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Summary Report of Consultants' Meeting

Improvements and Extensions to IRDF (International Reactor Dosimetry File (IRDF-2002))

IAEA Headquarters, Vienna, Austria
5 – 7 May 2010

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December 2010

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Abstract
The main aim of this Consultants' Meeting was to discuss the appropriate manner for implementing improvements and extensions to the current IRDF-2002 reactor dosimetry library. It was important to assess the applications requiring a dosimetry library, to discuss if a library that would meet the requirements of these varied applications could be produced and, if so, to define an approach for producing such an updated version.

This report summarises the presentations and discussions undertaken in order to achieve these goals, followed by the recommendations and conclusions resulting from the meeting.

December 2010

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1. Introduction

The International Reactor Dosimetry File (IRDF-2002) was released in 2005, based on cross section evaluation work started over a decade ago, and is widely used for reactor dosimetry applications. As nuclear power reactors age, assessment relating to reactor lifetime management becomes ever more important and of international concern. In addition, emerging applications are requiring dosimetry data up to ever higher energies with an equivalent level of accuracy and uncertainty information. Hence, it was deemed a timely action to arrange a Consultants' Meeting to discuss future dosimetry needs and the potential for an updated library.

2. Objectives

The main objective of the Consultants' Meeting was to discuss and decide whether the International Reactor Dosimetry File (IRDF-2002) should be improved and extended to higher neutron energies, principally for application at higher energy neutron sources that are used to irradiate fusion reactor materials, such as the International Fusion Materials Irradiation Facility (IFMIF). An affirmative decision requires the formulation of specific action items and recommendations regarding the evaluation, testing, and issuance of a new neutron cross section file.

3. Summary of Presentations

Following the welcome address of Robin Forrest, Section Head of the IAEA Nuclear Data Section (IAEA-NDS), Roberto Capote (IAEA-NDS) summarised the work that has been undertaken since the release of IRDF-2002, including cross section evaluation work (see presentation below), and previous meetings. He made it clear that the current library is the *de facto* reactor dosimetry library adopted by all major evaluation projects (most no longer produce their own), but that work was required so that the library would meet the needs for fusion and accelerator applications, i.e. there was a need to extend IRDF-2002 to higher energies, and further covariance data are required for all applications.

Prior to any formal presentations, each participant was asked to comment on their expectations for the meeting, and possible involvement in work to improve the dosimetry library. The relevant points are summarised here.

1. Robin Forrest clarified the project options available for improvements to IRDF-2002, i.e. a Coordinated Research Project (CRP) or a Data Development Project (DDP).
2. Eva Zsolnay commented that she had a PhD student involved in work related to IFMIF at FZK Karlsruhe. Thus she hoped that this connection would be useful in defining the needs for a future dosimetry library.
3. Andrej Trkov stated that funding for nuclear data is difficult to obtain, and that users unrealistically expect data to be provided without funding.

3.1. R. Capote (IAEA Nuclear Data Section)

At fission reactor energies, the IAEA-NDS has, over the past three years, sponsored new cross section evaluations by K.I. Zolotarev of IPPE Obninsk, Russia that should be tested for eventual inclusion in a new, evaluated nuclear data file to replace IRDF-2002. The methodology used for this work and the complete details are available in the following three

IAEA INDC(NDS) series reports written by K.I. Zolotarev and available from the IAEA-NDS website (http://www-nds.iaea.org/reports-new/indc-reports/indc-nds/):

1. *Re-evaluation of Microscopic and Integral Cross-Section Data for Important Dosimetry Reactions*, INDC(NDS)-0526;
2. *Evaluation of Cross-section Data from Threshold to 40-60 MeV for Specific Neutron Reactions Important for Neutron Dosimetry Applications*, INDC(NDS)-0546; and
3. *Evaluation of Cross-Section Data from Threshold to 40 MeV for Some Neutron Reactions Important for Fusion Dosimetry Applications*, INDC(NDS)-0584).

The cross section evaluations concerned have been carried out for the dosimetry reactions listed in Table 1.

