-2.1 (see Section on updates for further details).

Further developments of activation data libraries were discussed by **Ignatyuk**. He pointed out that there is strong interest in the astrophysical R-process that involves nuclides far from the stability line and, therefore, hardly available for experimental investigation. An extensive use of nuclear modelling for these cases led to certain improvements in level density parameterization and in systematics (especially for (n,α) reactions). These results could be used to produce new generation of more reliable activation data libraries relevant to all applications. To this end **Ignatyuk** called for establishment of a long term (5 to 10 years) international collaboration.

Deficiencies

During the discussion several examples of deficiencies in FENDL/A-2.0, observed in integral and differential measurements, were reported.

Integral Measurements

The existing integral validation has used a 14 MeV spectrum and as a consequence only threshold reactions have been tested. The FNS experiment indicated the following major deficiencies:

- ^{63}Cu(n,α)^{60g}Co is too small (~15%)
- ^{92}Mo(n,2n)^{91g}Mo is too high (20 %)
- ^{58}Ni(n,t) is too high (200 %)

- ^{62}Ni(n,α) is too small (30 %)
- ^{169}Tm(n,2n) is too large

Several other examples were presented for EAF-97, but it remains to be checked if these apply to FENDL/A-2.0.

Differential measurements

Manokhin noted deficiencies in the differential data for following reactions:

- ^{23}Na(n,2n) - lower cross sections are supported by experiments and systematics,
- ^{23}Na(n,np) - shape of excitation function is unphysical,
- ^{42}Ca(n,α) - cross section maximum is shifted considerably towards threshold,
- ^{42}Ca(n,nα) - shape of the excitation function needs to be reanalysed,
- ^{160}Gd(n,2n) - decrease of the excitation function above the (n,3n) threshold seems too steep,
- ^{32}S(n,np) - peak cross section too high compared to systematic.

Filatenkov noted a number of deficiencies when comparing FENDL/A-2.0 with differential neutron measurements between 13 and 15 MeV. The most serious are:

- ^{27}Al(n,2n)^{26}Al - new experimental data obtained in international collaboration headed by IRK should be taken into account.
- ^{63}Cu(n,α)$^{60m+g}$Co **-** the FENDL/A-2.0 evaluation should be increased by about 15%.
- ^{90}Zr(n,α)^{87m}Sr - the FENDL/A-2.0 evaluation should be decreased by about 20%.
- ^{106}Cd(n,np)^{105}Ag and ^{106}Cd(n,2n)^{105}Cd - the sum of cross sections is correct but individual reactions deviate from experimental data by factor of 2.

Miscellaneous

It was noted in EAF-97 that about 350 reactions had incorrect multigroup cross sections due to incorrect interpolation laws in the original evaluations. Similar problems are expected to occur in the FENDL/A-2.0 sublibrary. This will be investigated and corrected if necessary.

Ignatyuk noted a few very serious differences between half-lives in FENDL/D-2.0 and other data sources e.g., Wallet cards. Examples are given in Table.2

Table 2

Isotope	FENDL/D (y)	Wallet cards (y)
^{60}Fe	**$7.515*10^{6}$**	**$1.5*10^{6}$**
^{79}Se	**$6.504*10^{4}$**	**$6.5*10^{5}$**
^{93}Mo	**$3.014*10^{3}$**	**$4.0*10^{3}$**
^{150}Eu	**$3.418*10^{1}$**	**$3.69*10^{1}$**
^{150m}Eu	**$1.441*10^{-3}$**	**$1.5*10^{-3}$**

Updates

Following the presentations there was a discussion of the sources of updates to the FENDL libraries. As discussed above modifications could be made to three libraries: FENDL /A-2.0, FENDL /D-2.0 and FENDL /DS-2.0.

FENDL /DS

It was noted that recently there were new developments in the field of neutron dosimetry. The new dosimetry file RRDF was released in December 1998 by the Obninsk Nuclear Data Center and the new JENDL dosimetry file is being prepared in JAERI. The present neutron dosimetry file in FENDL-2.0 consists of cross sections taken from the IAEA dosimetry file IRDF-90.2. The data in this file are already 10 years old and updating of these data is needed. It is proposed to do this on the basis of the 2 new dosimetry files mentioned above.

For this purpose a comparison of the three files should be performed and candidate cross sections for inclusion in the new FENDL dosimetry file will be analysed by the JAERI and Obninsk NDC.

The new dosimetry file should be internally consistent and give better unfolding results for the benchmark sample problems chosen during the international intercomparison exercise. The data for these sample problems are contained in the IAEA NMF-90 file. The final selection of the cross sections will depend on the results of benchmarking.

