International Atomic Energy Agency

INDC(NDS)-395
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INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

VALIDATION AND IMPROVEMENT OF THE FENDL-2.0 TRANSPORT SUBLIBRARIES

Report on an IAEA Consultants' Meeting

IAEA Headquarters, Vienna, Austria

12 – 14 October 1998

Prepared by

M. Herman

IAEA Nuclear Data Section
Vienna, Austria

March 1999

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

The present report is a summary of the Consultants' Meeting on the transport sublibrary of the Fusion Evaluated Data Library version 2.0. It contains results of recent validations and benchmark experiments, reports on sublibrary status and improvements, and defines procedures and requirements for further updates.

March 1999

TABLE OF CONTENTS

I. 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 co-ordinator 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. The general purpose sublibraries (known also as transport sublibraries) were released on 15 May 1998, both as basic evaluated data and in processed form.

II. OBJECTIVES

The objectives of the present Meeting were:

- review recent testing and validation of the FENDL-2.0 sublibraries /E, /MC, and /MG,
- consider inclusion of the new experimental benchmarks,
- discuss and establish procedures for updating/revisions of the current evaluations,
- identify needs for library improvements and extensions,
- review Web-access tools for FENDL-2.0 and other dissemination issues.

III. ORGANIZATION AND ATTENDANCE

The Meeting was held in the IAEA Headquarters in Vienna from 12 to 14 October 1998. It was attended by five internationally recognized experts from five countries and three staff members of the NDS (see Appendix 5).

IV. PROCEEDING AND RESULTS

The Meeting was opened by D.W. Muir, Head of the Nuclear Data Section. He stated that 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.

U. Fischer (Forschungszentrum Karlsruhe) was elected as Chairman and the Agenda of the Meeting (see Appendix 4) was adopted.

Following the main aim of the Meeting, the discussion concentrated on the results of integral benchmark experiments and their comparison with the predictions of various calculations using FENDL-2.0 and other nuclear data libraries. Particular attention was paid to the validation of the ^{56}Fe evaluation. F. Maekawa and J. White reported on the problems which were encountered in application of the processed sublibraries. The status of the FENDL-2.0 transport sublibraries was presented by M. Herman. Finally, the procedure for acceptance of new evaluations in further releases of the FENDL library was discussed and agreed. The conclusions of the Meeting are reported below. More details can be found in the individual contributions presented during the Meeting, included in this report as attachments.

V. STATUS OF THE FENDL-2.0 TRANSPORT SUBLIBRARIES

Following recommendations of the last FENDL meeting in March 97 evaluations for ^{3}He, ^{4}He, ^{197}Au (ENDF/B-VI), and Ti (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 which revealed a number of minor deficiencies. Typical problems included:

- energies out of order
- width deviates too much from the average (typical for light nuclei)
- E_{pmax} incorrect
- distribution negative (but negligible $2*10^{-4}$)
- average energy exceeds available energy
- different energy ranges for different isotopes in natural material evaluations
- abundance of an isotope inconsistent
- Q-value for an isotope inconsistent
- normalization different from 1.0
- improper mass.

The authors were asked to correct the evaluations and most of these inconsistencies were removed. The remaining ones are deemed to have no impact on practical calculations. This rectification 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), 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 γ's, contrary to the version present in the EFF-3.0.

There are two recommendations of the FENDL AGM in March 97 which are still 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. Participants of the Meeting reviewed and approved contents of the new WWW-site.

FENDL-2.0 can still be downloaded through the classical ftp protocol from the NDS ftp-server: iaeand.iaea.or.at (username: FENDL2), or obtained on the CD-ROM. Users interested in the latter option should send a request for IAEA-NDS-CD-06 to the NDS.

Following the discussion on FENDL-2.0 deficiencies (see section VII) the participants of the present meeting decided to correct obvious errors in the basic and derived files for ^{29}Si and ^{56}Fe. After the replacement of the erroneous files the FENDL-2.0 library has been frozen and should be 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).

VI. VALIDATION AND BENCHMARKING

Comprehensive benchmarking of FENDL-2.0 candidate evaluations has been reported previously (Ref., e.g., Karlsruhe Meeting '96). The most remarkable achievement of 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-2.0 sub-libraries 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).

The results of the above benchmarking were reported during the meeting and are summarized in the attachments. 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, recommends to perform additional benchmark analyses. Reference can be made to the experiments compiled in the SINBAD data base which should serve as primary source of benchmark data in the future, substituting the collection of benchmarks in the FENDL-2.0 library. This substitution is justified by the fact that SINBAD data base is constantly maintained, better documented, and already contains most of the benchmarks collected in FENDL-2.0.

Recognizing the lack of integral data for some important materials like Sn, Nb, Al, Si, Ti and Zr, integral experiments on these materials are strongly recommended by the CM.

Five participants 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.

VII. 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 during the meeting:

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 FENDL-2.0 version of January 14, 1999.

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 which do not follow agreed uniform specifications.

5. The smallest σ_0 value for Cu data in FENDL/MG-2.0 is 10. Since the pure copper would be used in a fusion reactor, σ_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 σ_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 the 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 the materials, while three numbers (00c, 07c, and 40c) are used in FENDL/MC-2.0. A unique *nnc* number would make the library more user-friendly.

   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.

VIII. FURTHER UPDATES AND IMPROVEMENTS OF THE FENDL-2.0 LIBRARY

Due to limited financial support, which does not allow for further Advisory Group Meetings, the Consultants' Meeting proposes the following formal procedure 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). The proposed evaluation should fulfill requirements listed in Appendix 1.

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 (see Appendix 3),
   - a review kit for the new evaluations or an updated one for revised evaluations. The review kit should follow the specifications given in the Appendix 2.

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 to the Meeting 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.

IX. CONCLUSIONS AND RECOMMENDATIONS

FENDL-2.0 has been extensively benchmarked and frozen. The Consultants' Meeting has concluded that it is currently the best available and validated nuclear data library for fusion applications. Therefore, it should be adopted as reference library in fusion reactor design calculations and related applications.

The procedure for inclusion of new evaluations in future updates of FENDL has been recommended. To be accepted new evaluations must prove to be superior to the ones contained in FENDL-2.0.

New integral experiments are recommended for important materials like Sn, Nb, Al, Si, Ti and Zr.

Appendix 1

Requirements for new evaluations

A candidate evaluation must fulfill the following requirements to be considered for inclusion in the next release of the FENDL library:

- Gamma-ray production included;
- Neutron and charged-particle emission in File 6 format;
- File 1 descriptive information included;
- Recoil distributions in File 6 format for major structural materials;
- Energy balance better than 2% at all energies.

The following additional features are desirable:

- Simplified File 6 recoil distributions for less important materials;
- Uncertainty information;
- Use of Standard Reference Data such as IRDF-90.2 or IRDL for MF=3.

It is recommended that isotopic evaluations for a given material be replaced only if the combination of isotopic evaluations is shown to be consistent with the experimental data for the natural material.

Appendix 2

Comparison plots for candidate evaluations

The following plots, comparing candidate evaluation with the respective one contained in FENDL-2.0, and with available experimental data, should be provided:

1. Comparison of File 3 – cross section data, including pointwise reconstruction of resonance region.

2. Comparison of File 4 – first 3 Legendre coefficients a1, a2, a3. If significant differences occur between evaluations, then comparisons should be made between evaluated angular distributions and experimental data.

3. Comparison of energy distributions for neutrons, charged particles, and recoils at 8, 11 and 14.1 MeV.

4. Comparison of neutron spectra with Vonach evaluation if possible, otherwise with angle-integrated data of Takahashi.

5. Comparison of charged-particle spectra with Grimes and Haight data at 14.1 MeV (if possible).

6. γ-ray production spectra at incident neutron energies of 8, 11 and 14.1 MeV.

7. Integrated γ-ray production cross sections as a function of neutron energy.

8. Comparison of capture γ-ray spectra at thermal neutron energy (as a minimum).

9. If uncertainty files are present, compare the variances as function of neutron energy for MF-33.

Appendix 3

Specifications for processing

The FENDL/E-2.0 sublibrary should be processed into the multigroup sublibrary /MG using the following specifications:

- Neutron groups: 175, in Vitamin-J structure
- Gamma groups: 42, in Vitamin-J structure
- Neutron weight function: VITAMIN-E (IWT=11 in NJOY)
- Gamma weight function: 1/E with roll-offs (IWT=3 in NJOY)
- Legendre order for neutrons and photons: P-6 for transport calculations correction to P-5
- Temperatures: 300 Kelvin
- Dilution factors: 10^{10}, 10^5, 10^4, 10^3, 300, 100, 30, 10, 3, 1, 0.3, 0.1, 0.001 (in barns), not more than 10 out of this list
- Reconstruction, linearization and thinning tolerances used in RECONR: 0.2%
- Reactions included:
    - all reactions contained in the evaluations
    - energy balance heating (MT=301)
    - kinematic heating (MT=443)
    - damage (MT=444)
    - gas production
    - no thermal data.

The specifications to be used in processing the FENDL/E sublibrary with NJOY/ACER module into the ACE (ASCII) format, intended for use in the Monte-Carlo code MCNP, are the following:

- Temperature: 300 Kelvin = 2.585E-8 MeV
- No thinning
- Reactions included:
    - all reactions contained in the evaluation
    - kinematic heating (MT = 443)
    - damage (MT = 444)
    - gas production.

NJOY 97.62 or higher should be used for processing.

Appendix 4

Consultants' Meeting on
Validation and Improvement of the FENDL-2.0 Library
Vienna, Austria, 12-14 October 1998

Agenda

Monday, 12 October

09:00 - 09:30 Opening Session

- Opening address

  D.W. Muir, Head, IAEA Nuclear Data Section

  M. Herman, IAEA Nuclear Data Section

- Election of Chairman
- Adoption of Agenda

09:30 - 12:30 Validation of the FENDL-2.0 transport sublibraries

(Part I: general)

- *F. Maekawa*: New benchmark experiments in Japan
- *P. Batistoni*: Analysis of fast neutron flux measurements in the streaming experiment at FNG, using FENDL-1/-2.0 and EFF-2/-3 libraries
- *H. Wienke*: Benchmark analyses at the OKTAVIAN measurements of neutron and gamma leakage spectra from Al and Si spherical shells
- *F. Maekawa*: Present status of JENDL evaluation
- *P. Batistoni*: Analysis of nuclear heating measurements in the streaming experiment at FNG, using FENDL-1/-2.0 and EFF-2/-3 libraries
- *U. Fischer*: Benchmark analyses for EFF-1, -3 and FENDL-1, -2 beryllium data

12:30 - 14:00 Lunch Break

14:00 - 18:00 Validation of the FENDL-2.0 transport sublibraries (Part II: 56-Fe)

- *U. Fischer*: Benchmark analyses for EFF-3.0, -3.1 and FENDL-1, -2 iron data
- *H. Wienke*: Benchmark analysis at the FNS-TOF iron slab experiment
- *U. Fischer*: Benchmark analyses for the ITER bulk shield experiment with EFF-3.0, -3.1 and FENDL-1, -2 nuclear cross-section data
- *A. Trkov*: Current status of the EFF-3.1 evaluation for iron-56 and some benchmark results
- *U. Fischer*: Benchmark analyses for the ITER streaming experiment with FENDL-1 and -2 nuclear cross-section data

- *F. Maekawa*: Analysis of FNS iron benchmark experiments
- *U. Fischer*: Monte Carlo uncertainty analysis for an iron shielding benchmark experiment

Tuesday, 13 October

08:30 - 12:30 Updates and Improvements

- *J. White*: Recent RSICC experiences with FENDL-2.0 processed multigroup data
- *F. Maekawa*: Bugs, inconsistencies and possible improvements of FENDL-2 library
- *H. Wienke*: Presentation of the improved evaluation for 15-N by A. Blokhin
- *M. Herman*: Status of the FENDL-2.0/E -/MG, and -/MC sublibaries
- Adoption of updates and improvements for FENDL-2.1 release
- Discussion of procedures for further updating and revising of the FENDL library

12:30 - 14:00 Lunch Break

14:00 - 17:00 Review of the Web-access tools for FENDL, documentation, and other dissemination issues

17:00 - 18:00 Discussion on the needs for further experiments for data validation

19:00 Dinner

Wednesday, 14 October

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

12:30 - 14:00 Lunch Break

14:00 - 17:00 Concluding Session

- Adoption of the meeting report
- Final discussion

Appendix 5

IAEA Consultants' Meeting on the

Extension and Improvement of the FENDL Library for Fusion Applications

12 - 14 October 1998
IAEA Headquarters, Vienna

LIST OF PARTICIPANTS

GERMANY
U. Fischer (Chairman)
Institut für Neutronenphysik und Reaktortechnik
Forschungszentrum Karlsruhe
Postfach 3640
D-76021 Karlsruhe
Tel.: +49 7247-82-2437
Fax: +49 7247-82-3824
E-mail: ulrich.fischer@inr.fzk.de

ITALY
P. Batistoni
Dipartimento Fusione
Divisione Neutronica
Centro Ricerche Energia Frascati
Via E. Fermi 27
I-00044 Frascati
Tel.: +39 6-9400-5739
Fax: +39 6-9400-5314
E-mail: batistoni@frascati.enea.it

JAPAN
F. Maekawa
Intense Neutron Source Laboratory
Japan Atomic Energy Research Institute
Tokai-mura, Nakagun
Ibaraki-ken 319-1195
Tel.: +81 29-282-6075
Fax: +81 29-282-5709
E-mail: fujio@fnshp.tokai.jaeri.go.jp

SLOVENIA
A. Trkov
Institute 'Jozef Stefan'
Jamova 39, 1000 Ljubljana
Tel.: +386 61-1885-324 (direct)
Fax: +386 61-1612-335
E-mail: andrej.trkov@ijs.si

UNITED STATES OF AMERICA
J. E. White
Radiation Safety Information Computational Center (RSICC)
P.O. Box 2008, MS-6362
Oak Ridge National Laboratory
Oak Ridge, TN 37831
Tel.: +1 423-574-6176
Fax: +1 423-574-6182
E-mail: jew@ornl.gov

I.A.E.A.
M. Herman (Scientific Secretary)
IAEA Nuclear Data Section
P.O. Box 100
Wagramerstrasse 5
A-1400 Vienna, Austria
Tel.: +43 1-2600-21713
Fax: +43 1-26007
E-mail: herman@iaeand.iaea.or.at

H. Wienke
IAEA Nuclear Data Section
P.O. Box 100
Wagramerstrasse 5
A-1400 Vienna, Austria
Tel.: +43 1-2600-21714
Fax: +43 1-26007
E-mail: wienke@iaeand.iaea.or.at

V. Proniaev
IAEA Nuclear Data Section
P.O. Box 100
Wagramerstrasse 5
A-1400 Vienna, Austria
Tel.: +43 1-2600-21717
Fax: +43 1-26007
E-mail: v.pronyaev@iaea.org

Appendix 6

Extended abstracts of technical papers

New benchmark experiments in Japan

F. Maekawa

Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun Ibaraki-ken 319-1195, Japan

Status of the experiments

Until 1995 a large number of fusion neutronics benchmark experiments had been performed in Japan.

1. FNS/JAERI TOF experiments on Li_2O, Be, C, N, O, Fe and Pb
2. FNS/JAERI In-situ experiments on Li_2O, Be, C, Fe, SS316, Cu and W
3. OKTAVIAN/Osaka Univ. Pulsed sphere experiments on Li, CF_2, LiF, Al, Si, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zr, Nb, Mo, W and Pb

Since 1996, we have started at the FNS facility in JAERI a new series of benchmark experiments for advanced fusion reactor materials (i.e., low activation structural materials and advanced breeding blanket materials). Present status of those experiments is as follows.

The clean benchmark experiment has the following unique features: (i) neutron spectra in the entire energy range from 15 MeV to thermal energy are measured inside of the experimental assemblies along with several dosimetry reaction rates, (ii) γ-ray spectra and γ-ray heating rates are also measured. The FNS-TOF experiment provides high energy resolution and angle-dependent neutron spectra leaking from several slab assemblies of different thicknesses and materials. Most of the experiments are scheduled to be completed by the end of 1999, and expected to contribute to further improvements of the FENDL library.

We have also completed a series of streaming experiments for ITER/EDA. Experimental assemblies made of iron with various types of gaps and ducts were used. Although the experiments are a kind of mock-up experiments rather than benchmark experiments, information useful for the validation of iron cross section can be extracted from the results. Especially, we can investigate deeply penetrating neuron fluxes through the iron shield assembly of 1.2 m in thickness.

Detailed results on vanadium

Using experimental results for the pure-vanadium and vanadium-alloy assemblies, validity of cross section data for vanadium in FENDL/E-2.0 (JENDL Fusion File), FENDL/E-1 (ENDF/B-VI) and EFF-3 was investigated with the MCNP code.

Neutron fluxes above 20 keV calculated with the three evaluations agree within 20% with the experimental data. However, there are some differences among the three calculations. They can be explained by the following facts: (i) the DDX data of FENDL-2.0 agree best with the experimental DDX. The DDX data in FENDL-1 are given as isotropic. (ii) total discrete cross sections for the inelastic scattering to the first discrete level in FENDL-1 and EFF-3 (3.8 mb at 15 MeV) are too small. (iii) fine resonance structure in the total cross section in the few MeV range is not included the FENDL-2.0, also total cross section data by Garg, et al. adopted for FENDL-2.0 should be replaced by those of Rohr et al. (as adopted in FENDL-1 and EFF-3 in the energy range above 100 keV).

The FENDL-1 and EFF-3 calculations predict well neutron flux below 1 keV while FENDL-2.0 calculations fall short in the low energy region. This can be attributed to the too small total cross section at ~2 keV in FENDL-2.0.

γ-ray spectra and heating rates calculated with FENDL-2.0 agree very well with the experimental data. γ-ray production cross section in FENDL-1 seems to be slightly larger, and discrete γ-ray peaks are not reproduced clearly. γ-ray production cross section in EFF-3 is too large.

Total cross section of vanadium in JENDL Fusion File is now under revision, and the revised data will be incorporated into JENDL-3.3. The vanadium data in JENDL-3.3 will be a candidate for the replacement of vanadium data in FENDL/E-2.0.

Low activation structural materials	Clean Benchmark	TOF
Pure vanadium	October 1996	June 1997
Vanadium alloy	April 1997	June 1997
SiC	in 1999	in 1999
Advanced breeding blanket materials		
Li2ZrO3	September 1997	December 1997
Li2TiO3	October 1998	December 1997
LiAlO2	in 1999	December 1998

Analysis of fast neutron flux measurements in the streaming experiment at FNG, using FENDL-1/-2.0 and EFF-2/-3 libraries

Paola Batistoni

Associazione Euratom-ENEA sulla Fusione, C. R. Frascati,
I-00044 Frascati (Rome), Italy

Introduction

Nuclear performance of the ITER shield blanket has been validated in recent neutronics experiments undertaken within the EDA R&D activities. The most remarkable achievement of 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.

However, in ITER the shielding efficiency is deteriorated by ***voids and penetrations*** with direct view to the plasma. The experimental validation of the capability of available codes and nuclear data to calculate correctly the effect of neutron streaming paths of various shapes, was considered indispensable for the confirmation of design safety margins. For this purpose, a ***Neutron Streaming Experiment***, has been performed at the Frascati Neutron Generator FNG that aims at validating the shielding efficiency of the mechanically bolted ITER blanket modules by taking into account the neutron streaming through the open channel (diam=3 cm).

Measurements and analysis

Neutron reaction rates by activation foils have been measured in the channel, in the cavity, and in the bulk shield behind the cavity up to the superconducting magnet (the shield module mock-up is shown in Fig.1). The ^{93}Nb(n,2n)^{92}Nb, ^{27}Al(n,α)^{24}Na and ^{58}Ni(n,p)^{58}Co reactions (effective energy thresholds are 10.8, 8.5 and 2.9 MeV respectively) were chosen to measure the integrated fast neutron flux (E>≈3 MeV) and its gradient along the void structure and behind it. The ^{197}Au(n,γ) was used to measure the thermal flux. All measurements were performed with the neutron source in front of the channel, at 5.3 cm distance from the block surface (IN-AXIS set-up). The measurements in the channel and in the cavity were performed also with the neutron source shifted laterally by 5.3 cm with respect to the channel axis to simulate the effect of the extended neutron source from the plasma (OFF-AXIS set-up).

The experimental results were analyzed by using the Monte Carlo code MCNP (versions A and B) using FENDL-1 (IAEA), FENDL-2.0 (IAEA), EFF-3.0 (distributed by ECN for FENDL benchmark), and EFF-3. All dosimetric reactions were taken from IRDF-90.

<u>*Measurements along the mock-up axis - IN-AXIS set-up:*</u>

- C/E values obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 and also with EFF-3.0/3.1 within the associated uncertainties in the calculations.

- In the case of very high threshold reactions, $^{93}Nb(n,2n)$ and $^{27}Al(n,\alpha)$, C/E values are very close to unity in the first position, within the total uncertainties, showing that the source and experiment modeling in the calculation is correct. Then, underestimation is found with increasing depth, also in the void channel, but especially in the bulk shield behind the cavity.
- In all cases, the results are similar to those obtained in the Bulk Shield Experiment.

Measurements in the cavity - IN-AXIS set-up

- A rather good agreement is found between calculations and measurements, generally within the total uncertainty, for all reactions and in all foil positions inside the void cavity.
- Again, C/E values obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 and also with EFF-3.0/3.1 within the associated uncertainties.