Table 1: Recent cross section evaluations by K.I. Zolotarev

Report	**INDC(NDS)-0526**	**INDC(NDS)-0546**	**INDC(NDS)-0584**
Reactions evaluated	^{24}Mg(n,p)^{24}Na	^{27}Al(n,α)^{24}Na	^{59}Co(n,3n)^{57}Co
	^{32}S(n,p)^{32}P	^{55}Mn(n,2n)^{54}Mn	^{89}Y(n,2n)^{88}Y
	^{60}Ni(n,p)$^{60m+g}$Co	^{59}Co(n,p)^{59}Fe	^{93}Nb(n,2n)^{92m}Nb
	^{63}Cu(n,2n)^{62}Cu	^{59}Co(n,2n)$^{58m+g}$Co	^{169}Tm(n,2n)^{168}Tm
	^{65}Cu(n,2n)^{64}Cu	^{90}Zr(n,2n)$^{89m+g}$Zr	^{209}Bi(n,3n)^{207}Bi
	^{64}Zn(n,p)^{64}Cu		
	^{115}In(n,2n)^{114m}In		
	^{127}I(n,2n)^{126}I		
	^{197}Au(n,2n)^{196}Au		
	^{199}Hg(n,n')^{199m}Hg		

Other sources of new evaluations to be considered include:

1. The Neutron Cross Section Standards library (see http://www-nds.iaea.org/standards/ and "International Evaluation of Neutron Cross Section Standards", A.D. Carlson et al., *Nuclear Data Sheets* **110** (2009) 3215-3324).
2. Evaluations from the thorium/uranium CRP (see http://www-nds.iaea.org/Th-U/ and *Evaluated Nuclear Data for Nuclides within the Thorium-Uranium Fuel Cycle*, R. Capote et al., STI/PUB/1435, IAEA, May 2010).
3. The on-going work at IRMM Geel, Belgium and IJS Ljubljana, Slovenia, on the cadmium evaluation.

It was also noted that, owing to the importance of having covariance data in a dosimetry library, one might consider adopting covariances calculated by nuclear model codes, e.g. from the latest version of TENDL (http://www.talys.eu/tendl-2010/).

Finally the required accuracy for fusion and accelerator applications needs to be documented in the same way that has been done for fission reactors.

3.2. A. Trkov (IJS Ljubljana, Slovenia)

Outlined some of the problems associated with processing IRDF-2002 with NJOY (R.E. MacFarlane and D.W. Muir, *The NJOY nuclear data processing system*, LA-12740-M, Los Alamos National Laboratory, (1994); RSICC Code Package PSR-368, (1999)) and/or

PREPRO (D.E. Cullen, *PREPRO 2007 ENDF/B Pre-processing Codes*, INDC(NDS)-39, International Atomic Energy Agency (2001)). These had now been removed following a combination of code updates and minor adjustments to the covariance files in IRDF-2002. (See section 4 for further details.)

Validation of IRDF-2002 had been carried out for relevant applications and it was re-iterated that one must take care to use the correct Westcott *g*-factor when validating against k_0 data. One must also correctly understand the use of resonance integrals when using the cadmium-ratio method.

Future improvements should address known problems, such as format issues, isomeric state definitions, extension to higher energies (including additional reactions), additional and better covariance data, and additional monitor reactions for fission reactors (specifically zinc).

3.3. L. Greenwood (Pacific Northwest National Laboratory, Richland, USA)

Summarised work on the experimental validation of IRDF-2002, including both research reactors and commercial ones. It was felt that for 14 MeV fusion sources, the current dosimetry library is sufficient, but that extensions will definitely be required for fusion material testing facilities. It was also queried as to whether a future dosimetry library for spallation sources was within the remit of this meeting?

A number of issues were raised for discussion, including:

- the envisaged upper energy limit,
- need for covariance data,
- what testing can be done (especially in accelerator and fast reactor spectra)?, and,
- what radiation damage and gas production data can be included?