The benchmark tests will be co-ordinated at the Khlopin Radium Institute in St. Petersburg by **Kocherov**. The results of benchmarking will be distributed to JAERI, Obninsk NDC and IAEA-NDS for discussion. The final selection should be made by consensus between all parties involved by the end of 2000.

FENDL /D

FENDL/D-2.0 will be compared to EAF_DEC-99 by **Forrest** and a report prepared summarising the differences. Any obvious errors will be corrected, but there will be no attempt to update all nuclides in FENDL/D-2.0.

FENDL /A

It is foreseen that there will be five main sources of updates for FENDL/A-2.0:

1. Replacement reactions in the new FENDL dosimetry file will be considered for inclusion in the FENDL activation file. (~50 reactions)
2. Modifications made to EAF-99 as a result of the various validation exercises (JAERI FNS and results from the three European experiments). (~35 reactions)
3. Experimental measurements made at St Petersburg by Filatenkov will be compared with existing FENDL/A-2.0 data and where ADL-3 evaluations agree with the data this source will be used. (~15 reactions)
4. Manokhin will check FENDL/A-2.0 cross sections for the reactions (n,np) and (n,na) on the light isotopes of medium elements (Ca – Mo) with thresholds below (n,2n) thresholds against systematics. (~20 reactions)
5. New evaluations of ^{106}Cd(n,np) and ^{106}Cd(n,2n) made by Manokhin based on the Filatenkov measurements. (2 reactions)

In total about 100 reactions will be considered as replacements.

The following procedure was agreed for selection of updates of FENDL/A-2.0.

1. The submittor will prepare a plot (in PostScript format) containing the proposed evaluation, the FENDL/A-2.0 data and any experimental data (EXFOR). This will be sent to NDS by March 2000 with a short justification and the evaluation in a pointwise format (EAF or ENDF). If there are any metastable daughter states then the evaluation must be split, not sent as the total.
2. NDS will confirm that the new replacement should be used, or in cases where there are more than one candidate replacement make an initial selection.
3. The list of replacements and the plots will be distributed to the participants of the present meeting in June 2000 for confirmation of proposed changes.
4. NDS will make the final decision on replacements in line with the recommendations of the CM participants. The recommendations must be returned by July 2000. Note that NDS has the responsibility in the case of any conflicts.
5. NDS and the CM participants will attempt to identify an organisation willing to process the replacements.
6. The set of pointwise replacements will be sent to the organisation for processing at the end of September 2000.
7. NDS will make FENDL/A-2.1 available through its web site and CD-ROM by the beginning of 2001.

Actions

1.	Compare RRDF-98, JENDL-Dos and IRDF-90.2 and merge them into IRDF-2000.	Maekawa/Manokhin	March 2000
2.	Transfer candidate replacements for FENDL/A-2.1 together with the justifications to NDS	Forrest, Manokhin, Filatenkov	March 2000
3.	Report on differences between FENDL/D-2.0 and EAF-DEC-99	Forrest	March 2000
4.	Investigate processing effort	Cheng	March 2000
5.	Send justifications and plots for candidate replacements to the Meeting participants for approval	NDS	June 2000
6.	Accept/reject candidate replacements	Participants	July 2000
7.	Send replacements for processing	NDS	Sept 2000
8.	Process replacements for FENDL/A-2.1	to be determined	Nov 2000
9.	Benchmarking of IRDF-2000 (if positive IRDF-2000 will be adopted as FENDL/DS-2.1)	Kocherov	Dec 2000
10.	Assemble FENDL/A-2.1	NDS	Dec 2000
11.	Distribute FENDL-2.1	NDS	Jan 2001

Conclusions and recommendations

The reports presented at the CM meeting gave evidence that many of the reactions tested by the integral experiments were well represented in FENDL/A-2.0. Thus this sublibrary is able to give accurate predictions of activation for many materials.

The same reports also indicated that there are a small number of reactions that could be improved. Some of these will be investigated during the next year and will lead to the improved sublibrary FENDL/A-2.1. Such a maintenance update of FENDL activation sublibrary is necessary to ensure that the sublibrary remains relevant to users.

The role of experimental measurements, both differential and integral, is crucial in validating FENDL and in providing corrections for updates. Work at Khlopin Institute and JAERI-FNS has been especially useful and this should be continued and extended.

Validation of non-threshold reactions is necessary but not easy in existing accelerator based facilities. The use of reactor based facilities should be encouraged like those carried out at BR-10.

It was recommended that the IAEA investigate the possibility of substantially improving the capabilities of the FENDL activation sublibrary by including data at energies greater than 20 MeV for applications other than fusion (e.g., accelerator driven systems). It is noted that major efforts in measurement of neutron-induced cross sections are likely to be carried out in the near future and that such an extended FENDL library would be a natural place to store and distribute such data to all users.