Measurements in the channel and in the cavity - OFF-AXIS set-up

- Along the open channel and inside the void cavity, the results show that there is a good agreement between the calculations and the measurements, generally within the total uncertainty for $^{93}Nb(n,2n)$ and $^{58}Ni(n,p)$ reactions in all foil positions.
- A slight underestimation of about 10% is observed for $^{27}Al(n,\alpha)$.
- Again, C/E values obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 and also with EFF-3.0/3.1 within the associated uncertainties.

Conclusions

The results of the analysis of activation foil measurements in the void structure allow to draw the following conclusions:

1. the fast neutron flux (E > 3 MeV) is calculated by MCNP-4A/B with FENDL-1/2.0 and with EFF-3.0/3.1 within an uncertainty margin of about 10% in the channel and cavity for the IN-AXIS and the OFF-axis cases,
2. in all cases, the C/E values obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 and with EFF-3.0/3.1 within the associated uncertainties in the calculations.

As far as the bulk shield behind the void structure is concerned, it can be concluded that:

1. the high energy neutron flux (E > 8 MeV) tends to be underestimated by calculations with increasing depth behind the void structure up to about 20% in deepest positions,
2. the C/E values obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 and with EFF-3.0/3.0rev within the associated uncertainties in the calculations.

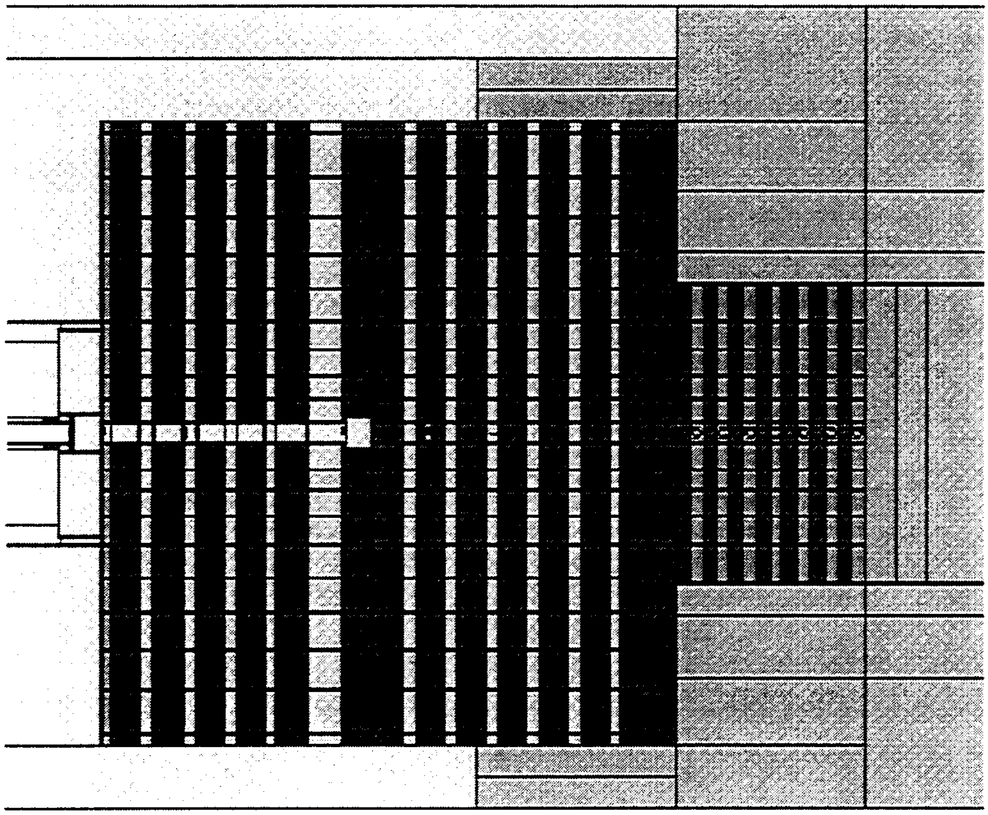

Fig.1 MCNP model of the shield mock-up used in the Neutron Streaming Experiment

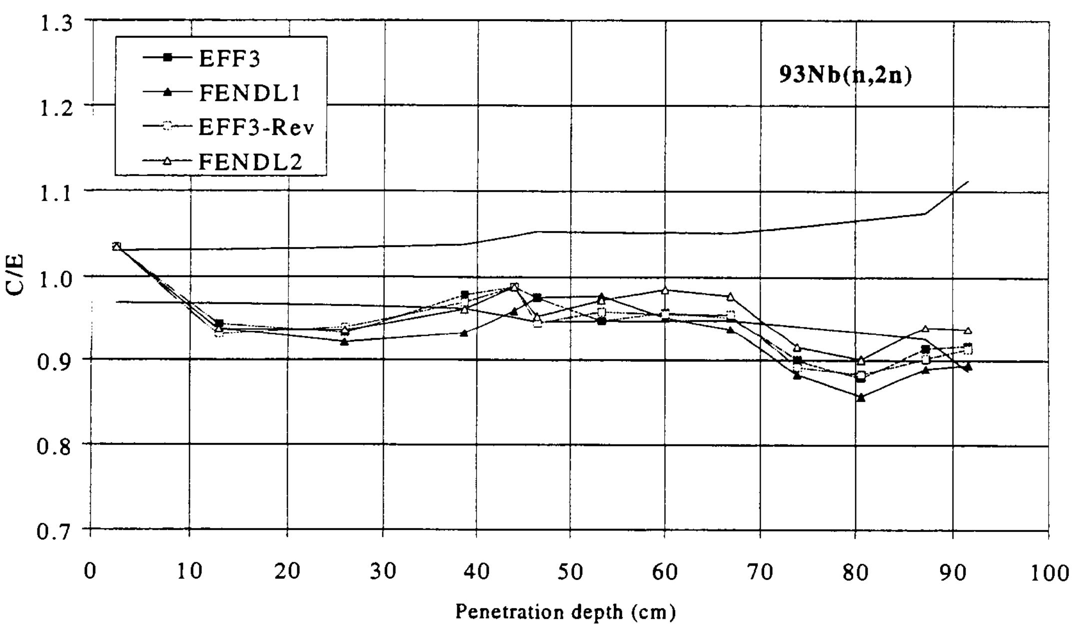

Fig.2 C/E values for ^{93}Nb(n,2n) reaction rate measurements along the mock-up axis (IN AXIS set-up) (EFF.3-rev is EFF3.1)

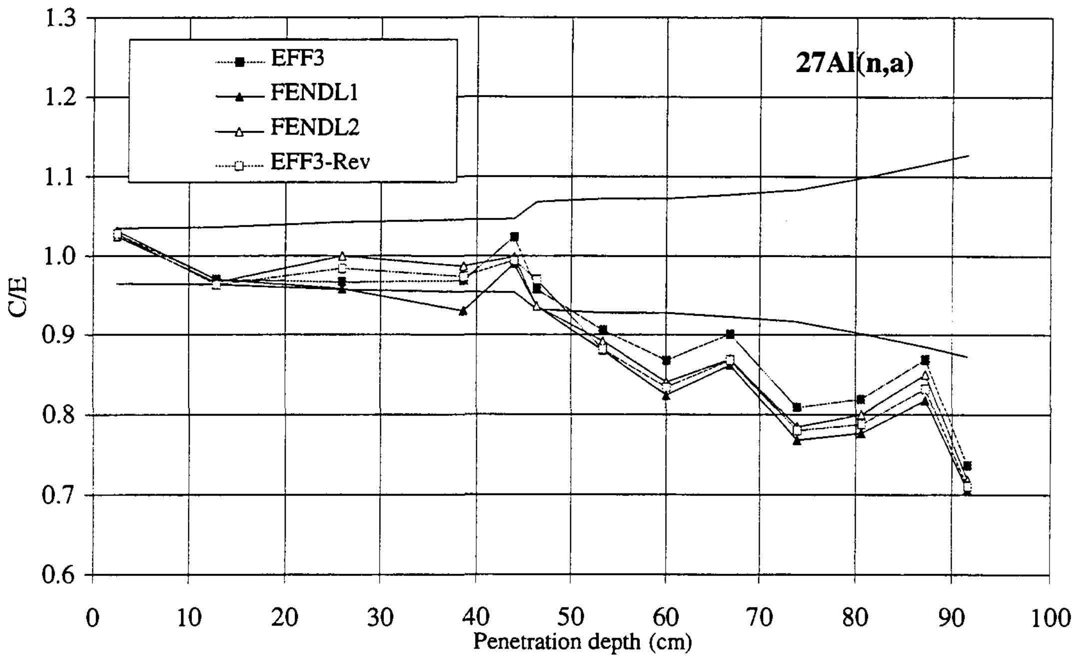

Fig.3 C/E values for ^{27}Al(n,a) reaction rate measurements along the mock-up axis (IN AXIS set-up) (EFF.3-rev is EFF3.1)

Benchmark analyses at the OKTAVIAN measurements of neutron and gamma leakage spectra from Al and Si spherical shells

H. Wienke

IAEA Nuclear Data Section
Vienna, Austria

The benchmarks consist of spectra of neutrons[1)] and gamma's[2)], leaking from spherical shells, measured with the Time-of-Flight method. The diameter of the Aluminium shell was 40 cm, the diameters of the Silicon shells were 40 and 60 cm. The inner radius of all shells was 10 cm. A D-T neutron source was placed in the centre of the shells. All shells had a cylindrical opening with a radius of 5 cm as beam duct.

Calculations were performed with the MCNP-4B code[3)] and FENDL-1 and FENDL-2 Monte-Carlo (ACE) libraries for Aluminium and Silicon. The calculated and experimental neutron-leakage spectra are shown in Fig. 1. For Aluminium the FENDL-2 result between 6 and 10 MeV is closer to the experimental data than the FENDL-1 calculation (Fig. 1a). The FENDL-2 calculations for Silicon agree much better with the experimental data in the energy range .04 – 16.5 MeV, than the FENDL-1 ones which strongly overestimate the data below 0.8 MeV and underestimate them above ~ 1.4 MeV.

The photon spectra are presented in Fig. 2. The calculations in Fig.'s 2a, 2b and 2c represent the combined contributions of photons produced in the shells and in the D-T target. The separate contributions for the FENDL-2 Aluminium calculation are shown in Fig. 2d together with the sum. The FENDL-2 results for Aluminium agree slightly better with the data than those of FENDL-1 (Fig. 2c). For Silicon the FENDL-1 and FENDL-2 results are comparable below 2.8 MeV, while above that energy the FENDL-2 calculations give a better description of the experimental data.

References:

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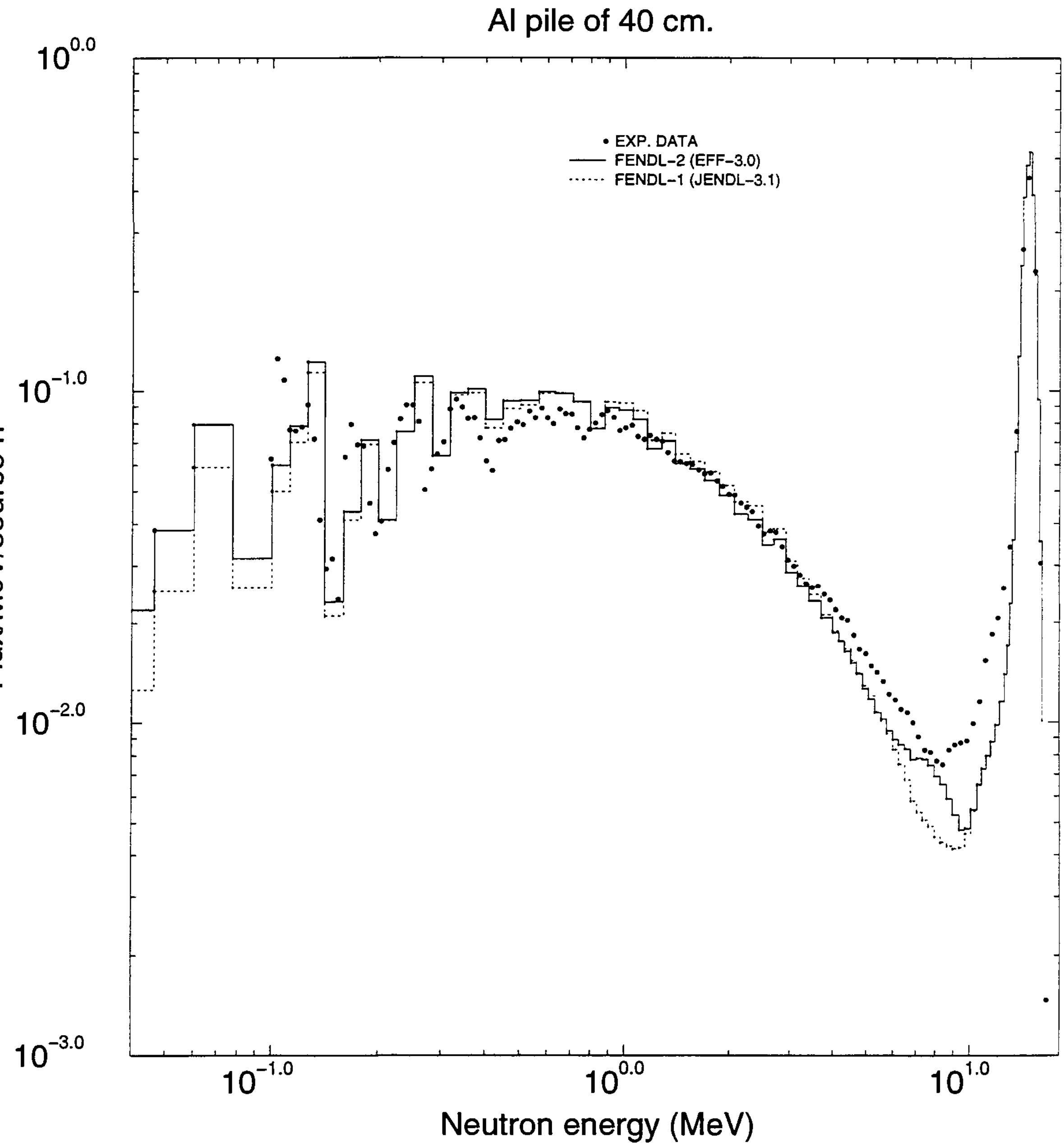
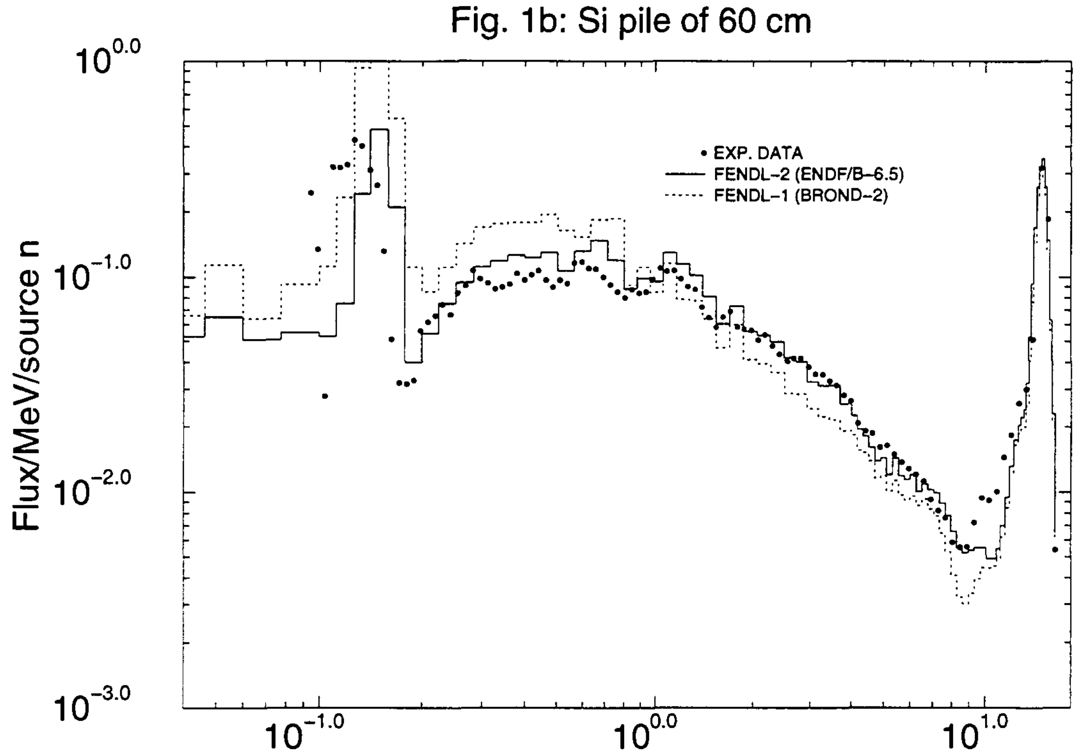


Fig. 1a: MCNP calculations with FENDL-1 (JENDL-3.1) and FENDL-2 (EFF-3.0) data at neutron leakage spectra of OKTAVIAN spherical Aluminium shell experiment.



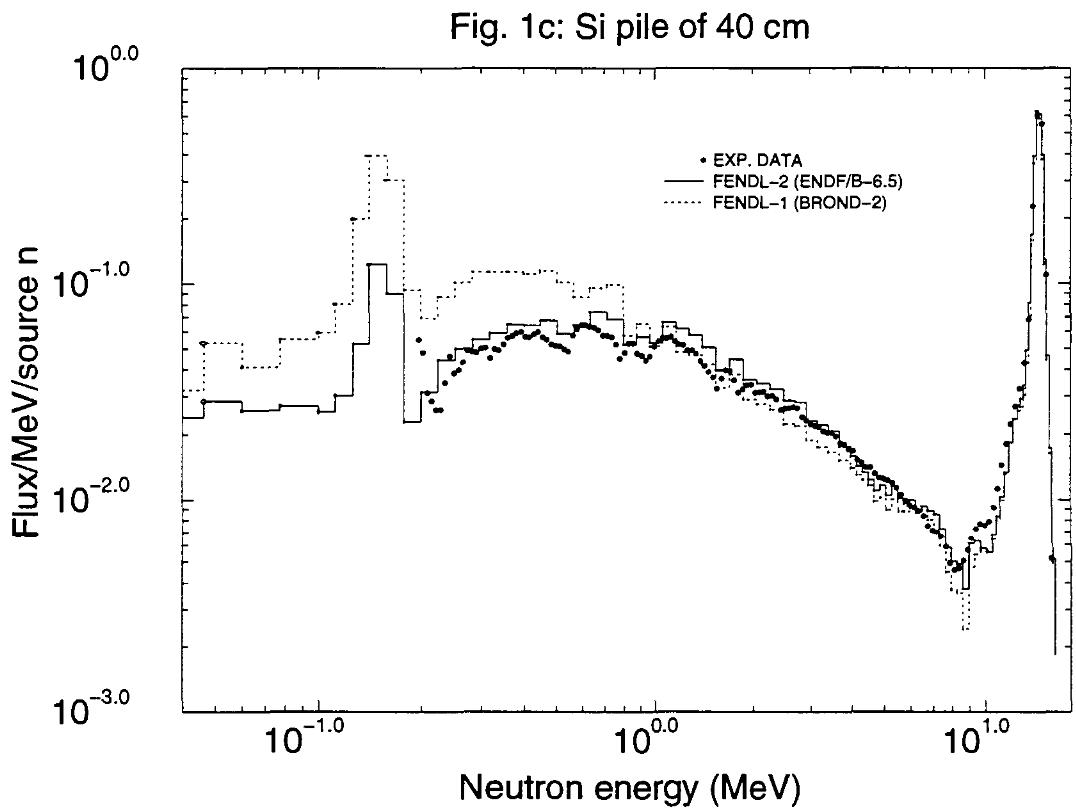


Fig. 1b,c: MCNP calculations with FENDL-1 (BROND-1) and FENDL-2 (ENDF/B-6.5) data at neutron leakage spectra of OKTAVIAN spherical Silicon shell experiments.