The requirement for the inclusion of damage cross sections was further highlighted with some examples. This provoked a discussion about the availability of suitable data and the ability for calculating damage cross sections, for example by using the NJOY processing code. Although NJOY can indeed calculate damage cross sections, the recoil spectra must be included in the original evaluations, which is not the case for those from Zolotarev. It was generally felt that damage cross sections should be taken from available sources, as was the case for IRDF-2002.

3.4. R. Capote (IAEA Nuclear Data Section)

A summary was given of the presentation made by P.J. Griffin (Sandia National Laboratories, USA) at the International Conference on Nuclear Data for Science and Technology, 26-30 April 2010, Jeju Island, Korea.

The talk discussed the use of model-based covariance data and their possible use for dosimetry purposes, as well as the availability of covariance data in the ENDF/B-VII library. It was noted that this library lacks a significant amount of covariance data and, although the possibility to use model-generated covariance data exists, it was stated as being absolutely fundamental that the covariance data must be produced using a methodology which matches that being used to produce the evaluated data. Both TALYS and EMPIRE can automatically produce covariance data, but an assessment of these data showed that TENDL-2008, for

example, contained uncertainties significantly larger (by a factor of 8 in some cases) than in IRDF-2002. It was also clear that a comparison of TENDL-2008 to experimental data showed a variation of greater than one standard deviation, highlighting the fact that this global version of the TENDL library is not suitable for dosimetry.

In the discussion that followed, it was noted that EMPIRE could be used to produce covariance data as "a prior" - to be combined with experimental data - more easily than TALYS and that this approach was sensible.

3.5. E. Zsolnay (Institute of Nuclear Techniques, Budapest, Hungary)

Presented, on behalf of herself and H.J. Nolthenius, the paper reproduced in Annex 1 to this report, which documents many of the fundamental issues relating to the extension of the IRDF-2002 dosimetry library.

This paper served as the basis for the subsequent discussions which took place. A summary of these discussions is given below, and the resulting actions, recommendations and work plan are presented thereafter.

4. Summary of Discussions

With regard to the status of nuclear data the attendees agreed that:

1. both new and improved cross section evaluations are available for fission reactor applications,
2. there is a need to produce a dosimetry library for use at higher neutron energies, e.g. for application at IFMIF or other accelerator-based fusion reactor relevant neutron sources,
3. sufficient cross section evaluations are available at higher neutron energies to allow the extension to higher energy, and
4. the new file should be called the International Reactor Dosimetry and Fusion File (IRDFF).

The general consensus was that sufficient cross section data evaluations (twenty-nine are listed in Annex 1) were currently available such that work could proceed on producing an update to IRDF-2002 (tentatively referred to as IRDFF) without the need for a Coordinated Research Project (CRP), which would take longer to organize, to provide these evaluations. It was felt that it would be possible to release the IRDFF in approximately two years due to the availability of evaluated cross sections and the effort required to create, test and issue the new file.

It was also noted that there are some minor problems in IRDF-2002 related to the processing of covariance files which have recently been solved by A. Trkov and others (A. Trkov, *IRDF-2002.1 Corrections to the IRDF-2002 Dosimetry Cross-Section Library (Covariance Processing Verification)*, INDC(NDS)-0576, IAEA, 2010). These corrections should be implemented in IRDF-2002 as soon as possible. Several reactions that are missing in IRDF-2002 were mentioned for inclusion in IRDFF, if possible, including ^{93}Nb(n,γ)^{94}Nb and ^{94}Zr(n,γ)^{95}Zr.

At higher neutron energies, cross sections have been measured and some evaluations are available. A list of dosimetry reactions that would be useful for IFMIF was presented from a paper by E. Zsolnay, H. Nolthenius, and A.L. Nichols (see Annex 1). This list should be viewed as a wish list such that evaluations of any of these reactions should be included in IRDFF. Reactions that have not been measured or evaluated should be included on lists of desired reactions for measurement and evaluation.