It was noted that consistency between activation, dosimetry and general-purpose libraries is a goal that should be aimed for in the long-term. However, it is recognised that the demands for using the best data in each library means that this goal should have low priority in the near term.

It was noted that the lack of processing capabilities at NDS is a serious obstacle to the successful realisation of FENDL/A-2.1. Although it is possible that processing effort may be found in this case it is recommended that the NDS take steps to ensure adequate in-house expertise in processing in the near future.

Appendix 1

International Atomic Energy Agency

Consultants' Meeting on
Extension and Improvement of the FENDL Activation Library
for Fusion Applications

Obninsk, Russia

22 – 24 June 1999

AGENDA

Tuesday, 22 June

09:00 – 09:30 Opening Session

- Opening addresses
  (Representative of FEI Obninsk; A. Pashchenko, FEI Obninsk;
  M. Herman, IAEA Vienna)
- Election of Chairman
- Adoption of Agenda

09:30 – 12:30 Review of recent testing, validation and application of the FENDL/A-2.0

- *F. Maekawa*: Validation of FENDL/A-2.0 library through the FNS decay heat experiment
- *A. Filatenkov*: Comparison of results of systematic cross section measurement with the FENDL/A-2.0 library
- *F. Maekawa*: Validation of FENDL/A-2.0 library through the FZK d-Be neutron irradiation experiment
- *A. Blokhin*: Benchmark testing of FENDL/A-2.0 cross section data on the basis of BR-10 and SNEG-13 integral measurements with vanadium alloys
- *F. Maekawa*: Utilization of FENDL/A-2.0 library in DCHAIN-SP code system for spallation neutronics analyses
- *R. Forrest*: Fusion Decay Power: Validation of FISPACT and FENDL-2.0

12:30 – 14:00 Lunch Break

14:00 – 18:00 New developments and possible improvements of FENDL/A-2.0

- *A. Ignatyuk*: Future development of activation data libraries
- *R. Forrest*: The evolution of the EAF library following FENDL/A-2.0
- *J. Kopecky*: Improvements of (n,γ) data in EAF-99
- *M. Herman*: Status of the Reference Neutron Activation Library
- *V. Manokhin et al.*: Improvement of the threshold reaction cross sections on the basis of current systematics

- *K.I. Zolotarev*: Evaluation He-production cross section data for ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr, ^{96}Zr and ^{nat}Zr
- *V. Manokhin* and *A. Pashchenko*: Evaluation of the $^{27}Al(n,2n)^{26g}Al$ reaction cross sections

18:00 – 19:30 Welcome drink

<u>Wednesday, 23 June</u>

08:30 – 12:30 New developments and possible improvements of FENDL/A-2.0

- *E. Cheng*: Recent fusion blanket concepts and activation data needs in the U.S.
- *F. Maekawa*: Status of a new activation experiment at FNS for further improvements of FENDL/A-2.0 library
- *A. Pashchenko*: Candidate replacements to improve FENDL-2 Activation Library
- Discussion of procedures for updating FENDL/A library

12:30 – 14:00 Lunch Break

14:00 – 17:00 Discussion of updates

17:00 – 18:00 Review of the Web-access tools for FENDL, documentation, and other dissemination issues

<u>Thursday, 24 June</u>

08:30 – 12:30 Drafting of the meeting report

12:30 – 14:00 Lunch Break

14:00 – 16:00 Drafting of the meeting report (continued)

16:00 – 17:00 Concluding Session

- Adoption of the meeting report
- Final discussion

International Atomic Energy Agency

Consultants' Meeting on

Extension and Improvement of the FENDL Activation Library for Fusion Applications

Obninsk, Russia
22 – 24 June 1999

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Appendix 3

Requirements for new evaluations

Each new evaluation proposed as replacement for FENDL/A-2.1 has to be clearly superior to the one existing in the current version of FENDL/A. This should be demonstrated by the "evaluation kit" consisting of:

1. Short description of the new evaluation (library of origin, evaluation method and nuclear model code used (if any)),
2. Justification for replacement (which way is the candidate evaluation superior to the current one),
3. Comparison plot in PostScript format (candidate evaluation compared against the current one and EXFOR data),
4. File with pointwise evaluated cross sections in EAF or ENDF format (see http://www-nds.iaea.or.at/fendl/fen-activation.htm). If there are any metastable daughter states then the evaluation must be split, not sent as the total.

The "evaluation kit" should be submitted in electronic form. The first three points must fit one A4 page when printed.

Technical input

Readers please note:

These contributions were prepared by the participants before the Meeting. The recommendations regarding FENDL updates contained therein do NOT necessarily agree with the conclusions worked out during the Meeting.