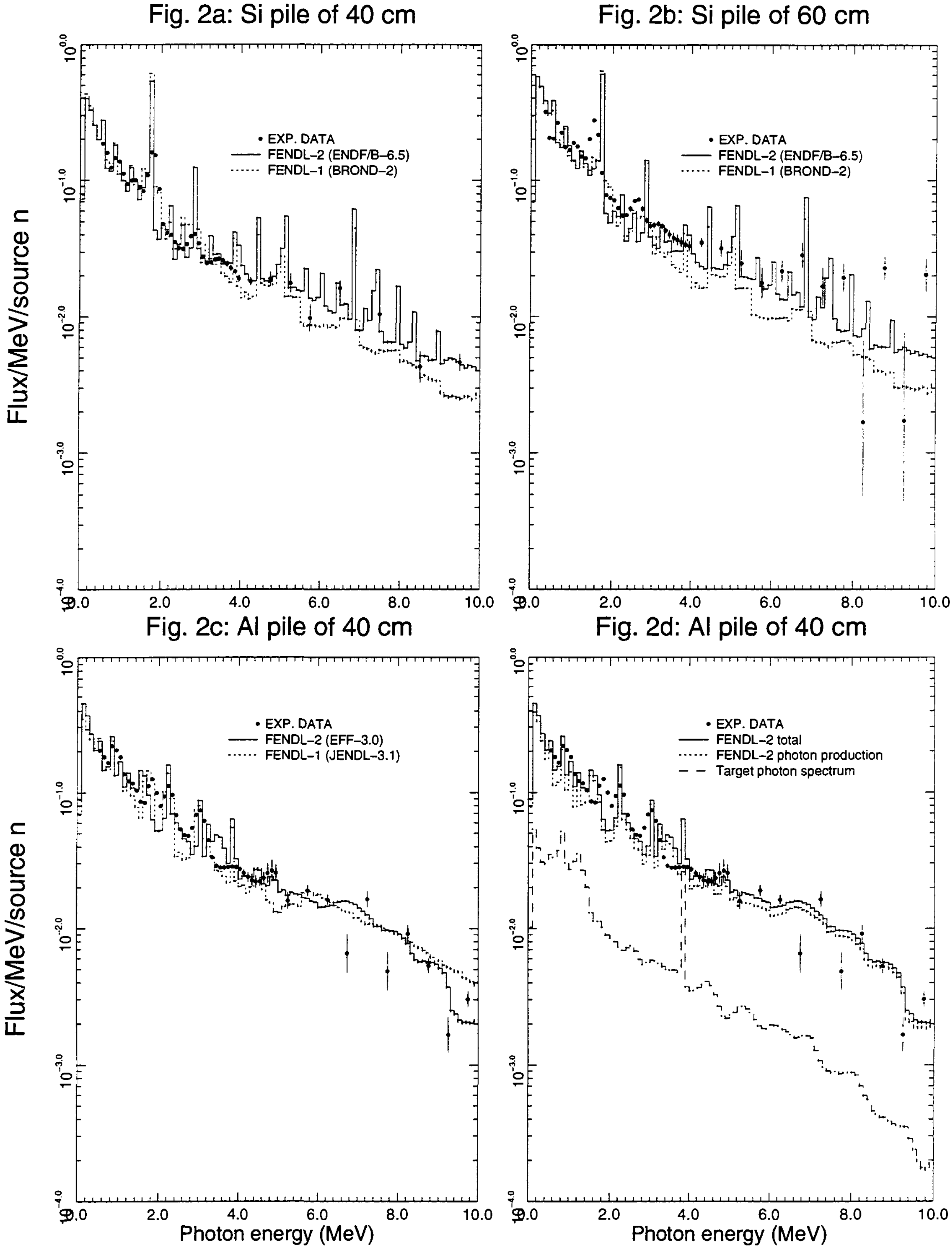


Fig. 2: MCNP calculations with FENDL-1 and FENDL-2 data at gamma leakage spectra of OKTAVIAN spherical shell experiments.

Present status of JENDL evaluation

F. Maekawa

Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun Ibaraki-ken 319-1195, Japan

The Japanese Evaluated Nuclear Data Library-3 revision 2 (JENDL-3.2) has been released in June 1994. The evaluation of JENDL Fusion File (JENDL-FF) has been completed by the end of 1995, and cross section data for some of nuclei in JENDL-FF have been selected for FENDL/E-2.0. In most cases, the File-3 data in JENDL-3.2 and JENDL-FF are identical, but the File-4 and 5 representation is adopted for JENDL-3.2 while FILE-6 is adopted for JENDL-FF. Now JENDL-3.2, is being revised to account for the feedback information collected after its release. The revised version, JENDL-3.3, is to be released by the end of 1999.

As regards FENDL/E-2.0, the most important material under revision is Vanadium. After the final selection of evaluations to be included in FENDL/E-2.0, new benchmark experiment for Vanadium was performed and analyzed at FNS/JAERI. The benchmark analysis showed that total cross section for Vanadium in JENDL-FF, (selected also for FENDL/E-2.0), is not accurate especially in the energy region between 0.1 to 4. This problem will be solved in JENDL-3.3. In addition, the revision of cross section data for Al, Ti, Cr., Co, Ni and Nb is also under way. These revised data will be submitted as candidates for future release of the FENDL library.

It has not yet been decided which representation for secondary neutrons, (i.e., File-4 and 5 or File-6), will be used in the JENDL-3.3. In the case File-4 and 5 representation is adopted, the JAERI Nuclear Data Center will provide File-6 version of JENDL-3.3 for the next FENDL library.

Analysis of nuclear heating measurements in the streaming experiment at FNG, using FENDL-1/-2.0 and EFF-2/-3 libraries

Paola Batistoni

Associazione Euratom-ENEA sulla Fusione, C. R. Frascati,
I-00044 Frascati (Rome), Italy

Experiment

In the frame of the Streaming Experiment (described in the previous report), nuclear heating was measured just behind the channel/cavity, in the shielding assembly and inside the superconducting magnet using CaF_2:Tm thermoluminescent detectors (TLD-300). The TLD-300 were calibrated, tested and used in previous experiments /1/. The measurements were done only for the IN AXIS set-up. TLD-300 were irradiated in 8 positions in the block and four positions in the coil, both in the stainless steel and copper plates. The absorbed dose in TLD-300 were measured with a total error of ±10% in the block and up to ±35% in the last position in the coils.

Analysis of experiment

The analysis of the experiments was carried out by means of the MCNP-4A/B code using:

1. FENDL-1 (IAEA),
2. FENDL-2.0 (IAEA),
3. EFF-2.4 (NEA),
4. EFF-3.0 (distributed by ECN Petten for FENDL benchmark),
5. EFF-3.1.

The neutron and photon absorbed doses in stainless steel and copper were calculated by track length estimator multiplied by KERMA factors (tally F6 of MCNP). The neutron dose includes the energy transferred by neutron-charged particle reactions and to the recoil nuclei.

The C/E comparison with TLD measurements requires the calculation of the absorbed dose in TLD with respect to the absorbed dose in the surrounding (stainless steel or copper) material. The calculational procedure is described in /1/.

Results and conclusions

<u>Gamma Heating Q_p:</u>

- The results obtained with FENDL-2.0 are very similar to those obtained with FENDL-1 within the associated calculation uncertainties, and are about 10% lower than those obtained with EFF-3.1.

- The results obtained with EFF-3.0 show high Q_p values, which result in a strong overprediction of the measured data. The problem, now well known and corrected in the updated version, was due to the erroneous double counting of photons (MT=3 reaction).

Neutron Heating Q_n:

- The results obtained for stainless steel with FENDL-2.0 are very similar to those obtained with FENDL-1 and with EFF-3.1, within the associated uncertainties.

- For Copper, Q_n in FENDL-2 is about a factor of three lower than in FENDL-1 and very close to EFF-3.1.

- The results obtained with EFF-3.0 show low Q_n values, as a result of the error in the MT=3 reaction connected with the use of the energy balance method.

C/E Comparison

A good agreement is found for FENDL-2.0 and for FENDL-1. EFF-3.1 gives results overestimated by about 10%.

/1/ P. Batistoni et al., Fus Eng. Design 36 (1997) 377-386

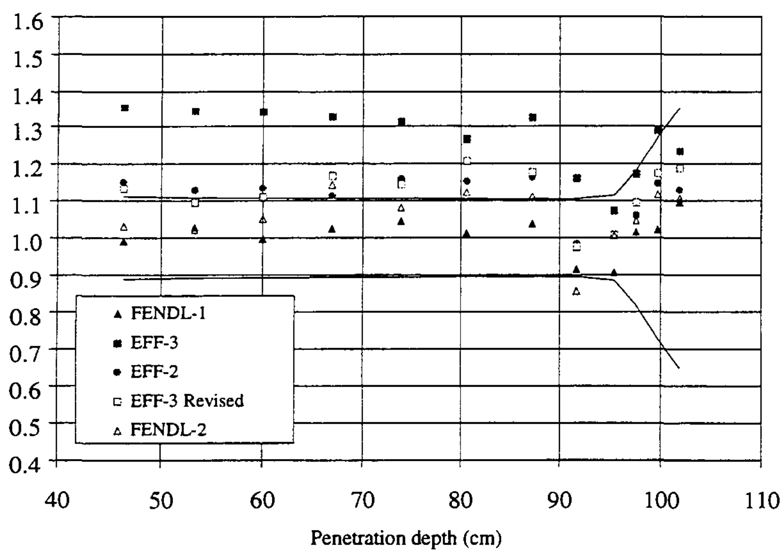


Fig.1 C/E Comparison for nuclear heating (EFF-3Revised is EFF3.1)

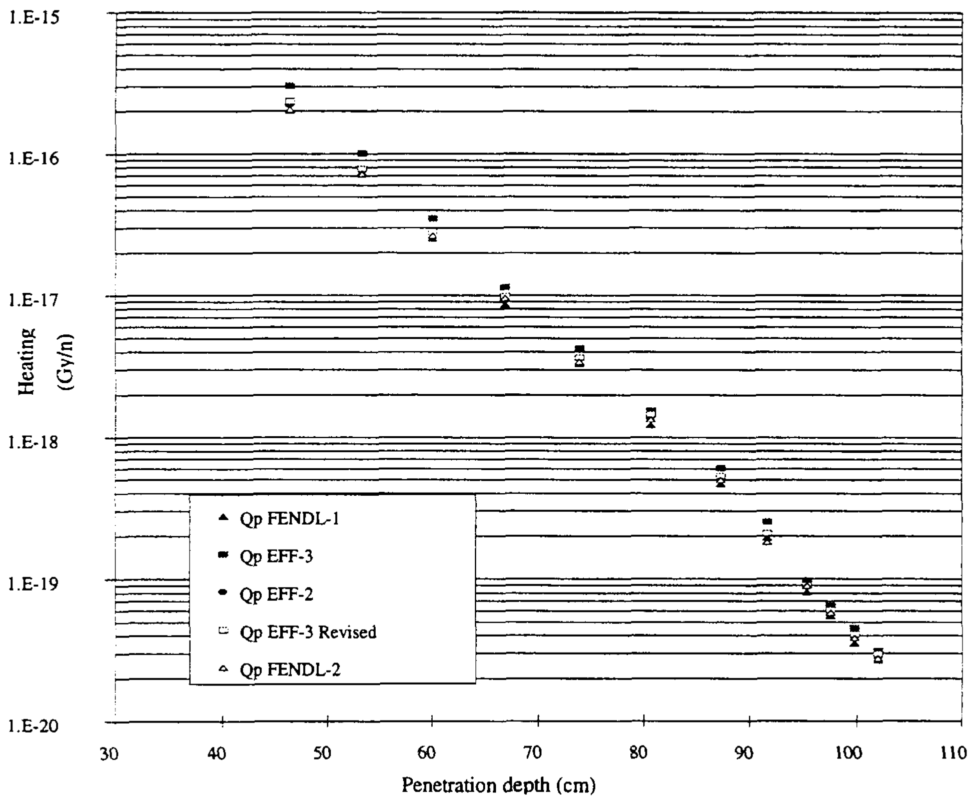


Fig.2 Calculated photon heating (EFF-3Revised is EFF3.1)

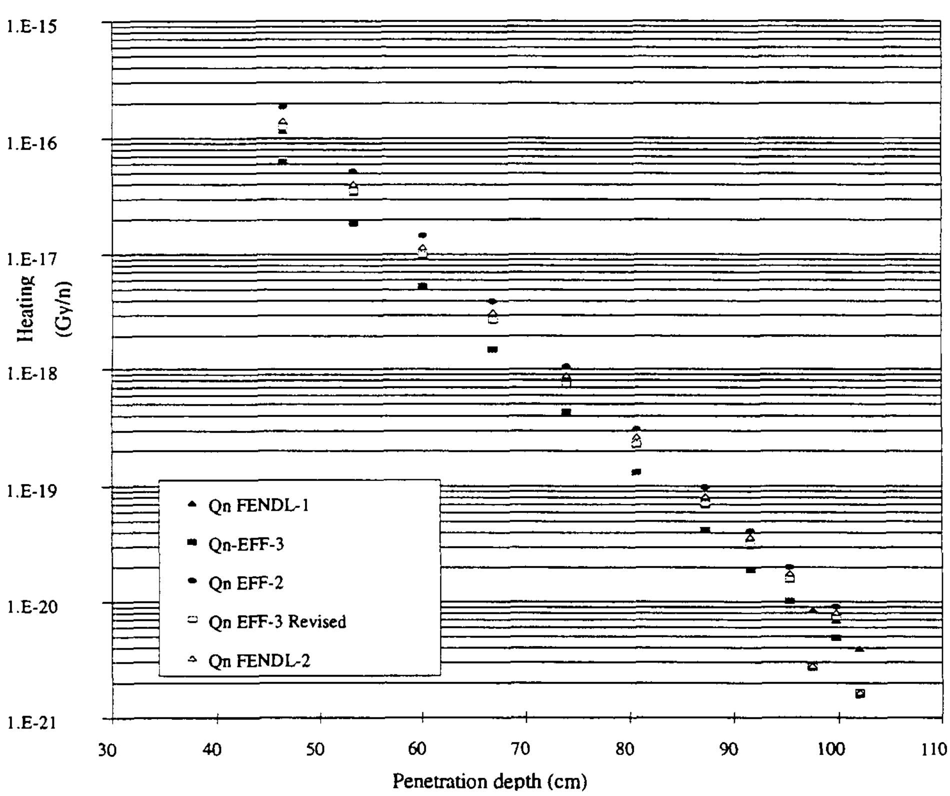


Fig.3 Calculated neutron heating (EFF-3Revised is EFF3.1)

Table 1. Measured dose il TDL-300 normalized to one source neutron

Depth (cm)	Dose in TLD-300 (Gy/n)	Experimental error (%)
46.35 SS	2.37E-16	10
53.3 "	7.79E-17	10
60.05 "	2.67E-17	10
66.9 "	8.77E-18	10
73.9 "	3.29E-18	10
80.6 "	1.42E-18	10
87.25 "	5.32E-19	10
91.65 "	2.53E-19	10
95.36 SS TFC	1.06E-19	11
97.56 Cu "	6.77E-20	18
99.76 SS "	4.13E-20	27
101.96 Cu "	2.67E-20	35

Benchmark analyses for EFF-1, -3 and FENDL-1, -2 beryllium data

U. Fischer(1), Y. Wu(2)

(1) Forschungszentrum Karlsruhe, Institut für Neutronenphysik und Reaktortechnik, Karlsruhe, Germany, e-mail: ulrich.fischer@inr.fzk.de

(2) Institute of Plasma Physics, Academia Sinica, Hefei, Anhui, P.R. China

Objective: Data testing and validation of new Beryllium evaluations through benchmark analyses of integral 14 MeV neutron experiments.

Methodology: Three-dimensional Monte Carlo calculations are performed with the MCNP4A-code to calculate and compare neutron leakage spectra as measured in suitable integral Beryllium benchmark experiments. In addition to graphical comparisons of calculated and measured neutron spectra, C/E (calculation/experiment) data are provided for integrated neutron flux spectra.

Data: ACE data files derived from the European Fusion File EFF, versions 1 and 3, and the Fusion Evaluated Nuclear Data File FENDL, versions 1 and 2 (FENDL/MC-1.0 and -2.0 as distributed by the IAEA/NDS), are used in the benchmark calculations.

Experiments: The following transmission experiments on spherical shell and slab-type Beryllium assemblies irradiated with 14 MeV neutrons and measurement of the neutron leakage spectra are considered:

- The Karlsruhe Neutron Transmission Experiment (KANT) [1] with a shell thickness of 17 cm. Neutron spectra were measured by the time-of-flight (TOF) method (thermal energy to 100 keV) and by the proton recoil spectroscopy (50 keV to 14 MeV). In addition, an independent measurement of the neutron multiplication factor was conducted with a Bonner sphere spectrometer [2].
- The OKATVIAN (University of Osaka) spherical shell experiment for a Beryllium shell of 11.65 cm thickness and measurement of the neutron leakage spectrum in the energy range 2.2 keV to 17 MeV with the TOF method [3].
- The FNS/JAERI transmission experiment [4] on a 15.24 cm thick Be cylindrical slab with measurement of the angular neutron flux spectra between 50 keV and 15 MeV at the angles of 0.0, 12.2, 24.9, 41.8 and 66.8 degree using the TOF-method with an NE-213 scintillation detector.

Results:

- The neutron (leakage) multiplication factor is reproduced within 3% with all considered ^{9}Be data evaluations (Table 1). As the experimental uncertainty is in the range of about 7% one can deduce that the neutron multiplication power of Beryllium can be satisfactorily predicted in design calculations with the ^{9}Be data evaluations in question.
- With regard to the neutron spectrum, there is an inconsistency between the results for the spherical shell and the slab experiments. In the spherical shell experiments, the old LANL ^{9}Be (as used e. g. in EFF-1) agrees best with the measured neutron spectra whereas all other evaluations give an underestimation. In particular, this is true for the 1-5 MeV energy range, where there is a significant underestimation with all data evaluations except EFF-1 (see e. g. Fig.1 for the KANT-spectra). The new EFF-3 ^{9}Be evaluation gives the largest underestimation and also underestimates the neutron population in the 5-10 MeV range.

- In the FNS slab experiment, on the other hand, both the FENDL-1, -2 and the EFF-3 evaluations agree in general better with the measured spectra, whereas the EFF-1 data show an overestimation over the whole energy range 1-10 MeV (except for larger angles) and an underestimation of the high energy (E>10 MeV) flux component (see Fig. 2 for C/E data in the FNS-experiment). Due to the resulting compensation effects EFF-1 finally gives good agreement (within 10%) for the total measured neutron flux. For FENDL-1, -2 and EFF-3, the deviation to the measured flux integrals in general is less than 10% except for the low energy component (E<1 MeV) at forward direction and the high energy flux (E>10 MeV) at 12.2 and 66.8 degree. This may be affected, however, by systematic uncertainties in the experiment.
- The inconsistency between the results for the spherical shell and the slab experiments can be explained by differences in the secondary energy distributions at backward angles. While the angle-integrated leakage spectra of the spherical shells are very sensitive to the backward component, this does not apply for the angular leakage spectra measured in the slab experiment at forward angles only. Thus the secondary energy-angle distribution should be carefully reconsidered to solve the observed discrepancy.

Table 1: Neutron leakage multiplication factors (M) for the KANT Beryllium spherical shell experiment (shell thickness 17 cm)

Experiment [1,2]		Calculation				
			EFF-1	EFF-3	FENDL-1	FENDL-2
	M	M	1.696	1.684	1.684	1.709
Integrated spectrum	1.661 ± 7%	C/E	1.021	1.014	1.014	1.029
Bonner spheres	1.695 ± 7%	C/E	1.001	0.994	0.994	1.008

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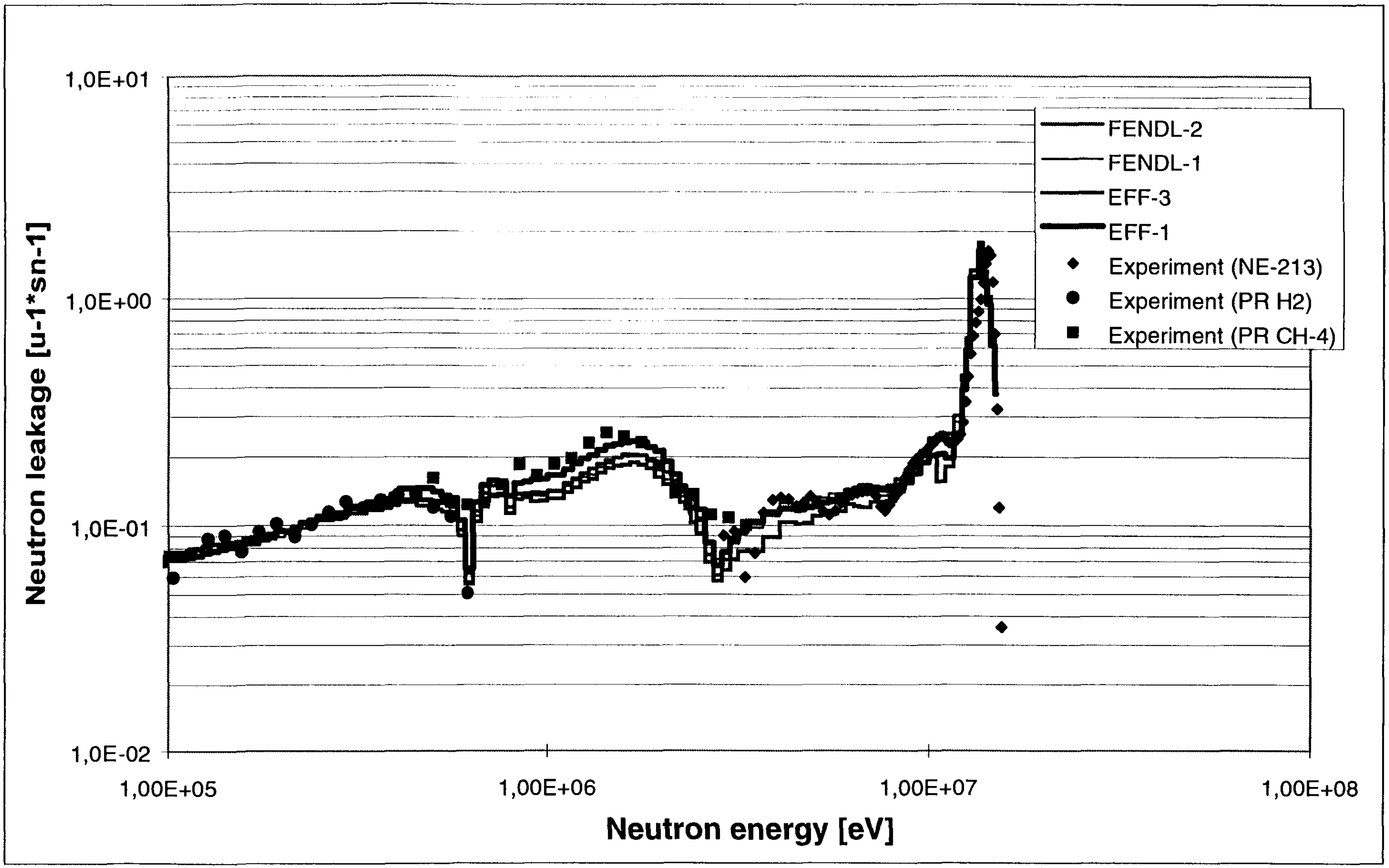