One of the main issues with higher energy reactions is that such files do not all extend to the same upper neutron energy and, more importantly, many of the files do not include covariance information. Regarding the upper neutron energy for IRDFF, the decision was made that all cross sections included in the file need to extend to 60 MeV, which is the upper neutron energy needed for neutron dosimetry at the proposed IFMIF. However, if an evaluated cross section extended to higher neutron energies, the decision was made to include the higher energy evaluations. IRDFF would thus contain evaluated cross sections to 60 MeV for all of the reactions in the file and higher neutron energies only as available in prior evaluations.

IRDF-2002 required the inclusion of covariances for all of the neutron cross sections. However, above 20 MeV, covariance information is not routinely available or included for many of the cross section evaluations. Ideally, it would be highly desirable to require the inclusion of covariance information. However, this requirement might delay the issuance of IRDFF for many years until such data become available. Recent work by Pat Griffin (P.J. Griffin, "Dosimetry User's Perspective on Covariance Needs", *Nuclear Data Sheets* **109** (2008) 2733-2738) and John Williams, et al (J. G. Williams, A. P. Ribaric and T. Schnauber, "NVSA-3: A Computer Code for Least-Squares Adjustment of Neutron Spectra and Measured Dosimeter Responses", *Proceedings of the 13th International Symposium on Reactor Dosimetry*, W. Voorbraak, L. Debarberis, P. D'hondt, J. Wagemans, editiors, World Scientific, London, 2008) suggest that this issue might be resolved by using nuclear model codes, e.g. EMPIRE and/or TALYS, to calculate the covariances. This was done for TENDL (see http://www.talys.eu/tendl-2010/), which was produced by the TALYS computer code. It was noted that TENDL cross sections gave poor results in integral testing compared to IRDF-2002. Nevertheless, covariance files calculated for TENDL may offer the best estimate of the true covariances at higher neutron energies since the calculations are based on nuclear physics models for all of the reactions. The decision was thus made to use the TENDL covariance files with high uncertainties assigned in all cases where covariance information is lacking or deficient above 20 MeV. It was noted that most of the TENDL covariance files have diagonal matrices which are also not desirable, but can be renormalized and assigned higher uncertainties as necessary. This option appears to be the only reasonable approach to issuing IRDFF in the near future.

There was agreement that IRDFF should include a decay data library as was the case with IRDF-2002. The decay data library should be updated and data will need to be included for all new reactions.

Radiation damage (dpa) cross sections have been developed for use with fusion neutron sources and it was recommended that damage cross sections be included with IRDFF for some of the most important engineering materials, where available. There was a discussion regarding whether pointwise, groupwise, or both types of cross section files, should be included with IRDFF. There was agreement that both were useful and that a new energy group structure beyond the 640 groups, as used for IRDF-2002, should be formulated for the

group cross sections in IRDFF. As with IRDF-2002, IRDFF should use a flat weighting spectrum for the group cross sections since it was agreed that spectral-weighting effects are not significant with such a fine energy group structure and that it is not at all clear what weighting spectra should be applied to a file that will be used for both fission and fusion reactor applications.

One of the concerns regarding the testing of IRDFF is that, whereas there are standard neutron reference fields such as ^{252}Cf for fission cross section testing, there are no available standard neutron fields for integral testing above 20 MeV. The KAYZERO database on integral constants for Neutron Activation Analysis should also be used for testing of fission cross sections due to the perceived accuracy of this database (F. De Corte and A. Simonits, "Recommended nuclear data for use in the k_0 standardization of neutron activation analysis", *Atomic Data and Nuclear Data Tables* **85** (2003) 47-67.). L. Greenwood mentioned that integral measurements have been published for higher neutron energies using time-of-flight neutron spectroscopy to measure the neutron spectra used for the integral measurements. (L.R. Greenwood and R.R. Heinrich, "Integral Tests of Nuclear Activation Cross Sections for ^{9}Be(d,n) Sources, Ed=14-40 MeV", *Nuclear Matter* **85** (1979) 473 and L.R. Greenwood, "Integral Testing of Spallation Cross Sections for Neutron Dosimetry at 113 and 256 MeV", *Reactor Dosimetry*, ASTM STP 1398, J. G. Williams, D. W. Vehar, F. H. Ruddy, and D. M. Gilliam, Eds., (2001) 409-416). Robin Forrest maintains a library of such activation data that could be used for testing (included in the European Activation System: EASY, see R.A. Forrest, A. Tabasso, C. Danani, S. Jakhar, and A.K. Shaw, *Handbook of Activation Data Calculated Using EASY-2007*, report UKAEA FUS 552, March 2009 and other documentation available from http://www.fusion.org.uk/EASY.aspx).