Fusion Decay Power: validation of FISPACT and FENDL/A-2.0

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Abstract

Integral experiments are a rich source of information with which a wide range of validation and comparison exercises can be made in the activation data field. Materials samples have been irradiated in a wide range of simulated D-T neutron fields at three European laboratories and at JAERI FNS. The later experiment is unique because decay heat rather than activity was measured. Some results from that experiment are reported here with some details of data corrections that have been made for EAF-99.

Introduction

Comparison with experimental measurements is essential to validate the calculation method (FISPACT inventory code) and the data libraries. A program of experimental measurements is in progress at three European laboratories. Measurements made at JAERI FNS [1] have generated decay heat results, which are reported here. The results of the different validation exercises, when correlated with other sources of information, led to a set of data corrections which have been implemented on the European Activation File EAF-99 [2].

JAERI FNS

14 MeV neutrons are generated by a 2 mA, 350 keV deuteron beam impinging on a stationary tritium-bearing titanium target. The total neutron flux at the sample location, can be up to 3.0 10^{10} n/cm^{2}s^{-1}. Irradiation times of 5 min and 7 hours were used. Measurements were made on 32 materials.

The decay energy in an irradiated thin sample was measured in the Whole Energy Absorption Spectrometer (WEAS) which comprises two large bismuth-germanate BGO scintillators in a geometric arrangement that provides almost 100% detection efficiency for both β and γ-rays. Using the highly sensitive WEAS method, both β and γ-ray decay energies were measured at selected cooling times as early as one minute after the irradiation ended. The overall experimental uncertainty totals between 6 to 10%.

Calculations

The European Activation System, EASY, has been used to perform the validation exercises. Two cross section data bases have been accessed using the 97 version of the FISPACT code [3]: EAF-97 [4] and FENDL/A-2.0 [5]. The decay data libraries used with the two cross sections libraries are also different: the EAF-97 decay data and the FENDL/D-2.0 data, respectively. In order not to bias the experimental spectral data, the groupwise libraries used in the calculational scheme both correspond to a 175 Vitamin-J groups structure collapsed using a flat micro flux weighting function.

Results

Figure 1 shows the results of the measurements made on copper, compared to predictions made using the EAF-97 and FENDL/A-2.0 libraries. At cooling time > 30 min there is a small under-prediction. The pathway analysis facility in FISPACT allows the likely reaction to be pin-pointed and the ^{63}Cu(n,α)^{60}Co [70.8 d/9.1 h] was investigated further. Figure 2 shows the change that was made to the data during the construction of EAF-99. The reaction to the ground state was increased by 15%; this change was guided both by the EXFOR database and the integral measurements.

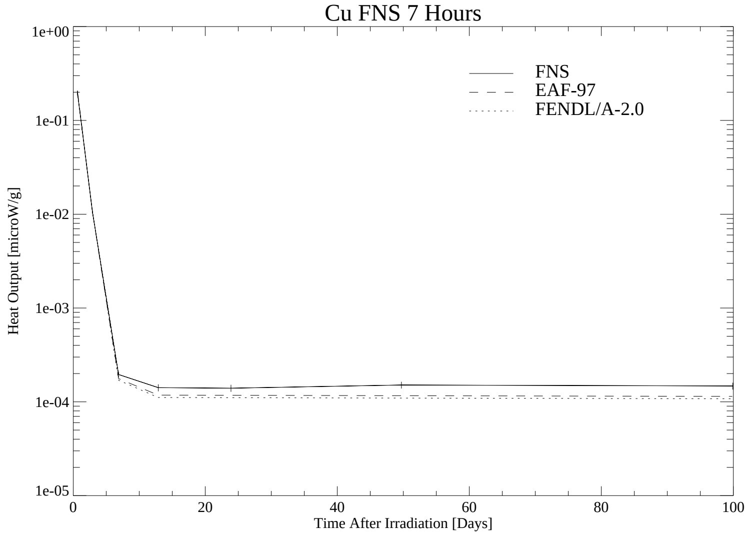

Figure 1 Decay curve for copper compared with EAF-97 and FENDL/A-2.0 predictions.