Fig. 1: KANT Beryllium spherical shell experiment [r_i = 5 cm, r_o = 22 cm]: comparison of neutron leakage spectra

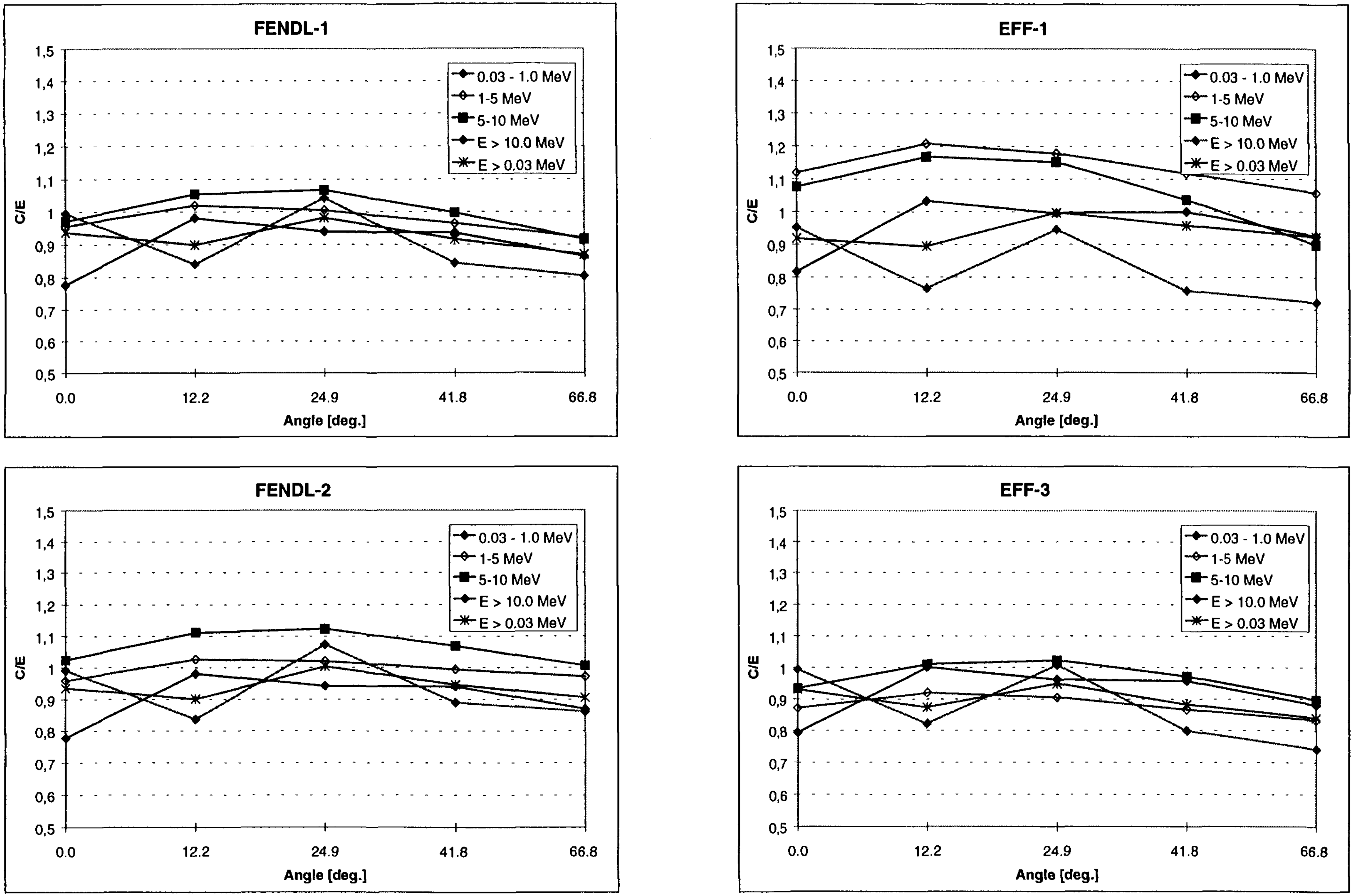

Fig. 2: FNS TOF Beryllium slab [t=15.2 cm] experiment: C/E comparison for neutron flux integrals

Benchmark analyses for EFF-3.0, -3.1 and FENDL-1, -2 iron data

U. Fischer(1), Y. Wu(2)

(1) Forschungszentrum Karlsruhe, Institut für Neutronenphysik und Reaktortechnik, Karlsruhe, Germany, e-mail: ulrich.fischer@inr.fzk.de

(2) Institute of Plasma Physics, Academia Sinica, Hefei, Anhui, P.R. China

Objective: Data testing and validation of new iron evaluations through benchmark analyses of integral 14 MeV neutron experiments.

Methodology: Three-dimensional Monte Carlo calculations are performed with the MCNP4A-code to calculate and compare neutron leakage spectra as measured in suitable integral iron benchmark experiments. In addition to graphical comparisons of calculated and measured neutron spectra, C/E (calculation/experiment) data are provided for integrated neutron flux spectra.

Data: ACE data files derived from the European Fusion File EFF, versions 3.0 and 3.1 for ^{56}Fe, and from the Fusion Evaluated Nuclear Data File FENDL, versions 1 and 2, (FENDL/MC-1.0 and -2.0 as distributed by the IAEA/NDS) are used in the benchmark calculations.

Experiments: The following transmission experiments on slab-type iron assemblies irradiated with 14 MeV neutrons and measurement of the neutron leakage spectra are considered:

- The TUD (Technical University of Dresden) experiment on an iron slab with a front surface of 100 cm x 100 cm and a thickness of 30 cm [1]. Neutron and photon leakage flux spectra have been measured above 1 and 0.4 MeV, respectively, at a distance of 349 cm from the target using a NE 213 scintillation detector. A set of different types of gas filled proportional counters has been used for measuring the low energy neutron spectrum (E≥0.03 MeV).
- The FNS/JAERI transmission experiment [2] on a 20 cm thick iron cylindrical slab with measurement of the angular neutron flux spectra between 50 keV and 15 MeV at the angles of 0.0, 12.2, 24.9, 41.8 and 66.8 degree using the TOF-method with an NE-213 scintillation detector.

Results:

- For the TUD iron slab experiment, there is a general good agreement between calculated and measured neutron leakage flux spectra (Fig. 1). The measured total neutron flux (E>0.1 MeV) is reproduced within 3% with all considered "state-of-the-art" EFF and FENDL data files (Fig. 2). There is included, however, an underestimation of the high energy flux component (E>10 MeV) by about 10% for EFF-3.0, -3.1 and FENDL-2 and by 20% for FENDL-1. In the 5-10 MeV energy range, EFF-3.0 shows a severe underestimation of the measured neutron flux by about 25%. This underestimation reduces to about 15% with EFF-3.1 and to 5% with FENDL-1, and -2. The shape of the photon flux spectrum is well reproduced by the calculations although the measured total photon flux is underestimated by about 20%.

- In the FNS slab experiment there is an excellent agreement between calculated and measured angular neutron flux spectra for all considered data files except FENDL-1 (Figs. 4, 5). This includes the 5-10 MeV energy where there is less structure than in the neutron spectrum of the TUD iron slab experiment. As FENDL-1 gives a significant overestimation in this energy range (cf. Fig. 4), a clear improvement can be stated with the more recent iron data evaluations of EFF-3.0, -3.1 and FENDL-2.

References:

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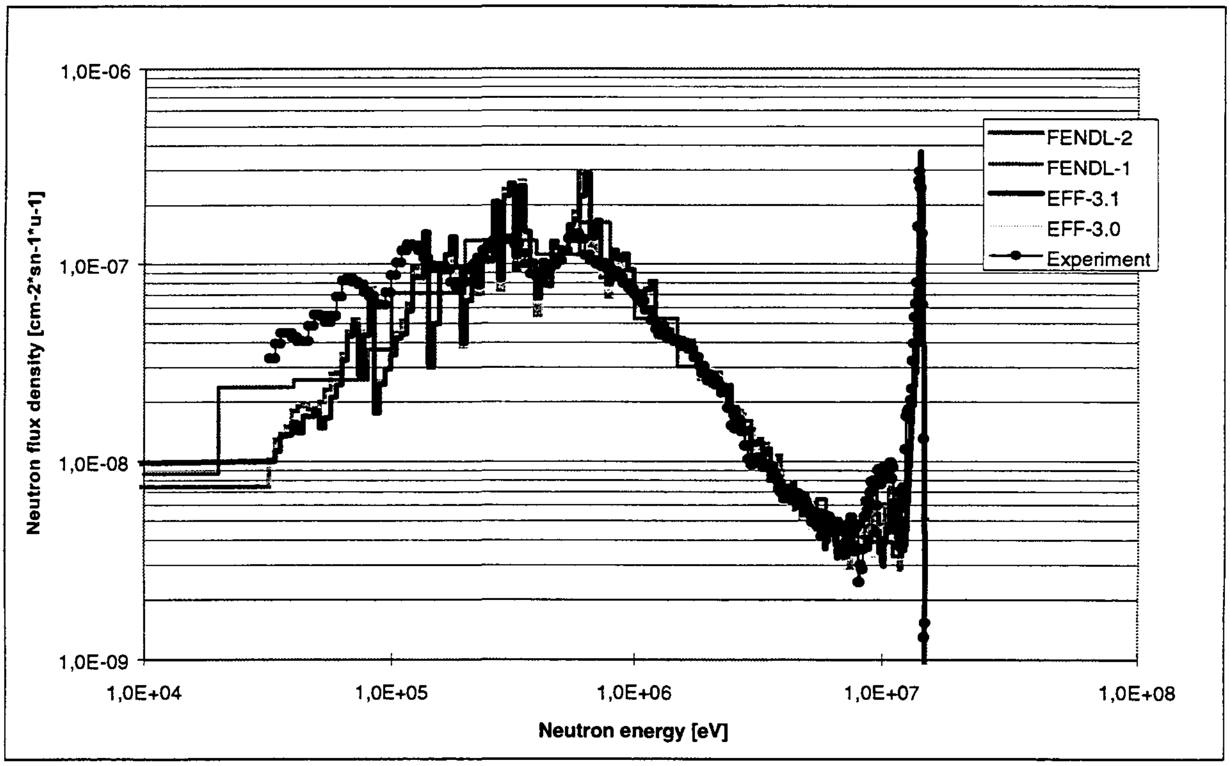

Fig. 1: TUD Iron slab experiment: comparison of neutron flux spectra

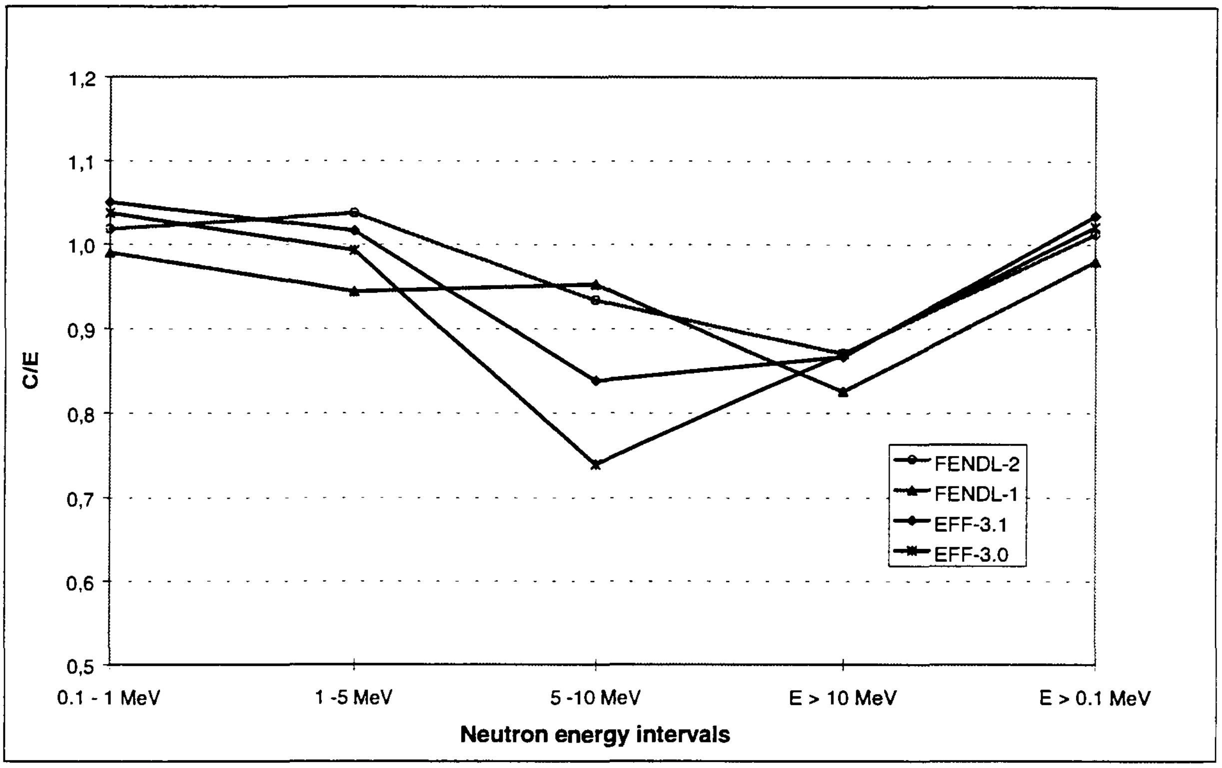

Fig. 2: TUD Iron slab experiment: C/E comparison for neutron flux integrals

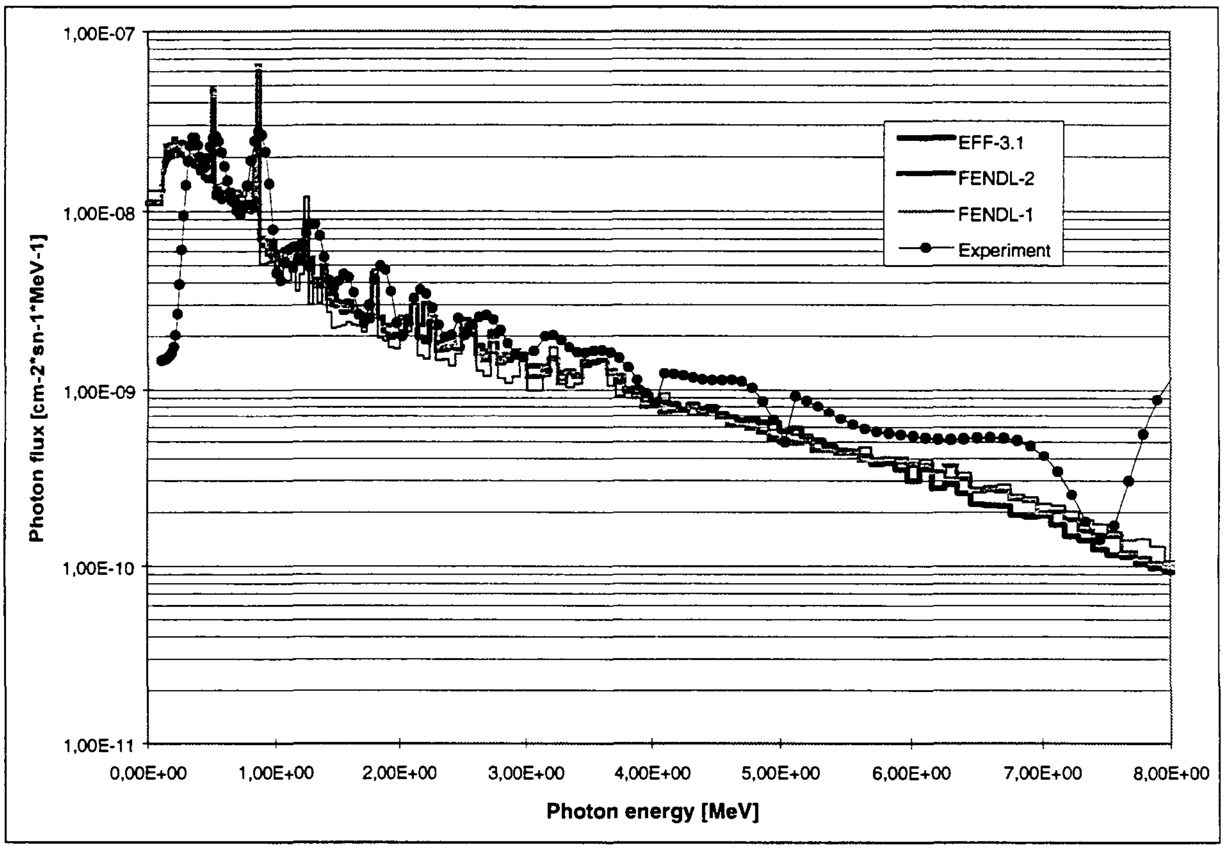

Fig. 3: TUD iron slab experiment: comparison of photon leakage spectra

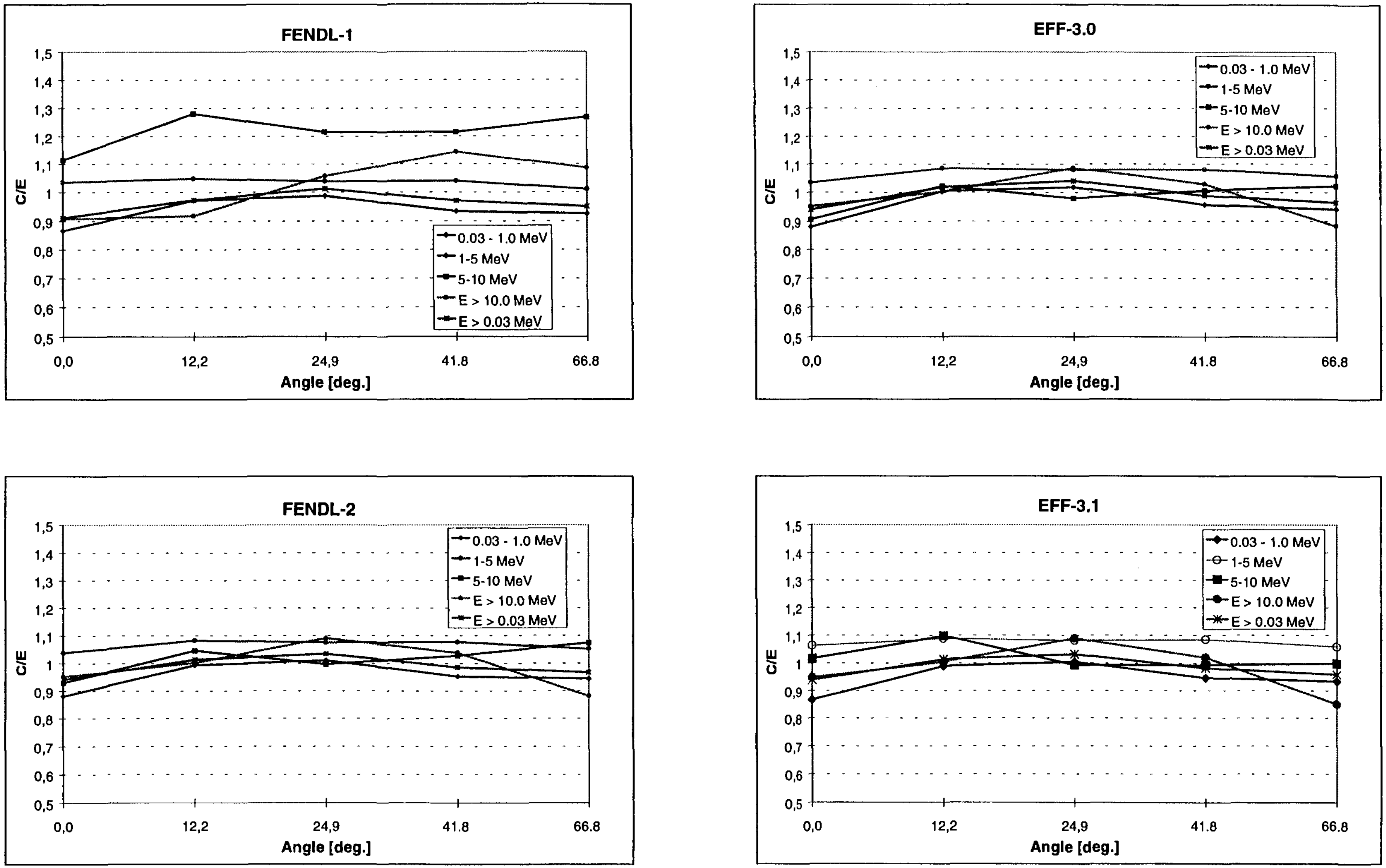

Fig. 4: FNS TOF Iron slab [t=20.0 cm] experiment: C/E comparison for neutron flux integrals