5. Summary of Actions

During the meeting a number of actions were discussed and allocated to the participants. The following list was agreed to by the attendees.

Regarding to the contents of the new dosimetry library, IRDFF:

1. Trkov: To investigate an appropriate group structure from 10^{-5} eV to 60 MeV, i.e. extending down from 10^{-4} eV to 10^{-5} eV and up from 20 MeV to 60 MeV, which the fusion, IFMIF and/or high energy community would wish to use. Depending on whether an appropriate group structure is forthcoming, it may be possible to make files available in this structure.
2. Capote: To ensure that the processing of files (with a flat-weighting spectrum) into the 640 group structure for all new evaluations, including 640 group structure for the covariances, is undertaken, including documentation.
3. Nolthenius: To produce the "metrology" format files for all new evaluations.
4. Zsolnay: Calculate the C/E values for all available experimental data, e.g. ^{197}Au, ^{55}Mn, ^{115}In(n,γ), in a ^{252}Cf average fission neutron spectrum and investigate the availability of data for other spectra.
5. Capote/Zolotarev: Ensure that the new ^{93}Nb(n,γ) evaluation correctly deals with the splitting between the formation of the ground and metastable states.
6. Capote/Zolotarev: Ensure correct priority assignment of proposed evaluations: ^{54}Fe(n,p), ^{58}Ni(n,2n), ^{169}Tm(n,3n), ^{115}In(n,γ)^{116m}In, etc.

7. All: Assess recently released evaluations, e.g. JENDL-4, ENDF/A (ENDF/B-VII.1), JEFF-3.1.1 (or JEFF-3.2 if available in time), for suitability, i.e. cross sections and covariances.
8. Kellett: Assess and provide the decay data requirements of IRDFF. Includes checking the compatibility of decay data used in recent evaluations by Zolotarev.
9. Greenwood: Review and recommend appropriate files for the dpa files by June 2011.
10. Trkov/Nolthenius: Produce 640 group covariance files by their own methods and assess their equivalence, e.g. ^{27}Al(n,α) and ^{235}U(n,f).
11. Capote/Zsolnay/Nolthenius: Assess the list of evaluations in IRDF-2002 and the proposed extensions for fusion and also ^{94,96}Zr(n,γ), etc. (see Annex 1 and references therein) to see if there are any more recent files (exercise last done in 2008), e.g. JENDL-4, ENDF/A (ENDF/B-VII.1), JEFF-3.1.1 (JEFF-3.2?), for suitability, i.e. cross sections and covariances. If appropriate evaluations are found, then Zsolnay/Nolthenius will assess their contents.
12. Kellett: Issue the Trkov report on the processing of MF40 covariance data as an INDC(NDS) report.
13. Kellett: Correct the 640 groupwise files of IRDF-2002, and release these as IRDF-2002.1 via the IRDF-2002 website, along with the corrected pointwise files from Trkov.

General:

1. Zsolnay: Contact W. Mannhart (PTB, Germany) to obtain the complete set of results for ^{252}Cf integral testing.

6. Summary of Recommendations

During the meeting a number of recommendations were formulated and discussed. The following list was agreed to by the attendees.

Regarding to the contents of the existing and future dosimetry libraries:

1. Corrections to IRDF-2002 (designated as IRDF-2002.1) should be carried out, i.e. to allow covariance processing, as soon as possible and prior to their adoption in IRDFF.
2. In the processed groupwise files, ensure the covariances are processed into the same group structure by using NJOY. (Using NJOY is necessary since GROUPIE only processes the cross sections, and NOT the covariances, into a new group structure.) It was nonetheless stated that an example GROUPIE file should be made available to allow users to produce their own groupwise cross section files.
3. Careful version control of evaluations needs to be ensured.