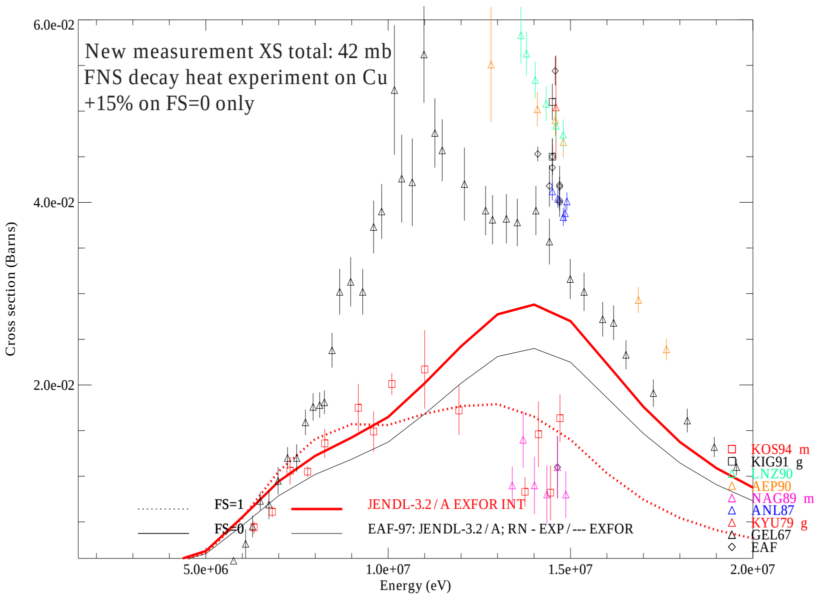

Figure 2 ^{63}Cu(n,α)^{60}Co data from EAF-97 and –99 compared to EXFOR results

Similar comparisons for the other materials were carried out. For the FENDL library about 2/3 of the reactions show good agreement (10-20%) between the predictions and experiment over the time period of 1 min – 3 months.

The ability of FISPACT to predict uncertainties based on the cross section uncertainties meant that these uncertainties could be compared with those found experimentally. In most cases these were similar.

Although this benchmark exercise is very positive, it must be remembered that the spectrum is much harder than found in typical fusion devices. It is therefore not possible to validate the non-threshold reactions, such as capture, that have been found to be important. Thus, in the FNS spectrum ^{64}Cu is produced by: ^{63}Cu(n,γ)^{64}Cu (0.8%) and ^{65}Cu(n,2n)^{64}Cu (99.2%), while in an ITER spectrum it is produced by: ^{63}Cu(n,γ)^{64}Cu (83.8%) and ^{65}Cu(n,2n)^{64}Cu (16.2%).

Conclusions

The calculational method used in the FISPACT inventory code is good. For many materials the cross section and decay data libraries are adequate to predict decay power. The low energy reactions were not tested by this experiment.

Acknowledgements This work was funded by the UK Department of Trade and Industry and Euratom.

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Evolution of the EAF library following FENDL/A-2.0

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Abstract

The European Activation File (EAF) project has been an ongoing process performed through European and worldwide co-operation that has led to the creation of succeeding EAF versions. EAF-4.1 was used in the construction of the FENDL/A-2.0 activation library. Since then versions EAF-97, EAF-97.1 and EAF-99 have been released. The latest release, EAF-99, has benefited from the results of integral experiments that have been used to adjust data. Details of some of the corrections used in the construction of EAF-99, and the library itself are described.

Introduction

The European Activation File (EAF) is the collection of nuclear data that is required to carry out inventory calculations of materials that have been activated following exposure to neutrons. One of the components of EAF is the collection of neutron-induced cross section data. EAF-4.1 was used in the production of the FENDL/A-2.0 activation library. Since that time, three successive further, and improved, releases have appeared EAF-97, EAF-97.1 and EAF-99. Summary details of the three libraries are presented. The current release, EAF-99, has benefited from the results of several integral experiments that enabled libraries to be validated and data corrections to be made. Some of the data corrections are described.

EAF-97

EAF-97 [1] was released in the summer of 1997. It contained data for 12,469 reactions on 766 targets. Special emphasis was put on improving the actinide and capture data. Many new data sources e.g., JENDL/A-3.2, were used and in total about 1000 reactions were improved. The pointwise file almost doubled in size to 114 MB.

EAF-97.1

A problem was noted when the EAF-97 pointwise and groupwise files were plotted and compared. In regions where there are limited data a difference was noted due to the use of an incorrect interpolation law when the groupwise file was produced. Corrections were made to 353 channels (mostly (n,γ)). This revised file [2] was released in January 1998.

EAF-99

The European Activation System (EASY) is a complete package for the calculation of activation. It was developed for fusion applications but is more general. It comprises the FISPACT code, the software tools, the neutron induced cross sections [3] and other data libraries. It is fully documented and validated.