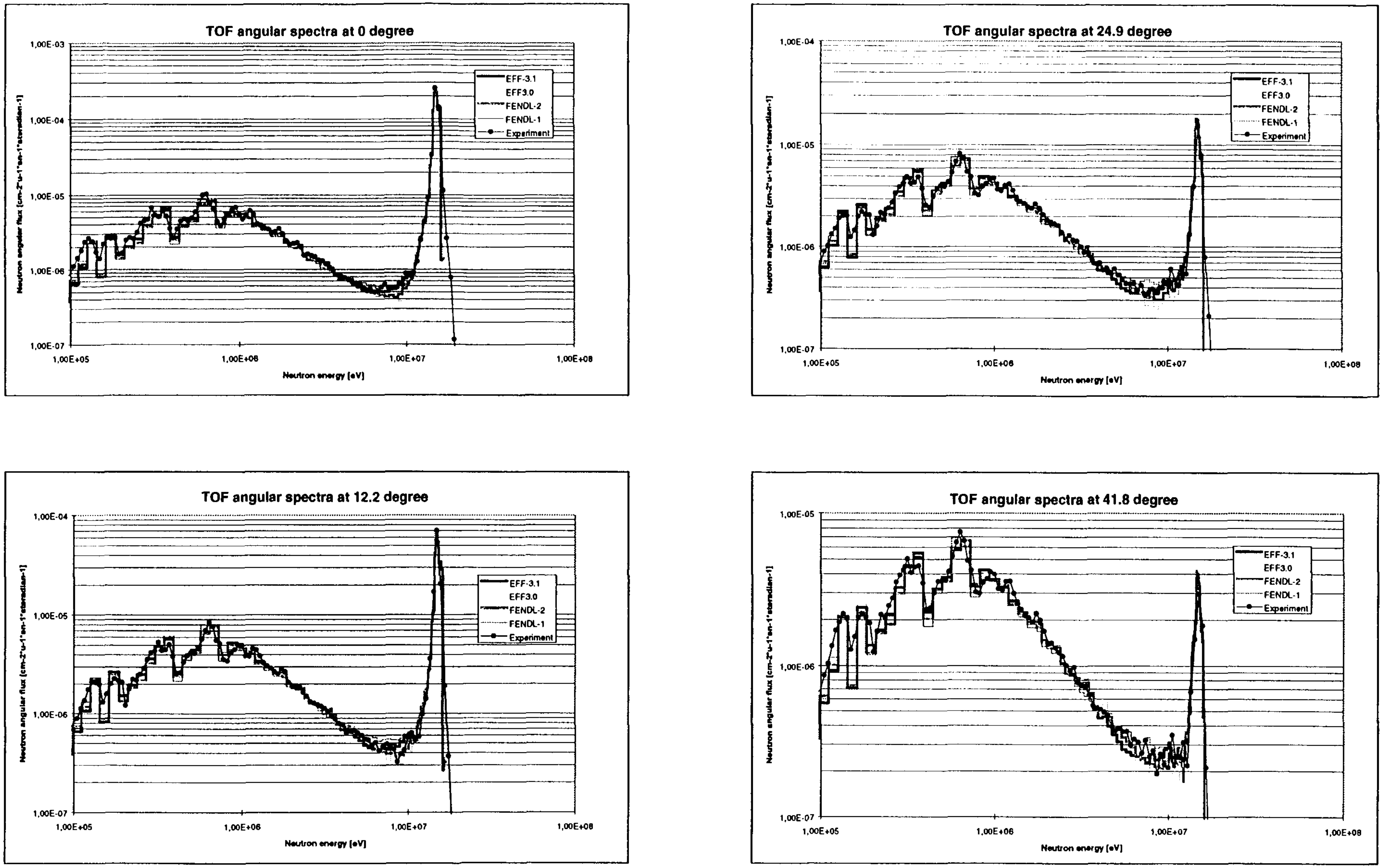

Fig. 5: FNS TOF Iron slab [t=20.0 cm] experiment: comparison of angular neutron flux spectra

Benchmark analysis at the FNS-TOF iron slab experiment

H. Wienke

IAEA Nuclear Data Section
Vienna, Austria

The benchmark experiment consists of angular flux spectra of neutrons leaking from cylindrical iron slabs, placed in front of a D-T neutron source, measured with the Time-of-Flight method at 0.0, 12.2, 24.9, 41.8 and 66.8 degrees with respect to the deuteron beam direction. The thicknesses of the cylindrical slabs were 5, 20, 40 and 60 cm, the slab radius was 50 cm[1,2].

Calculations were performed with the MCNP-4B code[3] and Monte-Carlo (ACE) libraries of FENDL-1, FENDL-2 and EFF-3.1. Two EFF-3.1 libraries were used, one prepared with the NJOY97/ACER module containing a patch which converts the double-differential (MF=6) data, represented by Legendre coefficients in the C.M system, into point wise energy-angle distributions in the lab system (MCNP4 law 67)[4], and one prepared with the unmodified ACER module which converts the MF=6 data into the usual Kalbach parameters. The patch was included as the Kalbach representation was supposed to be not adequate for the detailed structure of the new MF=6 data incorporated in the EFF-3.1 evaluation.

Fig. 1 shows that the use of the patch results in removal of a drastic overestimation of the 20 cm slab data between 8 and 13 MeV for most angles. The EFF-3.1 results (with patch) compete with those of FENDL-1 in describing the experimental data, both being superior to the FENDL-2 calculation, except for 12.2 deg., where the latter gives the best fit, and at 66.8 deg., where all three are about equally close to the data. The 40 cm slab calculations with FENDL-1, FENDL-2 and EFF-3.1 (with patch) are presented in Fig.'s 2a and 2b. At the two largest angles all three tend to underpredict the data between 4 and 10 MeV (Fig. 2a). In the energy region 0.05-1 MeV they all are shifted towards higher energies with respect to the data (Fig. 2b). This may be due to multiple scattering in the slab which has not been accounted for in converting the TOF spectra into energy spectra[5]. The results for the 60 cm slab (not shown here) reveal a similar but slightly larger shift. Therefore also a 40 cm slab calculation was performed for EFF-3.1, with the neutron arrival time as independent variable. The resulting time spectra were then converted into energy spectra according to the procedure described in Ref. 1, in order to keep the Monte-Carlo simulation as close as possible to the experiment. Fig. 2c shows the resulting spectra together with the conventional ones calculated with the neutron energy as independent variable. The time-converted spectrum gives clearly a better fit to the data below 0.4 MeV and the shifts, present in the conventional calculation, don't show up.

From the present study the following can be concluded: for Fe-56 from EFF-3.1 a continuous energy-angle representation of Mf=6 data is more adequate than Kalbach parameters; the FENDL-1 and EFF-3.1 results in general agree about equally well with the data and are both superior to FENDL-2. In the case of the 40 cm slab benchmark at low energies, where multiple scattering is predominant, the time-converted calculation described above is clearly more reliable for comparison with the experimental data than the conventional Monte-Carlo calculation with the neutron energy as independent variable.

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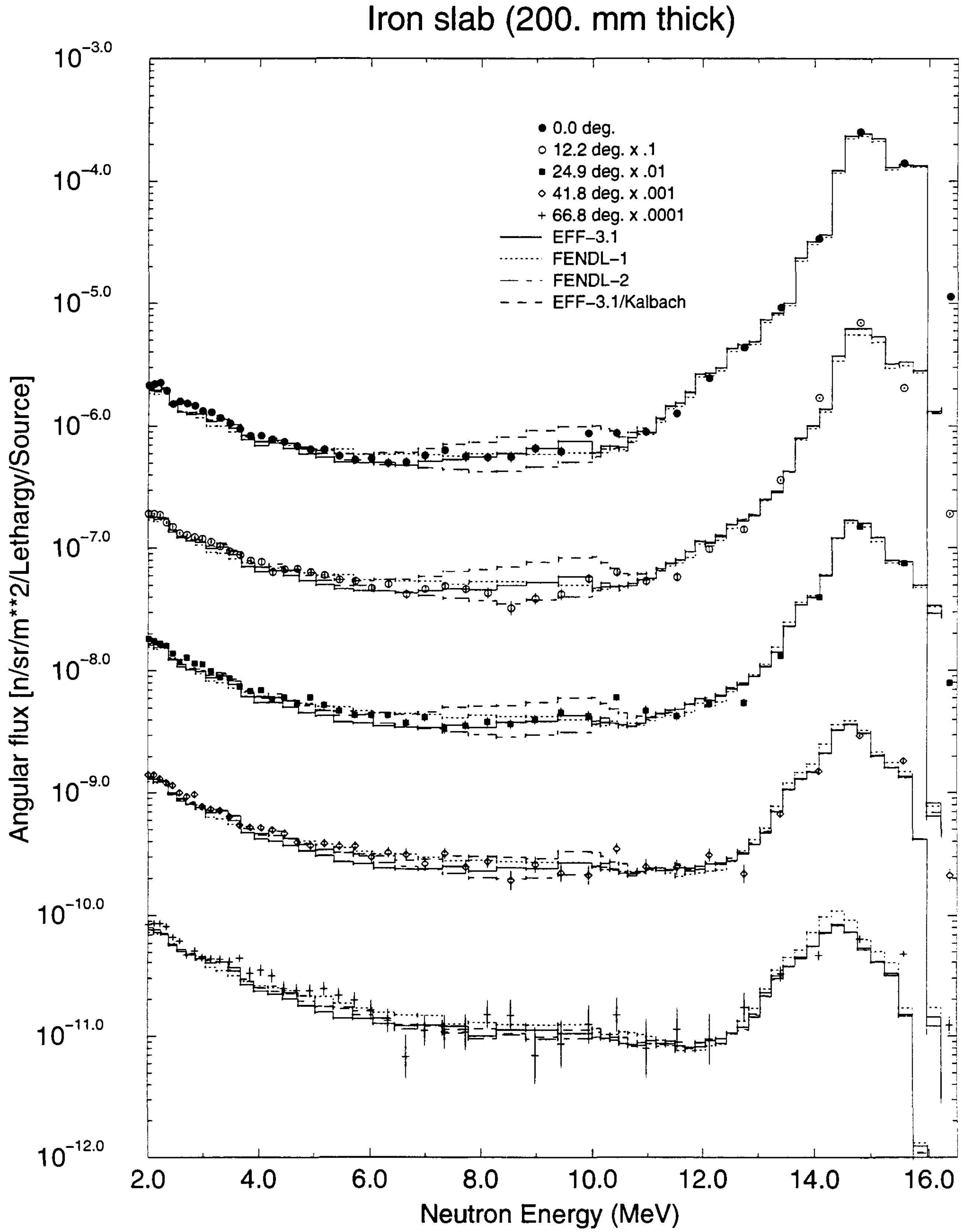

Fig. 1: MCNP calculations at the FNS-TOF 20 cm Iron slab benchmark experiment with Iron data from EFF-3.1, FENDL-2 and FENDL-1 in the energy range 2.0-16.5 MeV.

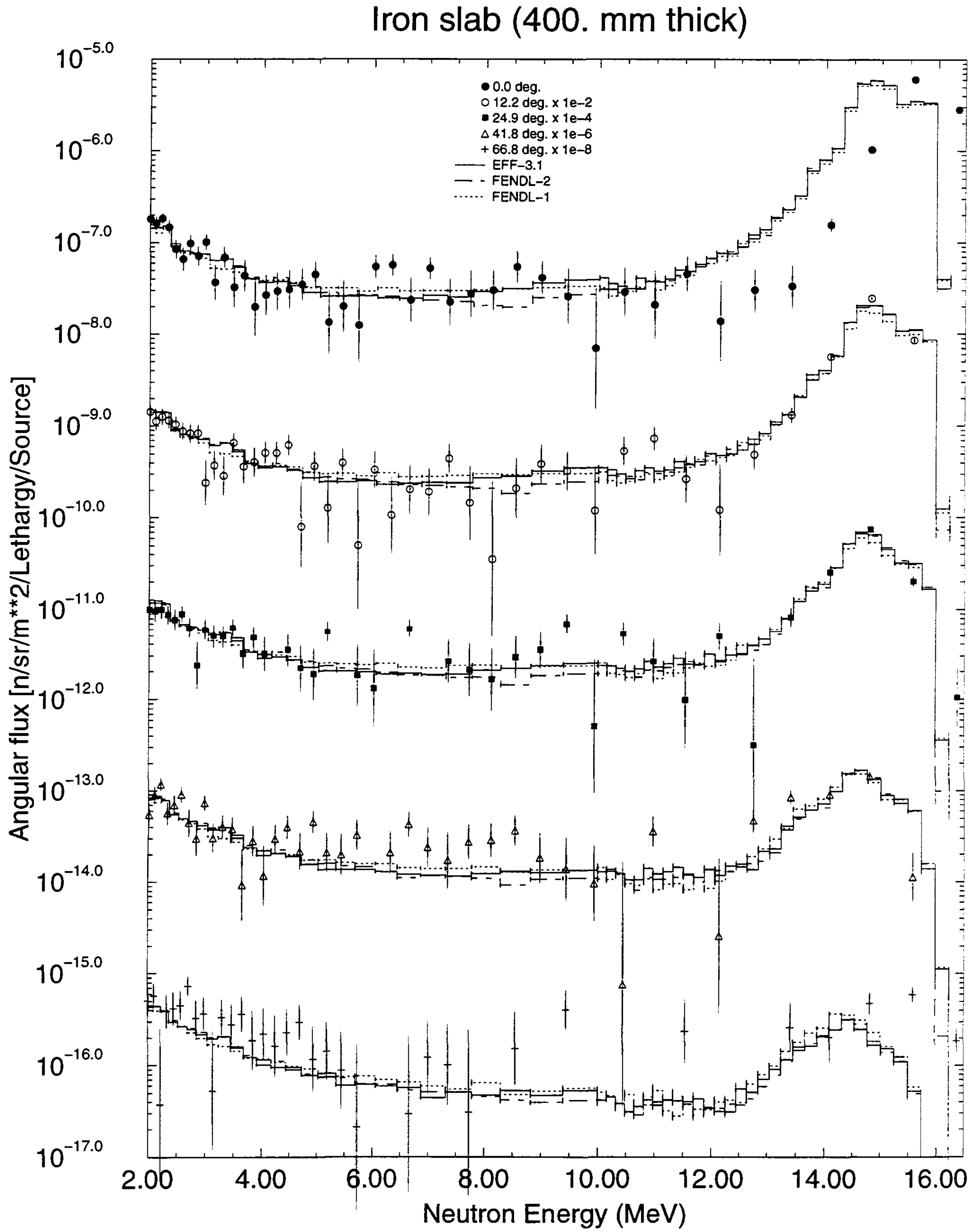

Fig. 2a: Results of MCNP calculations at the FNS-TOF 40 cm cylindrical Iron slab experiment in the energy range 2.0-16.5 MeV, with Iron data from EFF-3.1, FENDL-2 and FENDL-1.

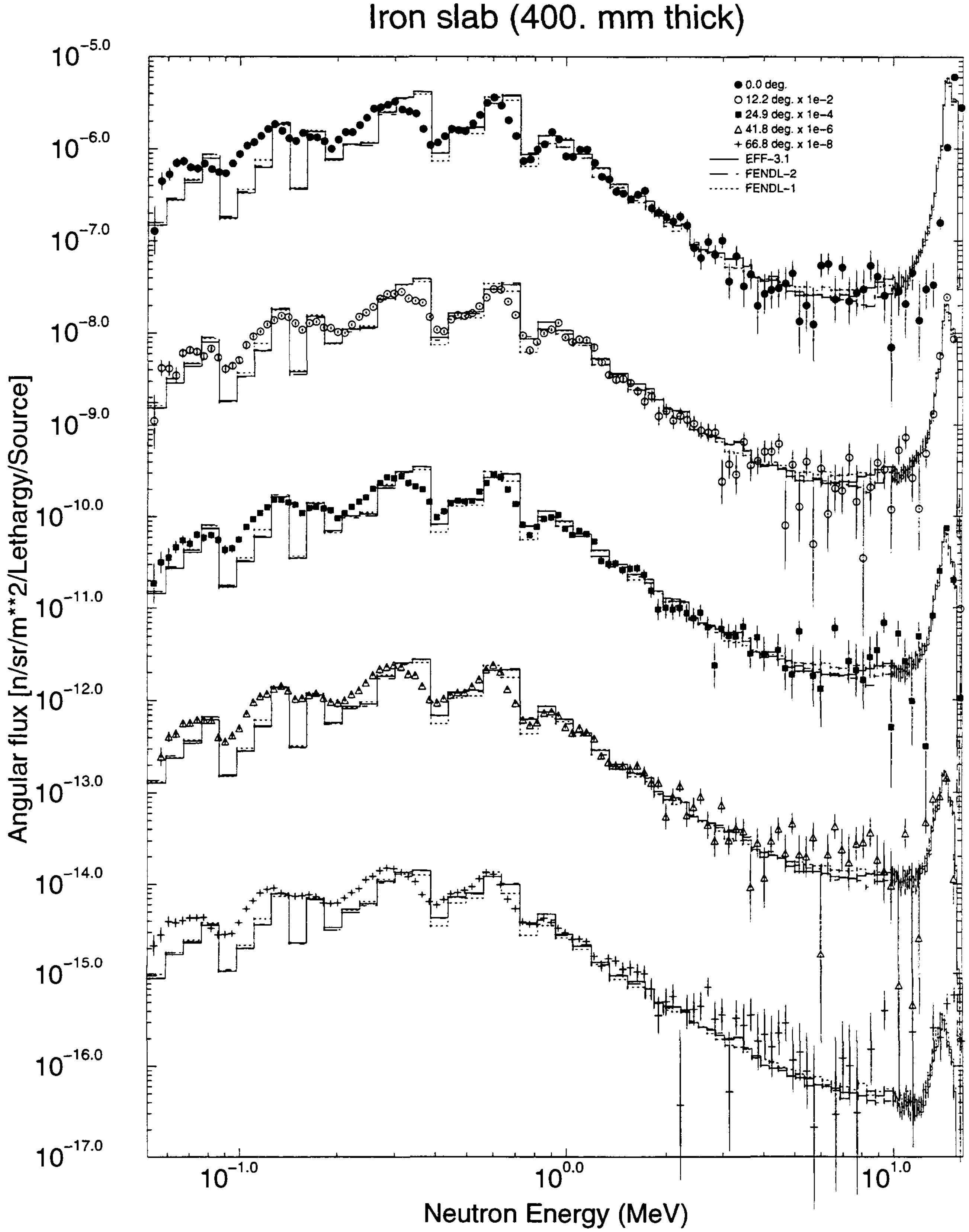

Fig. 2b: Results of MCNP calculations at the FNS-TOF 40 cm cylindrical Iron slab experiment in the energy range 0.05-16.5 MeV, with Iron data from EFF-3.1, FENDL-2 and FENDL-1.

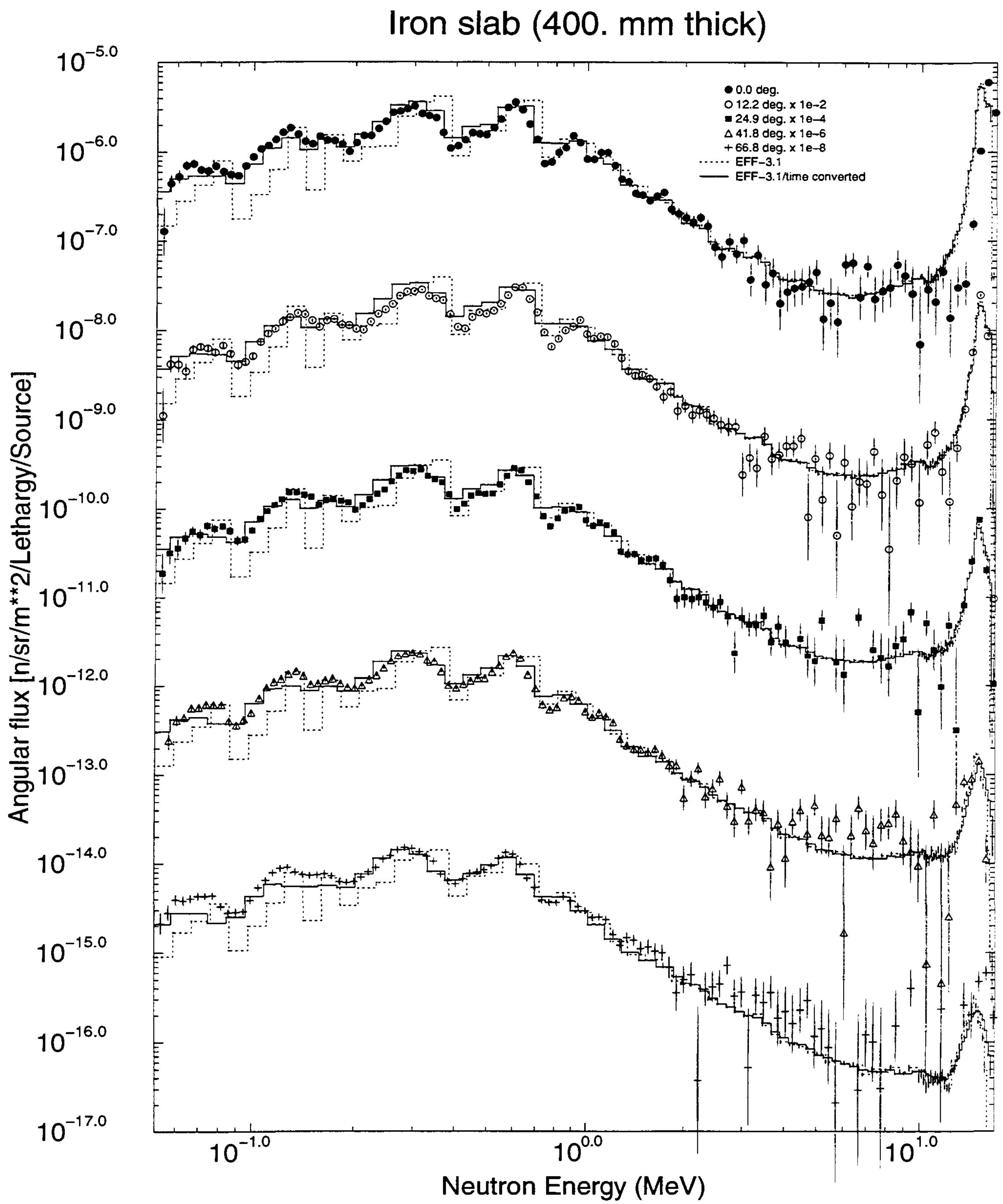

Fig. 2c: MCNP calculations with Iron data from EFF-3.1 at the FNS-TOF 40 cm slab benchmark experiment in the neutron-energy range 0.05 - 16.5 MeV. Dotted line: results of conventional MCNP calculation. Solid line: results obtained by converting the calculated time of arrival spectra into neutron energy spectra, as described in the text.

Benchmark analyses for the ITER bulk shield experiment with EFF-3.0, -3.1 and FENDL-1, -2 nuclear cross-section data

U. Fischer(1), Y. Wu(2), W. Hansen(4), D. Richter(3), K. Seidel(3), S. Unholzer(3)

(1) Forschungszentrum Karlsruhe, Institut für Neutronenphysik und Reaktortechnik, Karlsruhe, Germany, e-mail: ulrich.fischer@inr.fzk.de
(2) Institute of Plasma Physics, Academia Sinica, Hefei, Anhui, P.R. China
(3) Technische Universität Dresden, Institut für Kern- u. Teilchenphysik, Dresden, Germany
(4) Technische Universität Dresden, Institut für Energietechnik, Dresden, Germany

Objective: Data testing of EFF-3 and FENDL-1, -2 nuclear data libraries through benchmark analyses for a design relevant integral 14 MeV neutron shielding experiment.

Methodology: Three-dimensional Monte Carlo calculations are performed with the MCNP4A-code to calculate and compare neutron and photon spectra measured in the ITER bulk shield experiment at the Frascati Neutron Generator (FNG) [1]. In addition to graphical comparisons of calculated and measured neutron spectra, C/E (calculation/experiment) data are provided for integrated neutron flux spectra.

Data: ACE data files derived from the European Fusion File EFF, versions 3.0 and 3.1 for ^{56}Fe, and from the Fusion Evaluated Nuclear Data File FENDL, versions 1 and 2, (FENDL/MC-1.0 and -2.0 as distributed by the IAEA/NDS) are used in the benchmark calculations.

Experiment: Neutron and photon flux spectra have been measured in a mock-up of the ITER inboard shield system at FNG, Frascati [2,3]. The mock-up consists of a shielding block with a thickness of 94 cm made of alternate plates of stainless steel SS-316 and of the water-equivalent material Perspex. The lateral dimensions amount to about 100 cm x 100 cm. The mock-up is backed by a 30 cm thick block of alternate SS-316 and copper plates simulating the TF-coils.

The measurements were carried out on the central axis of the assembly at the two positions A and B (Fig. 1). Position A with a penetration depth of 41.4 cm corresponds to the back plate of the shielding blanket while position B at 87.6 cm depth is located at the back of the vacuum vessel near the TF-coil mock-up. Neutron spectra were measured in the energy range between about 20 keV and 15 MeV. A set of gas-filled proportional counters and a stilbene scintillation spectrometer were used in the energy range up to 3 MeV. Between 1 and 15 MeV a NE-213 scintillation spectrometer was applied. The spectra were determined on an absolute scale as fluences per source neutron. The NE-213 spectrometer was also used for the simultaneous measurement of the photon flux spectra above 0.2 MeV.

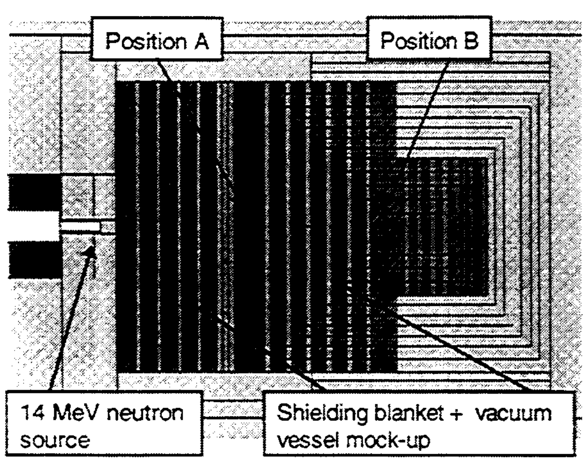

Fig. 1: ITER bulk shield mock-up assembly with measurement positions indicated

Results:

- The measured total neutron flux spectra are underestimated, in the order of 10% at the back of the shielding blanket (41.4 cm penetration depth) and up to 30% at the back of the vacuum vessel mock-up (87.6 cm penetration depth). The same is true for the high energy (E>10 MeV) neutron flux at the shallow position A. At the deep position B, this component is underestimated by up to 20% with FENDL-1 and -2 data. This underestimation is reduced when using the more recent EFF-3.1 ^{56}Fe data both for the high energy (E>10 MeV) component and the total fast neutron flux (E>0.1 MeV, see Tables 1, 2).
- The measured photon flux spectra can be well reproduced by the calculations, both at the shallow position A and the deep position B (Tables 3, 4 , Figs. 4, 5). At the latter position there is a slight underestimation in the order of 10% with FENDL-1 and -2 data and again good agreement with the more recent EFF-3.1 ^{56}Fe data. Note that the photon production is largely due to thermal neutron capture reactions in this case.

In summary it is concluded that the neutron and gamma flux attenuation in a design relevant bulk shield system can be satisfactorily described by MCNP based calculations using the "state-of-the art" fusion nuclear data libraries. It is noted, however, that this includes an underestimation of the fast (E>0.1 MeV) neutron flux by up to 30% with FENDL-1 data at about 1 m penetration depth. Some improvement has been obtained with FENDL-2 while a better agreement is being observed with the more recent EFF-3.1 ^{56}Fe data.

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Table 1: Neutron flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER bulk shield experiment and calculation-to-experiment (C/E) ratios at position A at the back of the shielding blanket mock-up.

Energy interval [MeV]	Experiment	C/E EFF-3.0	EFF-3.1	FENDL-1	FENDL-2	Stat. Error [%]
0.1 - 1	$(2.76\pm0.28)\cdot10^{-6}$	0.90	0.90	0.85	0.87	0.06
1 - 5	$(1.43\pm0.08)\cdot10^{-6}$	0.97	0.96	0.87	0.93	0.08
5- 10	$(2.47\pm0.13)\cdot10^{-7}$	1.03	1.00	1.05	1.00	1.0
E > 10 MeV	$(5.42\pm0.14)\cdot10^{-7}$	0.98	1.05	0.99	0.96	0.9
E > 0.1 MeV	$4.98\cdot10^{-6}\pm6.1\%$	0.93	0.94	0.88	0.90	0.4

Table 2: Neutron flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER bulk shield experiment and calculation-to-experiment (C/E) ratios at position B at the back of the vacuum vessel mock-up.

Energy interval [MeV]	Experiment	C/E EFF-3.0	EFF-3.1	FENDL-1	FENDL-2	Stat. Error [%]
0.1 – 1	$(8.78\pm0.89)\cdot10^{-9}$	0.73	0.76	0.68	0.71	0.08
1 – 5	$(2.37\pm0.13)\cdot10^{-9}$	0.85	0.88	0.78	0.77	0.09
5- 10	$(2.69\pm0.14)\cdot10^{-10}$	1.08	1.02	1.00	0.88	1.5
E > 10 MeV	$(5.79\pm0.15)\cdot10^{-10}$	0.87	0.86	0.81	0.80	1.5
E > 0.1 MeV	$1.20\cdot10^{-8}\pm7.5\%$	0.77	0.79	0.71	0.73	0.7

Table 3: Photon flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER bulk shield experiment and calculation-to-experiment (C/E) ratios at position A at the back of the shielding blanket mock-up.

Energy interval [MeV]	Experiment	C/E EFF-3.0	EFF-3.1	FENDL-1	FENDL-2	Stat. Error [%]
0.4 - 1	$3.18\cdot10^{-6}$	1.15	1.02	0.99	0.98	0.6
1 – 10.5	$4.29\cdot10^{-6}$	1.19	1.09	1.05	1.03	0.6
E > 0.4 MeV	$7.47\cdot10^{-6}\pm2.5\%$	1.17	1.06	1.02	1.01	0.5

Table 4: Photon flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER bulk shield experiment and calculation-to-experiment (C/E) ratios at position B at the back of the vacuum vessel mock-up.

Energy interval [MeV]	Experiment	C/E EFF-3.0	EFF-3.1	FENDL-1	FENDL-2	Stat. Error [%]
0.4 - 1	$4.50\cdot10^{-9}$	1.06	0.97	0.89	0.91	1.0
1 – 10.5	$6.20\cdot10^{-9}$	1.05	1.01	0.90	0.90	0.9
E > 0.4 MeV	$1.07\cdot10^{-8}\pm2.8\%$	1.06	0.99	0.89	0.91	0.8

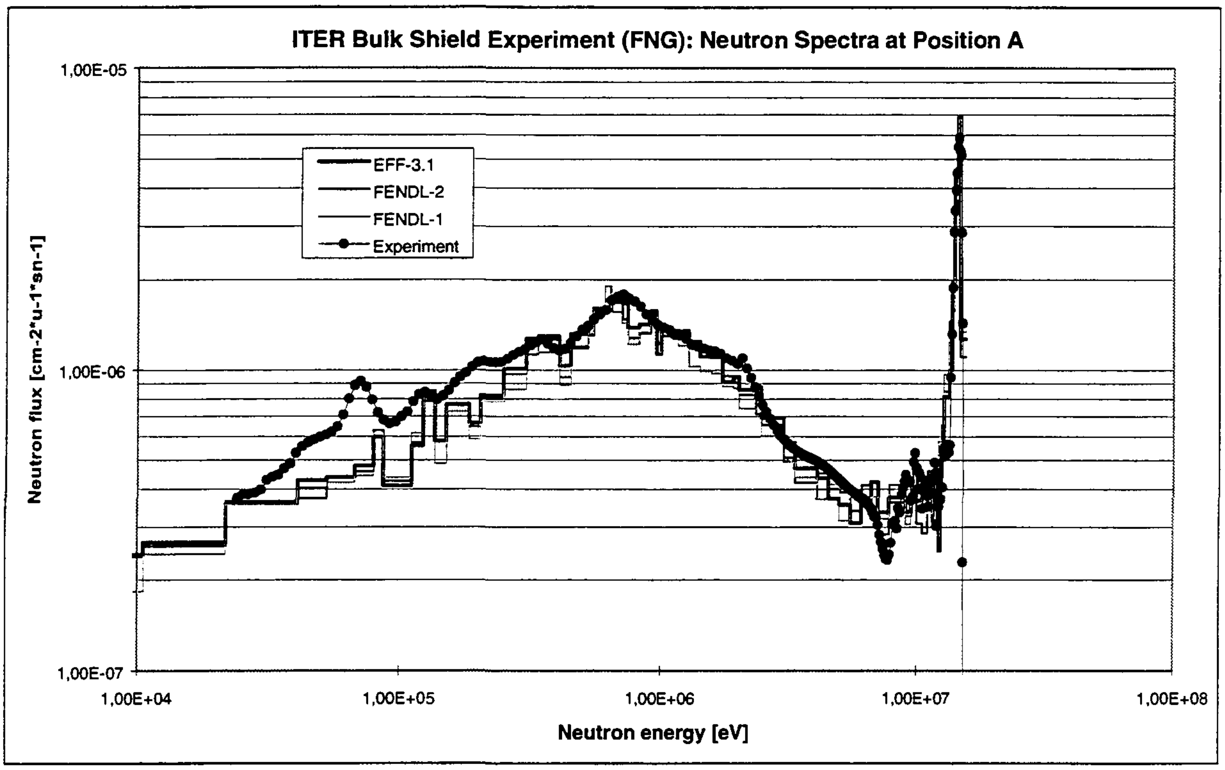

Fig. 2: Neutron flux spectra at the back of the shielding blanket mock-up

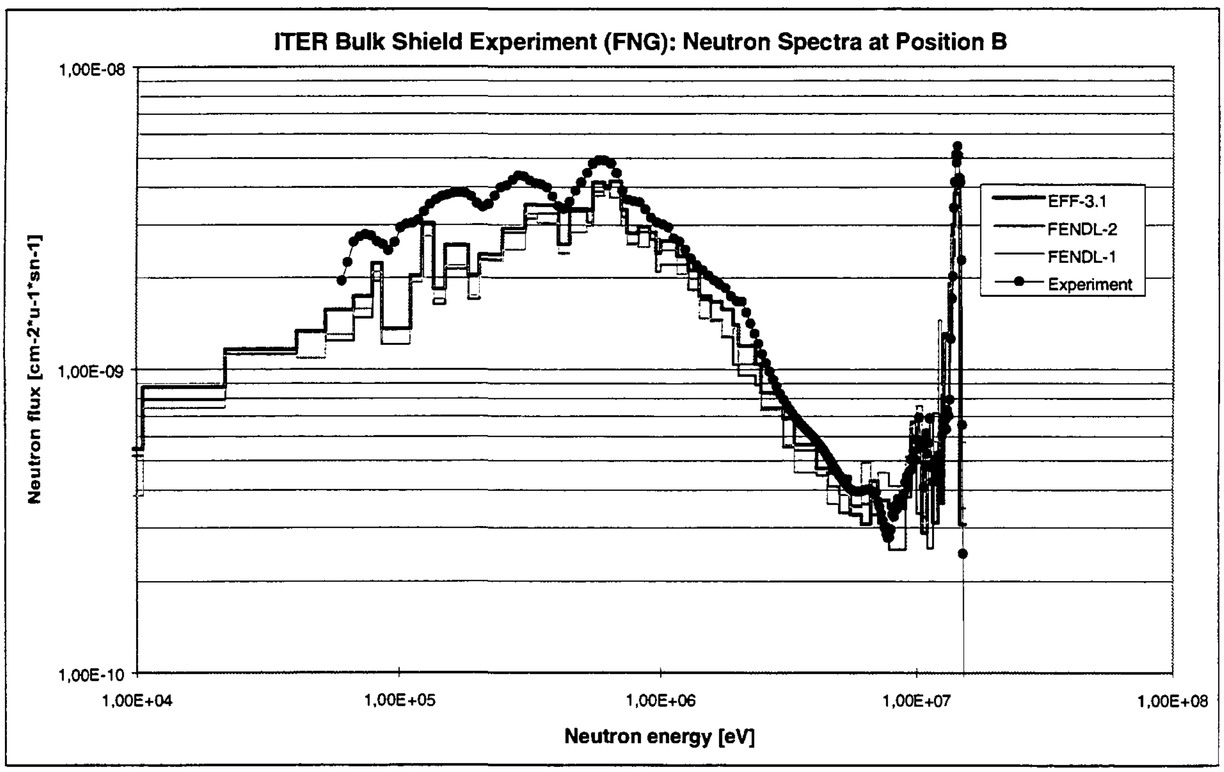

Fig. 3: Neutron flux spectra at the back of the vacuum vessel mock-up

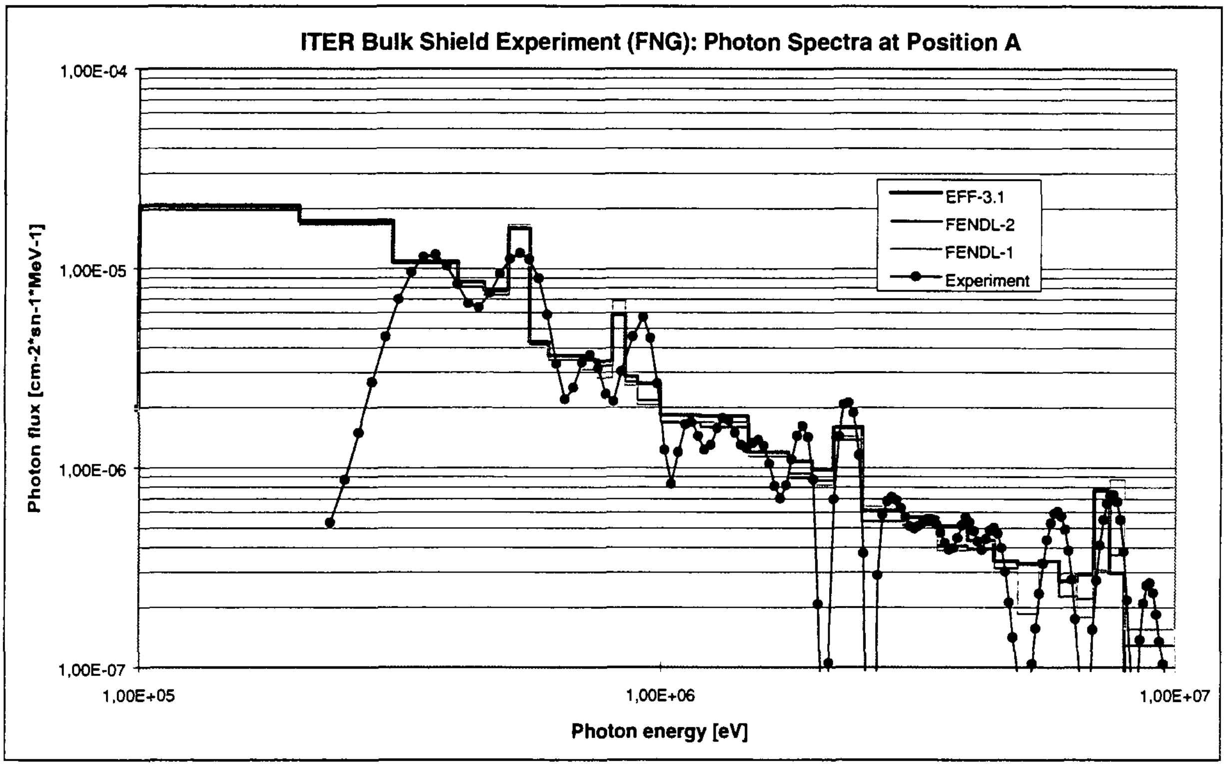

Fig. 4: Photon flux spectra at the back of the shielding blanket mock-up

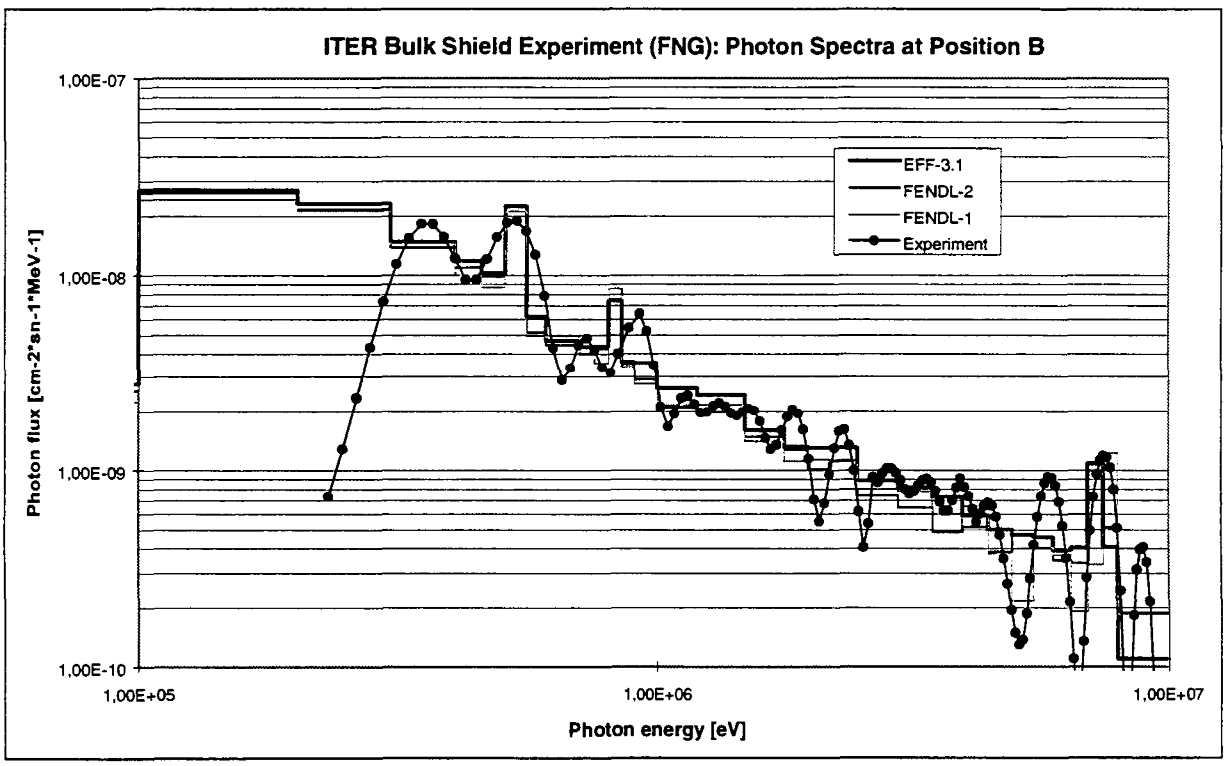

Fig. 5: Photon flux spectra at the back of the vacuum vessel mock-up

Current status of the EFF-3.1 evaluation for iron-56 and some benchmark results

Andrej Trkov

Institute 'Jozef Stefan', 1000 Ljubljana, Slovenia

Introduction

Iron is an important structural material, therefore its properties for neutron and photon transport must be accurately known. The most abundant isotope of the element is ^{56}Fe. The EFF-3.0 evaluated nuclear data file for this isotope was selected for the FENDL-2 library for fusion neutronics calculations. There exists a slight difference between the FENDL-2 file and the official EFF-3.0 file. Namely, a correction to the correlated energy-angle distributions was omitted in the EFF-3.0 file. Since the release of the EFF-3.0 file, several improvements to the nuclear data for ^{56}Fe were made. The revised file is referred to as EFF-3.1 and the improvements are described below.