The EAF-99 neutron induced cross section file contains data on 12,468 reactions on 766 targets and about 750 of these have been significantly modified since the previous version. The main improvements are due to:

- Extensive comparison with EXFOR database
- Results of integral experiments which have been used to adjust the data
- Selection of new evaluations: RDF, IRK, HEPRL, RNAL, LANL and Mengoni, Shibata, Kopecky
- New systematics formulae for (n,p), (n,α), (n,d) (n,n'p), (n,d+n'p), and (n,h)
- Corrected *Q*-values formula using the Audi-Wasptra mass excess table and the Duflo-Zuker empirical mass formula
- Improved uncertainty data: derived from EXFOR plots and/or integral experiment validation results
- Resonance integral validation

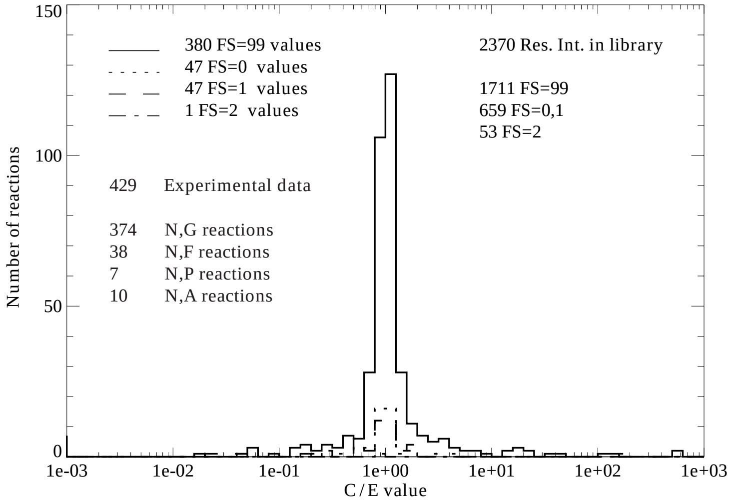

Figure 3 C/E distribution of resonance integrals for EAF-99

During the creation of the library several checks were made to monitor the quality of the data. As an example, Figure 1 shows the comparison between resonance integral values from the library and the experimental database. It can be seen that for the majority of reactions where there is experimental data there is good agreement with the measurements. Similar comparisons have been made with the reactions at 0.0253 eV, 30 keV and 14.5 MeV. Comparisons have been made with integral experiments made at three European laboratories and JAERI. These comparisons have allowed about 130 reactions to be validated and about 30 to be improved. Figure 2 shows one example of a change from EAF-97 due to experimental results. The JAERI decay heat results indicated an underprediction, and this was confirmed by the EXFOR data. EAF-99 was modified to use a new data source (ADL-3) that solves both problems. Full details of the validation exercise are available [4].

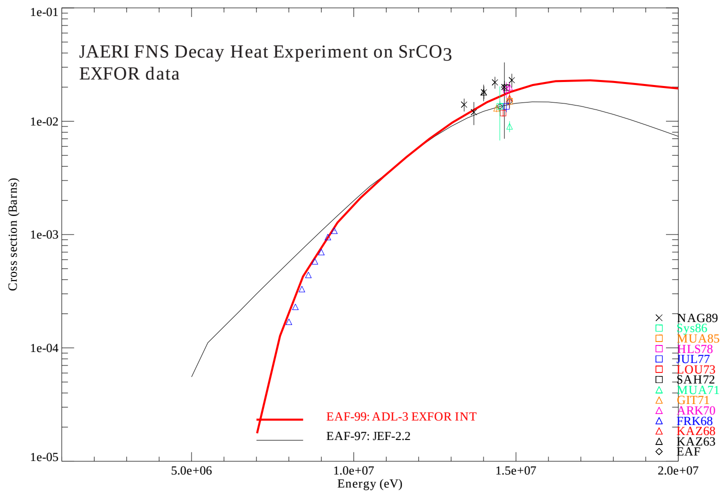

Figure 4 ^{88}Sr(n,p)^{88}Rb data from EAF-97 and EAF-99 compared with experimental data from EXFOR.

The future

A new EAF version is planned for the beginning of 2001. This will complete the comparison with EXFOR and new ongoing experiments.

Acknowledgements This work was funded by the UK Department of Trade and Industry and Euratom.

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Improvements of NG Data in EAF-99

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As part of a systematic validation of EAF-99 against the differential data, primarily originating from the EXFOR data base, the capture reaction data have been reviewed. Out of a total of 1001 reactions, 442 reactions can be tested against experimental information, such as the thermal cross sections (1/v region), resonance integrals (resolved resonance region) and against experimental data in the statistical or pre-equilibrium regions (up to 20 MeV). The remaining reactions (with no experimental data) have been tested against several systematics. A number of revisions have been performed. In the statistical region 39 reactions have been rejected and replaced by new calculations with the code NGAMMA. Examples of these replacements will be shown.

Candidate replacements to improve FENDL/A-2.0 activation sublibrary

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The FENDL AGM-97 [1] authorized the release of the FENDL-2.0 Library, with the exception of the general purpose file FENDL/E-2.0 and its processed form. The AGM strongly recommended the IAEA/NDS that following the completion of FENDL/A-2.0 a mechanism be found to maintain and develop the activation library. The AGM recommended that an attempt be made to produce FENDL/A-2.1, which should correct possible errors and make improvements to a small number of reactions, which are of significant impact on fusion relevant applications. The necessity for improvements may arise because of improved measurements, calculations or evaluations.