The EFF-3.1 Evaluation for Iron-56

As a result of benchmark testing and with the availability of new measured data, an evaluated nuclear data file EFF-3.1 for ^{56}Fe was prepared [1], containing the following improvements:

- The resolved resonance parameters, re-evaluated by Fröhner (F.H. Fröhner, European Fusion Technology Programme, NDB1-6, Dec. 1995), are substituted by manually editing the data from the listing in the report by MacMahon, JEF/DOC-631). The energy range up to 850 keV is adopted consistently, to correct the error where the total cross section in the range 850 to 862 keV was counted twice.

- In EFF-3.0 the total cross section in the range 0.850 - 10 MeV is the EXFOR data [2] translated into ENDF-6 format, scaled to the Pronyaev evaluation [3] over broad groups. To reduce the number of data points, piecewise linear smoothing is applied.

- The EXFOR data are for natural iron. The revised total cross section for ^{56}Fe is defined such that in combination with the cross sections for the other isotopes, the reconstructed total for the natural element is reproduced. The total cross section data for ^{54}Fe from ENDF/B-VI Rev. 3 and for ^{57}Fe, ^{58}Fe from EFF-2.4 (Fröhner's recommendation, JEF/DOC-650) are assumed. In several energy intervals this correction to the total cross section exceeds 40%.

- The cross section fluctuations modulating function was recalculated, based on the new total cross section. Following the example of the original EFF-3.0 data, the fluctuations were implemented only on the inelastic cross sections for the discrete levels and the continuum [4]. The "smooth" cross sections on which the fluctuations are implemented were taken from the file by Pronyaev et al.

- The newly measured inelastic cross sections for ^{56}Fe by Dupont et al. [5] are still preliminary. After consultation with the author, the shape of the measured cross section is imposed on the Pronyaev et al. evaluation by constructing a modulating function, similarly like for the total cross section.

- To ensure cross sections consistency, the total inelastic cross section in the file is reconstructed by summing the partials. Similarly, the elastic cross section is defined as the difference between the new total and the reconstructed non-elastic cross section.

- The energy-angle correlated outgoing particle distributions were recalculated with the EMPIRE code, which uses the Multistep Direct (MSD), Multistep Compound (MSC), and Hauser-Feshbach models. The MSD model predicts the structure in the spectrum around 10 MeV of outgoing neutron energy, which is caused by the concentration of the l=2 transfer strength at this particular energy range. Consequently, structure appears also in the angular distributions. This structure is partly supported by the experimental evidence. Indirectly, it is confirmed by the independent calculations of angular distributions for the inelastic scattering to the first excited 2^+ state in the ENDF/B-VI evaluation.

- The size of the file is significantly reduced, without loss of information.

Benchmark calculations

Several benchmarks from the Fusion Benchmarks collection [6] and from the Sinbad [7] compilation were considered. The main difficulty was to identify clean and reliable benchmarks, which are sensitive enough to discriminate between different data sets. Calculations with the MCNP-4B Monte Carlo code were performed. The input models were not developed locally but taken from the literature or obtained by private communication with other experts in this field. Specific results are presented by other authors on the meeting.

In the course of investigating the apparent contradiction between the Dresden Iron Slab and the Livermore Pulsed Sphere benchmarks it became clear that the treatment of the energy-dependent angular distributions in the ACER module of NJOY is inadequate, when generating the library for the MCNP-4B code. A patch was prepared to convert the distributions to the laboratory co-ordinate system in tabulated form. The patch is available on request from the author.

Conclusions

- A revised EFF-3.1 evaluation for ^{56}Fe is completed and is offered to FENDL-2 as a replacement.

- From the benchmarks considered, the results using the new data are at least as good or better than those, calculated with the older data set.

- Current approximations in the preparation of the library for the MCNP Monte Carlo code are in some cases inadequate. A patch for the ACER module of NJOY97 is available from the author.

- Preliminary benchmarking of data is useful even at the evaluation stage. The following suggestions are made:
  - The benchmark descriptions in the Fusion Benchmarks collection and the Sinbad compilation are not always consistent. It is suggested to adopt the Sinbad and contribute to its reliability.
  - Reference input models for benchmarks should be an integral part of benchmark specifications. There exists a danger that differences in the results are erroneously attributed to the data while in fact they may originate from different assumptions in the input models.

Acknowledgement

The work was supported by the ENEA, Bologna.

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Benchmark analyses for the ITER streaming experiment with FENDL-1 and -2 nuclear cross-section data

U. Fischer[(1)], W. Hansen[(3)], D. Richter[(2)], K. Seidel[(2)], S. Unholzer[(2)]

(1) Forschungszentrum Karlsruhe, Institut für Neutronenphysik und Reaktortechnik, Karlsruhe, Germany, e-mail: ulrich.fischer@inr.fzk.de

(2) Technische Universität Dresden, Institut für Kern- u. Teilchenphysik, Dresden, Germany

(3) Technische Universität Dresden, Institut für Energietechnik, Dresden, Germany

Objective: Data testing of FENDL-1 and -2 nuclear data libraries through benchmark analyses for a design relevant integral 14 MeV neutron shielding experiment with streaming channel.

Methodology: Three-dimensional Monte Carlo calculations are performed with the MCNP4A-code to calculate and compare neutron and photon spectra measured in the ITER streaming experiment at the Frascati Neutron Generator (FNG) [1]. In addition to graphical comparisons of calculated and measured neutron spectra, C/E (calculation/experiment) data are provided for integrated neutron flux spectra.

Data: ACE data files derived from the Fusion Evaluated Nuclear Data File FENDL, versions 1 and 2, (FENDL/MC-1.0 and -2.0 as distributed by the IAEA/NDS) are used in the benchmark calculations.

Experiment: Neutron and photon flux spectra have been measured in a mock-up of the ITER inboard shield system with open channel at FNG, Frascati [2,3]. The mock-up consists of a shielding block with a thickness of 94 cm made of alternate plates of stainless steel SS-316 and of the water-equivalent material Perspex. The lateral dimensions amount to about 100 cm x 100 cm. The mock-up is backed by a 30 cm thick block of alternate SS-316 and copper plates simulating the TF-coils The Mock-up assembly includes an open channel on the central axis (inner diameter: 2.8 cm) crossing the first wall and the shielding blanket and a cavity positioned symmetrically at the end of the channel (inner dimensions: 14.8 cm x 4.8 cm x 5.2 cm, see Fig. 1).

Neutron and photon flux spectra have been measured at positions A (z = 41.4 cm) and B (z = 87.6 cm) including a series of measurements with the neutron source on the channel axis, and a second one with the source shifted off the axis (A0S, B0S with a lateral source shift of 5.3 cm). Additionally, the detectors were shifted. The detector positions A0 and B0 are located on the channel axis, whereas A1, A2 and B1 are shifted off the axis by 7.5 cm, 15.0 and 9.0 cm, respectively (Fig. 1).

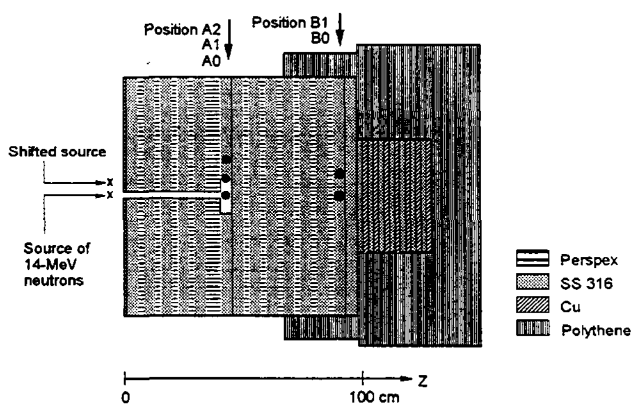

Fig. 1: ITER mock-up assembly with streaming channel and measurement positions indicated

A NE213 scintillation spectrometer has been used for neutron spectra measurements in the energy range between about 1 MeV and 15 MeV and for flux spectra of γ-rays with energies E >0.2 MeV. A set of gas-filled proportional counters was applied for the lower neutron energies, down to about E = 30 keV.

Results:

- With regard to the capability of the applied code and data to predict the measured neutron and photon flux spectra, very similar results are obtained in the ITER streaming experiment and the compact bulk shield experiment:

  1. The measured total neutron flux spectra in general are underestimated, in the order of 10% at the back of the shielding blanket (41.4 cm penetration depth) and in the order of 30% at the back of the vacuum vessel mock-up (87.6 cm penetration depth). The same is true for the high energy (E>10 MeV) neutron flux, although this component is well reproduced in the compact bulk shield experiment at the shallow measuring position A. In the streaming experiment, however, there is one peculiarity for the neutron spectra obtained at the bottom of the streaming channel (Table 1: "A0 - source on axis") where the high energy (E>10 MeV) neutron flux is underestimated by as much as 20% while, at the same time, the flux component below 10 MeV is largely overestimated (Table 1). This behaviour requires further investigations in view of its significance to properly describe the neutron streaming through design relevant void channels and ducts. It may be caused by an insufficient description of the angular distribution of the neutron scattering in the calculation.
  2. The measured photon flux spectra can be well reproduced by the calculations, both at the shallow position A and the deep position B (Table 2, Fig. 3). At the latter position there is a slight underestimation in the order of 10%. This is again in full agreement with the results obtained for the compact bulk shield experiment. Note that the photon production is largely due to thermal neutron capture reactions in this case.

- With regard to FENDL-1 and -2 data, there is no large difference in the spectra calculated for the two locations in the ITER streaming experiment, although there is a clear trend for a better reproduction of the photon spectra with FENDL-2 at deep locations (Table 2).

In conclusion, the comparison of MCNP-calculations with FENDL-1 and -2 data and measured flux spectra show that the fast neutron and γ-ray radiation can be predicted within an uncertainty margin of about 30% for a design relevant shield mock-up assembly with streaming channel. The same result had also been obtained for the corresponding compact shield mock-up system.

References:

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Table 1: Neutron flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER streaming experiment and calculation-to-experiment (C/E) ratios for FENDL-1 and -2 data.

	Energy range / MeV			
	0.1 ... 1 MeV	1 ... 5 MeV	5 ... 10 MeV	> 10 MeV
A0 – source on axis				
Experiment	(3.74 ± 0.38)E-6	(3.64 ± 0.20)E-6	(1.04 ± 0.10)E-6	(3.98 ± 0.10)E-5
FENDL-1 C/E	1.39 ± 0.14	1.32 ± 0.08	1.83 ± 0.18	0.78 ± 0.02
FENDL-2 C/E	1.39 ± 0.14	1.37 ± 0.08	1.76 ± 0.17	0.78 ± 0.02
A0 – source shifted				
Experiment	(2.25 ± 0.23)E-6	(1.71 ± 0.10)E-6	(0.42 ± 0.04)E-6	(1.65 ± 0.04)E-6
FENDL-1 C/E	1.13 ± 0.11	0.96 ± 0.06	1.08 ± 0.11	0.84 ± 0.03
FENDL-2 C/E	1.13 ± 0.11	0.95 ± 0.05	1.01 ± 0.10	0.89 ± 0.03
A1- source on axis				
Experiment		(2.10 ± 0.12)E-6	(4.79 ± 0.46)E-7	(1.26 ± 0.03)E-6
FENDL-1 C/E	-	0.85 ± 0.05	0.99 ± 0.10	0.89 ± 0.03
FENDL-2 C/E	-	0.89 ± 0.05	0.99 ± 0.10	0.87 ± 0.03
A2 – source on axis				
Experiment	-	(1.25 ± 0.07)E-6	(2.75 ± 0.26)E-7	(5.97 ± 0.16)E-7
FENDL-1 C/E	-	0.88 ± 0.05	0.97 ± 0.09	0.92 ± 0.03
FENDL-2 C/E	-	0.87 ± 0.05	0.89 ± 0.09	0.85 ± 0.03
B0 - source on axis				
Experiment	(3.26 ± 0.33)E-8	(1.45 ± 0.08)E-8	(0.26 ± 0.03)E-8	(2.19 ± 0.06)E-8
FENDL-1 C/E	0.72 ± 0.07	0.81 ± 0.05	1.07 ± 0.11	0.62 ± 0.02
FENDL-2 C/E	0.77 ± 0.08	0.89 ± 0.05	1.07 ± 0.11	0.66 ± 0.03
B0 – source shifted				
Experiment	(8.32 ± 0.84)E-9	(2.95 ± 0.16)E-9	(0.49 ± 0.05)E-9	(1.26 ± 0.03)E-9
FENDL-1 C/E	0.73 ± 0.07	0.79 ± 0.05	0.90 ± 0.09	0.67 ± 0.03
FENDL-2 C/E	0.77 ± 0.08	0.81 ± 0.05	0.95 ± 0.10	0.79 ± 0.03
B1– source on axis				
Experiment	-	(1.19 ± 0.07)E-8	(1.84 ± 0.18)E-9	(6.71 ± 0.17)E-9
FENDL-1 C/E	-	0.64 ± 0.04	0.88 ± 0.09	0.61 ± 0.02
FENDL-2 C/E	-	0.71 ± 0.04	0.88 ± 0.09	0.67 ± 0.02

Table 2: Photon flux integrals [cm^{-2}(source neutron)$^{-1}$] measured in the ITER streaming experiment and calculation-to-experiment (C/E) ratios for FENDL-1 and -2 data.

	Energy range / MeV	
	0.4 ... 1 MeV	> 1.0 MeV
A0 – source on axis Experiment	(0.81 ± 0.02)E-5	(1.43 ± 0.04)E-5
FENDL-1 C/E	0.85 ± 0.03	0.79 ± 0.03
FENDL-2 C/E	0.86 ± 0.03	0.82 ± 0.03
A0 –source shifted Experiment	(4.27 ± 0.12)E-6	(6.91 ± 0.19)E-6
FENDL-1 C/E	0.99 ± 0.03	0.99 ± 0.03
FENDL-2 C/E	1.01 ± 0.03	0.97 ± 0.03
A1- source on axis Experiment	(4.32 ± 0.12)E-6	(7.16 ± 0.20)E-6
FENDL-1 C/E	1.01 ± 0.03	1.02 ± 0.03
FENDL-2 C/E	1.06 ± 0.03	1.02 ± 0.03
A2 – source on axis Experiment	(3.13 ± 0.09)E-6	(5.16 ± 0.14)E-6
FENDL-1 C/E	1.00 ± 0.03	0.97 ± 0.03
FENDL-2 C/E	1.01 ± 0.03	0.94 ± 0.03
B0- source on axis Experiment	(2.52 ± 0.07)E-8	(3.65±0.10)E-8
FENDL-1 C/E	0.77 ± 0.03	0.80 ± 0.03
FENDL-2 C/E	0.86 ± 0.03	0.85 ± 0.03
B0 – source shifted Experiment	(0.68 ± 0.02)E-8	(1.02 ± 0.03)E-8
FENDL-1 C/E	0.85 ± 0.03	0.93 ± 0.04
FENDL-2 C/E	0.91 ± 0.03	1.26 ± 0.34
B1– source on axis Experiment	(1.97 ± 0.06)E-8	(2.91 ± 0.08)E-8
FENDL-1 C/E	0.74 ± 0.02	0.75 ± 0.02
FENDL-2 C/E	0.84 ± 0.03	0.94 ± 0.14

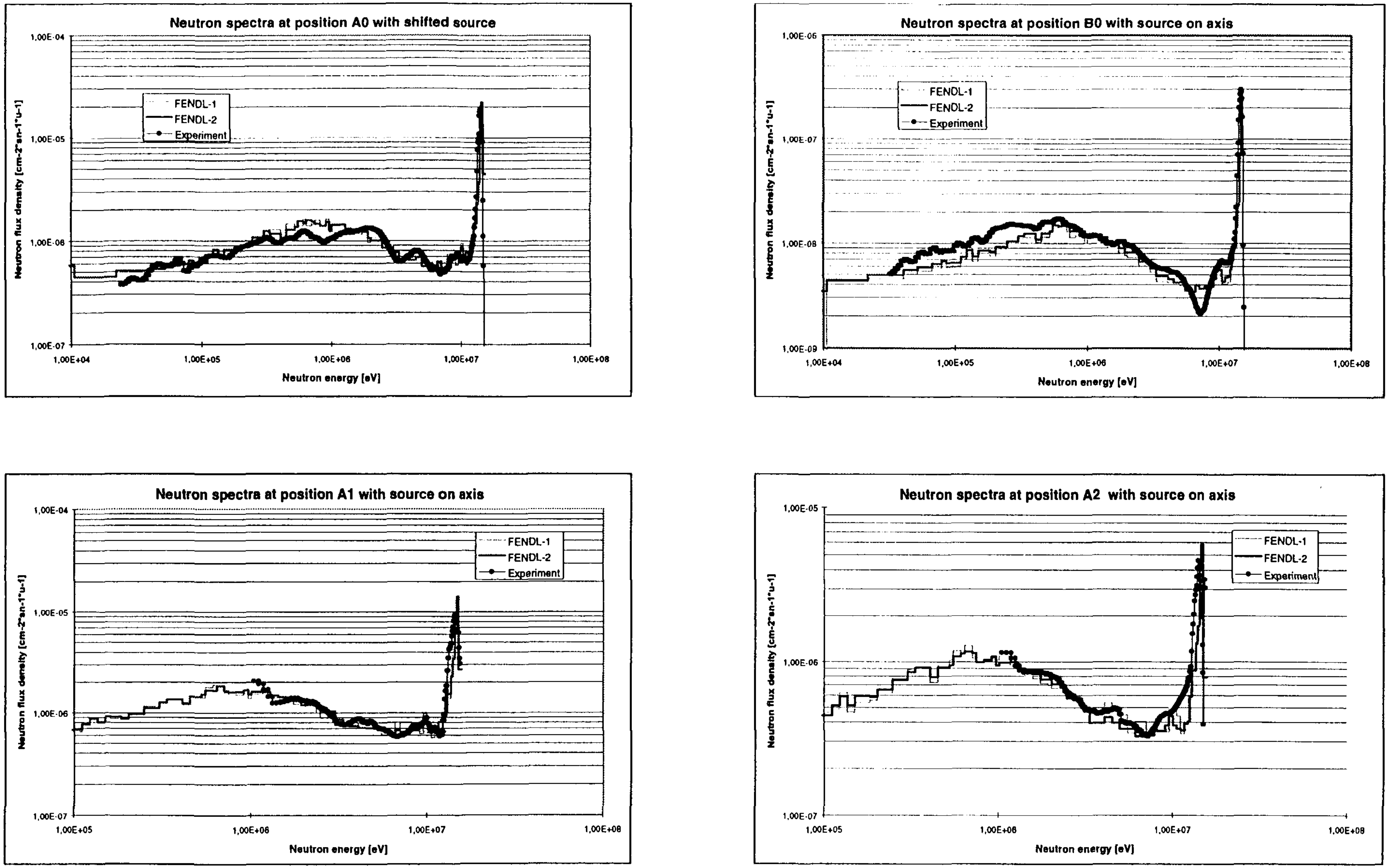

Fig. 2: ITER streaming experiment: comparison of neutron flux spectra at different positions

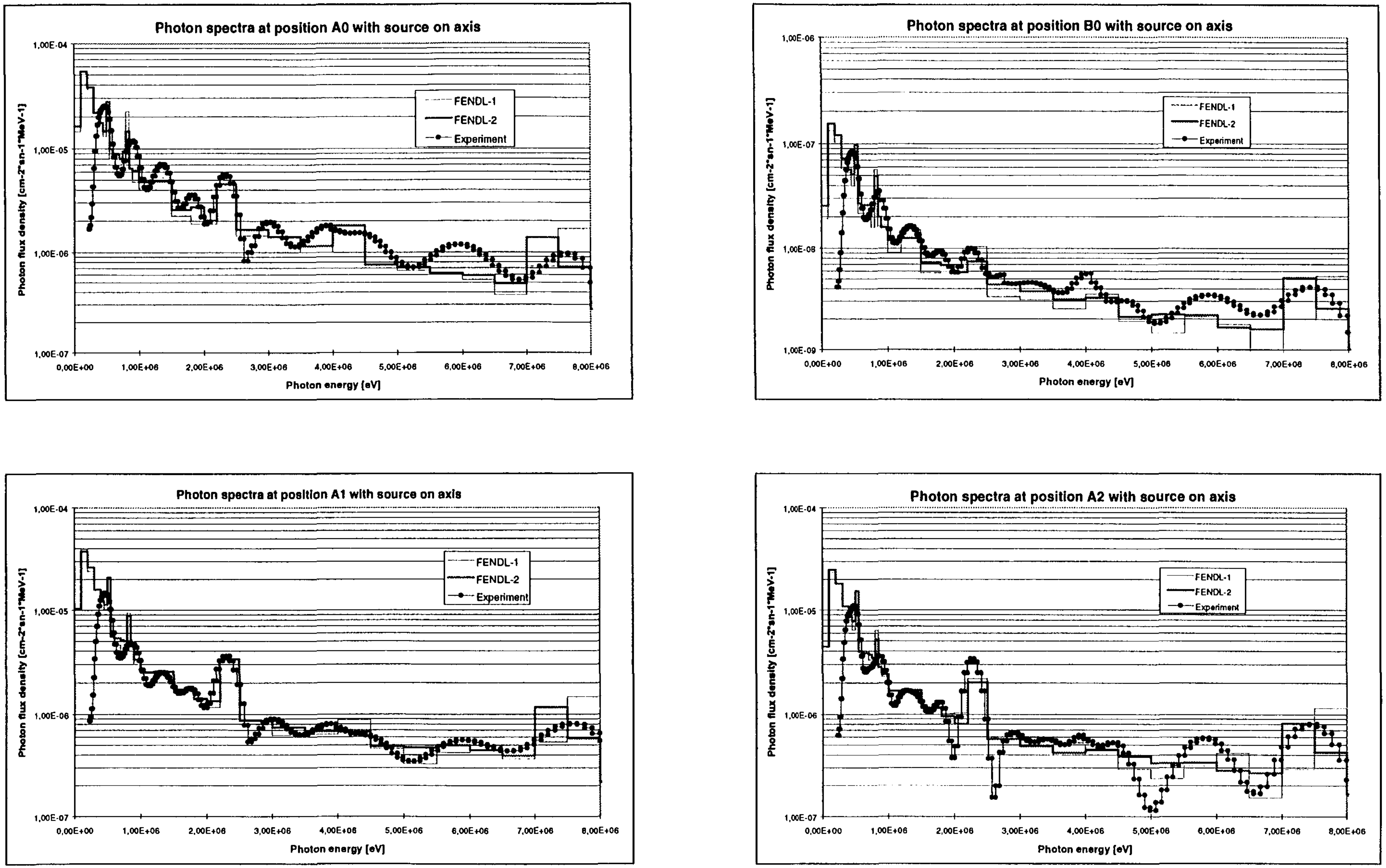

Fig. 3: ITER streaming experiment: comparison of photon flux spectra at different positions

Analysis of FNS iron benchmark experiments

F. Maekawa

Japan Atomic Energy Research Institute
Tokai-mura, Naka-gun Ibaraki-ken 319-1195, Japan

Clean Benchmark Experiment

In the FNS clean benchmark experiment, neutron spectra, dosimetry reaction rates, gamma-ray spectra, and gamma-ray heating rates were measured inside an iron shield assembly of 1 m diameter and 0.95 m thickness. Benchmark analyses of the experiment were performed by MCNP with the following three nuclear data sets:

(a) FENDL/E-1.0 (ENDF/B-VI for all Fe isotopes)

(b) EFF-3.0 for ^{56}Fe and FENDL-1 for the other iron isotopes

(c) FENDL-2.0 (EFF-3 for ^{56}Fe and FENDL-1 for the other Fe isotopes)

All the calculations agree very well with neutron spectra in the energy range from 1 eV to 1 MeV up to the depth of 810 mm. As for threshold reaction rates and integral neutron fluxes in the six energy intervals, a very good agreement, typically within 10%, with the experimental data are achieved in all three calculations. However, with increase of the iron thickness there is a slight trend for underestimation of the 14 MeV neutron flux.

Very large C/E ratios for γ-ray heating rates in iron are obtained when using the EFF-3 + FENDL-1 libraries in the calculation (case-(b)). The maximum value of ~ 1.7 is reached at 100 mm depth in the iron assembly. This problem is due to the double counting of γ-ray production cross sections in MT=3 and MT=12~15 of the ^{56}Fe evaluation, which has been corrected in FENDL/E-2.0. The FENDL/E-1.0 and FENDL/E-2.0 calculations provide very good results for the γ-ray heating rates since for both the C/E ratios are within the experimental uncertainty of ~ 10%. The γ-ray spectra calculated using cross sections of (a) and (c) also agree well with the experimental data. These results indicate validity of the γ-ray production cross sections for the threshold reactions as well as the (n,γ) reactions.

Analysis of Cross Section at ~14 MeV

Possibilities to improve the underestimation of 14-MeV neutron flux penetrating through iron shield were investigated by Dr. Konno, FNS/JAERI. The FNS Iron clean benchmark experiment was analyzed with FENDL/E-1, FENDL/E-2.0 and JENDL-FF. All the calculations underestimated the neutron flux above 10 MeV by 10 ~ 30% at 716 mm depth position.

First, sensitivity of the neutron flux to the replacement of File-3 data for ^{56}Fe among the three evaluations were estimated. It was found that the File-3 data in FENDL-1 gave the C/E ratios closest to 1.0 while those in JENDL-FF gave the lowest C/E ratios, when the same cross sections except file MF=3 were used. This indicate that the C/E ratios approach 1.0 when cross sections for such reactions as the continuum inelastic scattering, (n,2n), (n,np), which remove neutrons from the 14 MeV range, are small. Still, all the C/E ratios are lower than 1.0 independently of any replacement of the file MF=3 data.

Next, the influence of the angular distributions of elastically scattered neutrons was investigated. At 0 degree, the cross section in FENDL/E-2.0 is the largest, while those of JENDL-FF and FENDL/E-1 are respectively 6% and 15% smaller. When the angular distributions for the elastic scattering in FENDL/E-1 were replaced by those of FENDL/E-2.0, keeping the rest of the data unchanged, the C/E ratios of the neutron flux above 10 MeV were close to 1.0.

Accordingly, two suggestions are proposed:

- It is worthwhile to investigate the possibilities of decreasing the removal cross sections for 14-MeV neutrons in ^{56}Fe evaluation in FENDL/E-2.0.
- Attention should be paid to angular distributions of elastically scattered neutrons at 14 MeV, because of the observed sensitivity of the 14 MeV neutron penetration through thick iron shields to the elastic angular distributions at forward angles.

Duct Streaming Experiment

A series of streaming experiments was conducted as a task for ITER/EDA. The experimental data were accumulated for various duct and gap configurations. Here, we select the small duct streaming experiment because it is the most suitable for testing nuclear data itself due to the large iron thickness of 1.2 m and the small duct diameter of 100 mm. Measured nuclear responses are dosimetry reaction rates, neutron spectra, gamma-ray heating rates, and gamma-ray spectra. The experimental data are compared with MCNP calculations using JENDL-FF, FENDL/E-1 and FENDL/E-2.0.

In spite of the rather complicated experimental configuration, as compared with that of the clean benchmark experiment, good agreement (typically within 20%) was achieved for all nuclear responses in all three calculations. A slight underestimation trend for the 14 MeV neutron flux was also confirmed in this experiment.

Monte Carlo uncertainty analysis for an iron shielding benchmark experiment

U. Fischer[(1)], R. L. Perel[(2)], H. Tsige-Tamirat[(1)], Y. Wu[(3)]

[(1)]Association FZK-Euratom, Forschungszentrum Karlsruhe, P.O. Box 3640,
D-76021 Karlsruhe, Germany, Institut für Neutronenphysik und Reaktortechnik,
e-mail: ulrich.fischer@inr.fzk.de, tsige@inr.fzk.de
[(2)] Hebrew University of Jerusalem, 91904 Jerusalem, Israel, e-mail: perel@vms.huji.ac.il
[(3)] Institute of Plasma Physics, P.O. Box 1126, Hefei, 230031, P.R. China,
e-mail: ycwu@ipnc1.hfcas.ac.cn

ABSTRACT

This work is devoted to the computational uncertainty analysis of an iron benchmark experiment having been performed previously at the Technical University of Dresden (TUD). The analysis is based on the use of a novel Monte Carlo approach for calculating sensitivities of point detectors and focuses on the new ^{56}Fe evaluation of the European Fusion File EFF-3. The calculated uncertainties of the neutron leakage fluxes are shown to be significantly smaller than with previous data. Above 5 MeV the calculated uncertainties are larger than the experimental ones. As the measured neutron leakage fluxes are underestimated by about 10 - 20% in that energy range, it is concluded that the ^{56}Fe cross-section data have to be further improved.

1 INTRODUCTION

Neutron and photon radiation penetrating the shielding system of fusion reactors results in crucial loads to the superconducting magnets. As a consequence, the safety margins for shielding related nuclear responses have to be known with high precision. A major neutronic task is to provide well qualified assessments of the related uncertainties and finally to assure the requested accuracy. This can be achieved by means of sensitivity and uncertainty calculations having been qualified by applications to integral benchmark experiments. Along this guide-line, this work is devoted to the uncertainty analysis of an iron benchmark experiment performed previously at the Technical University of Dresden (TUD) [1]. The analysis is based on the use of the Monte Carlo sensitivity approach for point detectors by applying the differential operator method and using covariance data from the European Fusion File EFF for calculating the resulting uncertainties.

2 COMPUTATIONAL ASPECTS

2.1 Sensitivity and Uncertainty Analysis

The usual approach in sensitivity and uncertainty analysis is to calculate the sensitivity to the involved data of a specified nuclear response on the basis of perturbation theory using direct and adjoint fluxes provided by discrete ordinates calculations. The resulting sensitivity profiles can be used to calculate the uncertainties when folding with the covariance matrices of the underlying nuclear cross sections. There are, however, several drawbacks with this approach. First of all, it is very difficult to properly calculate two- and three-dimensional problems as they are typical in fusion applications. A further drawback is the necessary use of group-averaged cross sections involving many approximations. In addition, a sensitivity calculation of many ("N") responses (e.g. neutron fluxes in N groups), necessitates one transport calculation of the direct flux, N transport calculations of the adjoint fluxes and N additional calculations to get the sensitivity for each of the N responses.

2.2 Monte Carlo Sensitivity Calculations

These drawbacks can be avoided when basing the sensitivity calculations on the Monte Carlo method. Any complex geometry thus can be handled without severe constraints, there are no numerical convergence problems and, in addition, the energy dependence of the cross sections can be accurately described when using the pointwise representation. Suitable computational tools allowing the calculation of sensitivities with the Monte Carlo technique became available recently. At the Hebrew University of Jerusalem [2], a computational technique has been developed for calculating point detector sensitivities based on the use of the differential operator method. This technique has been implemented into a local update to MCNP4A [3] and allows to calculate all the sensitivities in one single Monte Carlo run. More recently, sensitivity capabilities have been incorporated into the MCNP4B code to enable sensitivity calculations for track length estimators.

2.3 Nuclear Cross-Section Data

Nuclear data are taken from the European Fusion File, versions EFF-2 and -3 [4], for the Monte Carlo transport and sensitivity calculation as well as for the uncertainty calculation. The focus, however, is on the new ^{56}Fe evaluation of EFF-3 which includes an accurate description of the total neutron cross section in the unresolved energy range above 0.85 MeV, based on ultra-high resolution measurements performed at IRMM Geel [5]. In addition, the EFF-3 ^{56}Fe evaluation includes a new evaluation of all reaction cross sections and their covariance data which resulted in significantly smaller uncertainties as compared to previous evaluations.

2.4 Covariance Data for Uncertainty Calculations

The covariance data have been generated from the basic EFF files in the VITAMIN-J 175 group structure with the help of the NJOY processing code [6]. Both libraries, EFF-3.0 and the basic version of EFF-2.4, include data for the cross sections of single reactions while the user version of EFF-2.4, on which the MCNP library is based, has for several reactions only lumped cross sections. In order to be able to determine the uncertainty in the responses, a set of reactions had to be defined for each library which describe all neutron reactions and for which all needed data - cross sections and covariances - are available; this set turned out to be different for each library.

3 TUD IRON BENCHMARK EXPERIMENT

This experiment has been previously conducted in the framework of the European Fusion Technology Programme at the Technical University of Dresden [1] to provide the database for benchmark tests of iron cross-section data. An iron slab with a front surface of 100 cm x 100 cm and a thickness of 30 cm has been irradiated with 14 MeV neutrons. A point-like radiation detector was placed at a distance of 349 cm from the target to record the neutron and photon leakage flux spectra. A NE 213 scintillation detector was used to measure the neutron and photon flux spectra above 1 and 0.4 MeV, respectively, while several types of gas filled proportional counters were used for measuring the low energy neutron spectrum ($E \geq 0.03$ MeV).

4 MONTE CARLO ANALYSIS

A full three-dimensional MCNP model of the experimental set-up including the collimator, the floor, the wall, the air, the assembly rack, the cooling and the target holder has been developed by TU Dresden [1]. This model ("full geometry"), complemented with a source routine to describe properly the anisotropic neutron emission from the target, was applied to calculate the neutron leakage spectra for comparison with the measured data. In addition, an "ideal geometry model" has been set up consisting of the point neutron source, the iron slab and the point detector. In the Monte Carl runs, typically 5 to 10 million source neutron histories were tracked.

4.1 Neutron Flux Spectra

Calculated and measured neutron leakage spectra are compared in Fig 1. C/E data (calculation/experiment) are shown in Table. 1. There is generally good agreement for the "state-of-the-art" data files (EFF-2, -3, FENDL-1, JENDL-FF) except for the high energy component (E> 10 MeV) which is underestimated by 10 to 20%. With regard to EFF-3 there is, in addition, an underestimation of the e neutron spectrum in the 5-10 MeV range by about 25%.

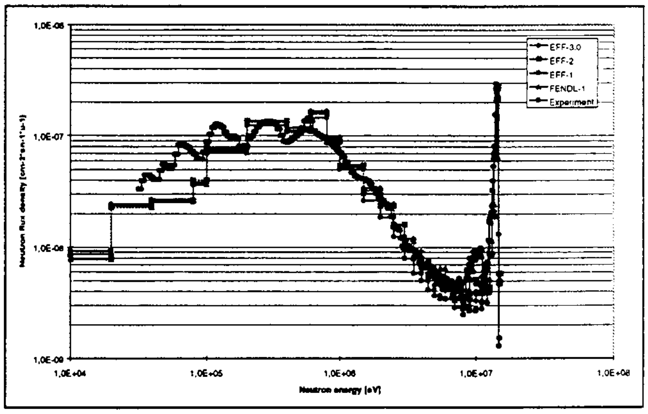

Fig. 1: Comparison of neutron leakage flux spectra

Energy range [MeV]	Experiment [n·cm^{-2}sn^{-1}]	C/E EFF-3	EFF-2	EFF-1	FENDL -1
0.1-1	$(2.56 \pm 0.28)\cdot 10^{-7}$	1.04	1.02	0.94	0.99
1-5	$(4.51 \pm 0.21)\cdot 10^{-8}$	0.99	0.98	0.83	0.94
5 – 10	$(3.42 \pm 0.19)\cdot 10^{-9}$	0.74	0.90	0.64	0.95
> 10	$(1.59 \pm 0.07)\cdot 10^{-8}$	0.87	0.91	0.72	0.83
> 0.1	$(3.2 \pm 0.31)\cdot 10^{-7}$	1.02	0.98	0.91	0.98

Table 1: C/E comparison of neutron leakage flux integrals in the TUD iron benchmark experiment.

4.2 Sensitivity Profiles

Monte Carlo point detector sensitivity calculations have been performed for the neutron leakage fluxes. Table 2 shows the relative sensitivities of the neutron leakage fluxes to the specified EFF-3 ^{56}Fe reaction cross sections in a coarse 5 group representation. An increase of 1% in the continuum inelastic scattering cross section (at all energies) e.g. would result in a decrease of 1.75% in the leakage flux above 10 MeV.

Table 2: Relative sensitivity [%/%]of the neutron leakage flux integrals in the TUD iron benchmark experiment to ^{56}Fe EFF-3 reaction cross sections integrated over all energies.

Energy range of leakage [MeV]	<0.1	0.1-1	1-5	5-10	>10	total
Elastic scattering (MT=2)	-2.39	-1.22	-1.32	-0.89	-0.61	-1.33
(n,2n) –reaction (MT=16)	0.19	0.11	-0.19	-0.54	-0.98	0.03
1st level inelastic scatt. (MT=51)	0.16	-0.01	-0.98	-0.18	-0.11	-0.11
Continuum inelastic scatt. (MT=91)	-0.22	-0.19	-0.25	-1.35	-1.75	-0.28

4.3 Uncertainty Analysis

By making use of the sensitivity profiles calculated in the VITAMIN-J 175 group structure along with the covariance data provided in the same group structure, the uncertainties of the neutron leakage flux integrals have been calculated. As shown in Table 3, there is a clear improvement of the new EFF-3 over the EFF-2 data in terms of reduced uncertainties. In particular, this is true for the high energy fluxes above 1 MeV. Due to correlations in the uncertainties originating from elastic and inelastic scattering, the uncertainties in the total neutron flux differ not very much. The uncertainties calculated with the full geometry model agree with that of the ideal geometry model except for the low energy group (E<0.1 MeV). This is caused by the fact that considerably more reaction events take place in the case of the full geometry model thereby decreasing the contribution to the total uncertainty of the single isotope ^{56}Fe. This effect is strongest for the lowest energy group which is populated by neutrons having undergone lots of multiple scattering events.

Table 3: Uncertainties [%] of calculated neutron leakage fluxes in the TUD iron slab experiment due to uncertainties in the ^{56}Fe cross section data and experimental uncertainty.

Energy range of leakage [MeV]	MC-calculation ideal geometry EFF-3.0	MC-calculation ideal geometry EFF-2.4	S_n calculation ideal geometry EFF-3.0	MC-calculation full geometry EFF-3.0	Experimental uncertainty
<0.1	9	9	-	3	-
0.1-1	3	4	3	3	11
1-5	1.6	20	2	1.5	2.2
5-10	8	27	10	6	2.9
>10	4	19	14	4	1.9
Total	3	4	-	2.5	-

Table 3 includes uncertainties calculated with the sensitivity/uncertainty code SUSD [7] on the basis of two-dimensional forward and adjoint S_N-calculations performed with the TWODANT discrete ordinates code [8] in (r,z) geometry. There is good agreement with the Monte Carlo results except for the high energy component where the two-dimensional S_N-calculation suffers from the ray effect. This has been further investigated by comparing the sensitivity of the neutron fluxes to the total neutron cross section with the sensitivity to the iron nuclide density. Good agreement was found for the Monte Carlo sensitivities while there was disagreement for the sensitivity profiles of the high energy fluxes as calculated by SUSD/TWODANT.

As compared to the experiment, the calculated uncertainties are lower than the experimental ones below 5 MeV but higher above that neutron energy. At the same time, the measured high energy flux is underestimated (Table 1) suggesting to decrease, in the first place, the inelastic scattering cross sections in the high energy range in agreement with the sensitivity results (Table 2).

CONCLUSION

The Monte Carlo approach for calculating sensitivities of point detectors has been applied to the TUD iron benchmark experiment thus providing the basis for assessing the uncertainties of the calculated neutron flux spectra due to the underlying cross-section uncertainties. It has been shown that this approach is a versatile computational tool for performing sensitivity and uncertainty analyses of fusion relevant benchmark experiments. As there is no restriction with regard to the geometry, the same basic approach can be applied to real fusion reactor configurations to assess the uncertainty of relevant nuclear responses. With regard to the EFF-3 ^{56}Fe data, it has been shown that further improvements are needed at high neutron energies to arrive at error levels within the experimental ones and to get better agreement with the measured neutron flux spectra.

ACKNOWLEDGEMENT

This work has been performed in the framework of the nuclear fusion programme of Forschungszentrum Karlsruhe and is supported by the European Union within the European Fusion Technology Programme.

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Recent RSICC experiences with FENDL-2.0 processed multigroup data

J.E. White

Radiation Safety Information Computational Center
Oak Ridge National Laboratory
Oak Ridge, TN 37831

The Radiation Safety Information Computational Center is a technical institute serving an international radiation community. RSICC selects, acquires, stores, retrieves, evaluates, analyzes, synthesizes, and disseminates information on radiation transport and safety. Since 1992, RSICC has been involved in working with the FENDL community to help meet the practical nuclear data needs of fusion analysts. In addition, RSICC has served as an unofficial liaison between the FENDL project and the ITER nuclear analysis group.

To provide nuclear data needed in radiation transport applications, RSICC participates in many data activities, with the most emphasis placed on nuclear cross sections. Through cooperation with others, RSICC assists in improving the quality of basic evaluated cross section data through participation in the U.S. Cross Section Evaluation Working Group. In addition, RSICC packages and disseminates various types of data libraries important for radiation transport. Since FENDL represents the most comprehensive collection of nuclear data targeted to address radiation problems in fusion systems, there is strong interest in making FENDL part of the RSICC data collection.

The accepted benchmark data testing exercises, which are performed to assess the suitability of FENDL-2.0 processed nuclear data for fusion applications, indirectly limit the scope of data testing to the ACE format used in MCNP. Because of the strong link between RSICC and the deterministic transport community, there was a need to help review the FENDL-2.0 data for use in discrete ordinates codes. During the last FENDL AGM, RSICC was asked to review the FENDL-2.0 processed multigroup data and perform simple physics checks before the final release. No serious discrepancies were detected by the RADE checking program as reported in a letter to IAEA/NDS on April 23, 1998.

While testing FENDL-2.0 multigroup data using ANISN, a problem in the magnitude of the gamma-ray flux for a steel/water configuration in a "typical" ITER design was identified. An investigation of the gamma-ray problem exposed an error in the Si-29 evaluated data file from ENDF. The nature of the error, in the description of the photon angular distributions from capture, was such that the error had no adverse impact on the generation of the ACE formatted data for MCNP.

In summary, the RSICC experiences highlight the reality that processed nuclear data should be used with caution.

Nuclear Data Section	e-mail: services@iaeand.iaea.or.at
International Atomic Energy Agency	fax: (43-1)26007
P.O. Box 100	cable: INATOM VIENNA
A-1400 Vienna	telex: 1-12645 atom a
Austria	telephone: (43-1)2600-21710

Online: TELNET or FTP: iaeand.iaea.or.at
username: IAEANDS for interactive Nuclear Data Information System
usernames: ANONYMOUS for FTP file transfer;
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Web: http://www-nds.iaea.or.at