Consistency

In the discussions during the FENDL AGM-97 regarding future activities, the consistency between the general purpose and the activation sublibraries of FENDL-2.0 was addressed. It was proposed to substitute certain reaction cross sections in the general-purpose library FENDL/E with the high precision results from FENDL/A-2.0 in the future release of the library. However, this should be a long-term task. The consistency between FENDL/DS-2.0 and FENDL/A-2.0 sublibraries should be considered as a first step for improvement of FENDL-2 database.

Dosimetry Library

The FENDL -2.0 Dosimetry Sublibrary is based on IRDF-90 version 2 data provided in multigroup form with 640 energy groups [2]. As demonstrated by H. Wienke at the AGM-97 the data should be available in pointwise form included in the original source to avoid processing histogram representation.

RRDF-98

The 1998 version of the Russian Reactor Dosimetry File (RRDF-98) contains original evaluations of cross sections performed at the Institute of Physics and Power Engineering (Obninsk) for 22 neutron induced dosimetry reactions [3]. The list of reactions contained in RRDF-98 is given in Table 1. The majority of evaluations included in previous versions of the Russian Reactor Dosimetry File (BOSPOR-80, RRDF-94 and RRDF-96 that were issued in 1980, 1994 and 1996 respectively) have been superseded by new evaluations.

The evaluations of excitation functions were performed on the basis of statistical analysis of corrected experimental data in the framework of generalized least squares method [4] taking into account the results of combined optical and statistical model calculations (codes STAPRE and GNASH). The experimental cross section data, including the most recent results, were critically reviewed and processed in this study. If necessary, the data were renormalised in order to adjust to the relevant cross section standards and decay data. In order to improve the accuracy and consistency of the experimental data, an update of the 1991 NEANDC/INDC Nuclear Standards Data File [5] was adopted for correction of measured values.

Table 1. RRDF-98. List of reactions

Isotope/Reaction	MAT	Threshold energy (MeV)	Authors	Date
$^{12}C(n,2n)^{11}C$	613	20.4095	K.I.Zolotarev, A.B.Pashchenko, M.V.Scripova	September 1998
$^{16}O(n,2n)^{15}O$	813	16.6481	K.I.Zolotarev, A.B.Pashchenko, M.V.Scripova	May 1998
$^{19}F(n,2n)^{18}F$	912	10.985	K.I.Zolotarev, A.B.Pashchenko	December 1993
$^{24}Mg(n,p)^{24}Na$	1225	4.9311	S.Badikov, K.I.Zolotarev	August 1994
$^{46}Ti(n,2n)^{45}Ti$	2212	13.4802	K.I.Zolotarev, S.Badikov, A.B.Pashchenko	January 1994
$^{46}Ti(n,p)^{46}Sc$	2212	1.6197	K.I.Zolotarev, S.Badikov, A.B.Pashchenko	January 1994
$^{47}Ti(n,x)^{46}Sc$	2222	9.0709	K.I.Zolotarev, A.B.Pashchenko,	October 1995
$^{48}Ti(n,p)^{48}Sc$	2232	3.2756	K.I.Zolotarev, A.B.Pashchenko	December 1993
$^{48}Ti(n,x)^{47}Sc$	2232	9.41396	K.I.Zolotarev, A.B.Pashchenko,	December 1993
$^{49}Ti(n,x)^{48}Sc$	2242	8.3077	K.I.Zolotarev, A.B.Pashchenko	November 1993
$^{51}V(n,\alpha)^{48}Sc$	2323	11.2688	K.I.Zolotarev, V.N.Manokhin, A.B.Pashchenko	November 1997
$^{54}Fe(n,2n)^{53m+g}Fe$	2613	13.6302	K.I.Zolotarev, A.B.Pashchenko, M.V.Scripova	August 1998
$^{54}Fe(n,\alpha)^{51}Cr$	2611	10^{-11}	K.I.Zolotarev	June 1996
$^{56}Fe(n,p)^{56}Mn$	2622	2.9709	K.I.Zolotarev	November 1992
$^{59}Co(n,\alpha)^{56}Mn$	2712	10^{-11}	K.I.Zolotarev	December 1997
$^{63}Cu(n,\alpha)^{60}Co$	2911	10^{-11}	K.I.Zolotarev	March 1997
$^{75}As(n,2n)^{74}As$	3312	10.3779	K.I.Zolotarev, V.N.Manokhin, A.B.Pashchenko	September 1994
$^{93}Nb(n,n')^{93m}Nb$	4112	0.03073	K.I.Zolotarev, S.Badikov	August 1996
$^{93}Nb(n,2n)^{92m}Nb$	4112	9.0523	K.I.Zolotarev, S.Badikov	August 1996
$^{103}Rh(n,n')^{103m}Rh$	4525	0.04	S.Badikov	August 1996
$^{115}In(n,n')^{115m}In$	4931	0.32	S.Badikov	August 1996
$^{141}Pr(n,2n)^{140}Pr$	5912	9.4607	K.I.Zolotarev, A.B.Pashchenko, M.V.Scripova	January 1994

Proposed replacements.

1. RRDF-98 - considering the progress which have been achieved in the development of the RRDF-98, and in view of the need for a single consistent data library, it is proposed to substitute 22 reaction cross sections in both FENDL/A-2.0 and FENDL/DS-2.0 sublibraries with the high precision RRDF-98 evaluations. These new evaluations met all requirements mentioned above for being considered as replacements. Pointwise data have been submitted to the IAEA/NDS together with the plots of new data compared to existing evaluations and available experimental data. The IAEA-NDS-193 report may serve as justification for replacements.
2. Evaluations proposed by Manokhin.
3. Zolotarev's evaluations for $^{90,91,92,94,96}Zr$ isotopes.

Benchmarks

Within the scope of integral checking and validation of FENDL/A sublibrary the IAEA experts, already during the FENDL AGM-91 [6], recognized that a compilation of a set of representative neutron spectra for activation purpose might be useful. This set would represent the blanket or power plant concepts that are being under consideration. As discussed with E. Cheng, such an exercise should collect contributions from ITER project as well as from EU, Russian, Japanese and US concepts. Such a recommendation could be formulated by the present Meeting, as representatives from all the above mentioned projects/countries will be present. The compilation of benchmarks should be updated continuously.

References.

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About improvement of some excitation functions from FENDL-2/A library

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Comparison of FENDL/A-2.0 against new measurements and empirical systematics shows that some excitation functions need reevaluation or corrections. In this report such examples regarding several excitation functions for threshold reactions are discussed.

^{23}Na(n,2n) and ^{23}Na(n,np)

The experimental data fall into two very discrepant groups. The ADL-3 evaluated excitation function, based on the higher group of data, was selected for FENDL/A-2.0. However, most of the differential and integral measurements as well as systematic trends support low group of data.

The ^{23}Na(n,np) reaction excitation function included in FENDL/A-2.0 was taken from EFF-2 that coincides with JENDL-3.2. The shape of this excitation function looks unphysical. There is a steep decrease of the cross section only 4-5 MeV above the threshold that is hard to understand. Therefore, the evaluation should be reanalysed.

It should be noted that, in general, the evaluated data for (n,np) and (n,nα) reactions are very discrepant and unreliable.

^{42}Ca(n,α) and ^{42}Ca(n,nα)

The ADL-3 evaluation was adopted for FENDL/A-2.0. The shape of the curve seems to be wrong. The position of the peak is shifted towards the threshold by 3 MeV as compared to the excitation functions for the same reactions on ^{44}Ca. The latter shapes are determined on the basis of experimental data and are more reliable. Both isotopes have a close difference of $Q_{nn\alpha}$ and $Q_{n\alpha}$ values and therefore approximately the same peak positions relative to the (n,α) reaction thresholds are expected. Taking into account the difference of 3 MeV in the (n,α) reaction thresholds for these two isotopes one would expect that the position of the ^{42}Ca(n,α) reaction reaches its maxiumum at 13 MeV instead of 11 MeV as in FENDL/A-2.0 evaluation.

The excitation function of the ^{42}Ca(n,nα) reaction, taken from JENDL-3.1, is unexplainable. The additional analysis is needed to understand the shape of the excitation function.

^{160}Gd(n,2n)

The JENDL-3.2 evaluation was selected for FENDL/A-2.0. It decreases sharply in the energy region above the maximum of the excitation function that indicates overestimation of the (n,3n) cross section. This feature is typical for JENDL-3.2 general-purpose file. In general, FENDL/A-2.0 contains improved excitation functions taken from JENDL-3.2/A, which are close to ADL-3 or agree with systematics. However, in some cases, including this one, data were taken from the general purpose JENDL-3.2 file and should be corrected.

^{32}S(n,np)

The adopted ADL-3 evaluation contradicts the systematics. The absolute value in the maximum of the excitation function seems to be too high by at least 100 mb.

One should note that there are difficulties in description of (n,np) reactions, especially when $Q_{nnp} < Q_{n2n}$.

Conclusions

Several examples show that FENDL/A-2.0 needs improvements. Obviously, some excitation functions must be reevaluated or corrected. The main problem is to determine how many reactions need to be improved. To this end, systematics and selected calculations can be used.

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