General:

1. The IAEA should continue to support the cross section evaluation effort, e.g. the work of K.I. Zolotarev.

2. The IAEA should organise a CRP devoted to the validation and improvement of IRDFF-1.0 for all applications, which should include the following activities:

a) Creation of reference neutron fields and corresponding experimental database of integral measurements in fission and fusion applications.

b) Assessment of newly released high fidelity evaluations with covariances in order to improve the existing dosimetry library for fission and fusion applications.

c) Use integral data e.g. KAYZERO, in order to reduce the uncertainty in existing evaluated cross sections and improve the consistency of the library (for many reactions in the low energy region (capture and inelastic), uncertainties are still too large.

d) Identification and correction of deficiencies in the library.

e) Complete documentation of the validation of the IRDFF-1.0 library for fission, fusion and IFMIF applications.

7. Production of the Next Version of the International Reactor Dosimetry Library

During the meeting a number of actions and recommendations were discussed and have been recorded elsewhere in this report. For clarity, those relating specifically to the agreed plan of work for producing the next version of the IRDF library are summarised below.

General recommendation:
Recommend that the new name will be IRDFF-1.0 and that it should be released by the end of 2011, including appropriate documentation.

Future IRDF library contents and schedule:

1. The upper limit of all evaluations must be at least 60 MeV. Evaluations going beyond this limit will be included without removing the part beyond 60 MeV.
2. The extension of evaluations up to 60 MeV, will be made by adding TENDL above the original upper energy limit, and ensuring a smooth connection at that point by renormalizing TENDL. Covariances from TENDL will be assessed and included if appropriate.
3. All new evaluations available up to June 2011 should be included.
4. Damage cross sections – need to take those available from IRDF-2002 at lower neutron energies and other evaluations above 20 MeV.

Actions:

1. Capote: Explore the use of TENDL covariances in the extended energy range.
2. Greenwood: Review and recommend appropriate files for the dpa files by June 2011.

8. Documentation for the Next Version of the International Reactor Dosimetry Library

A list of chapters for the final documentation was agreed upon and each one was allocated to one or more participants. *It was also agreed that drafts are to be sent by 30 September 2011 to R. Capote.*

Chapters required and allocation:

1. INTRODUCTION
   R. Capote and L.R. Greenwood
2. SPECIFIC EVALUATIONS FOR REACTOR AND FUSION DOSIMETRY
   K.I. Zolotarev
3. SELECTION OF ADDITIONAL SUITABLE CROSS-SECTIONS (Fission and Fusion)
   R. Capote, E.M. Zsolnay, H.J. Nolthenius, L.R. Greenwood
4. ASSEMBLY AND VERIFICATION OF THE IRDFF-1.0 LIBRARY
   Assembly, verification – format and processing, ACE and group file production, tabulations of calculated σ_0, RI, Cf-252 reference field, and other reference fields
   A. Trkov
5. INITIAL VALIDATION OF IRDFF-1.0
   a. Fission (U-235 spectrum (Zolotarev uses ENDF/B-VI), Maxwellian, 1/E, Cf-252, KAYZERO)
   b. Fusion (14 MeV)
   c. IFMIF

   E.M. Zsolnay, H.J. Nolthenius, L.R. Greenwood (R.A. Forrest – for fusion)
6. RADIATION DAMAGE FILES AND COMPUTER CODES
   L.R. Greenwood
7. DECAY DATA AND ISOTOPIC ABUNDANCES FOR DOSIMETRY APPLICATIONS
   M.A. Kellett

9. Conclusions

The consensus of the attendees at this Consultants' Meeting was that there is a need for revision of the IRDF-2002 nuclear data library to extend the library to higher neutron energies for use at accelerator-based neutron sources used for fusion materials studies and to include new nuclear data evaluations that will improve and expand the library for fission reactor dosimetry applications. It was agreed that sufficient new nuclear data cross section evaluations are available to warrant creation of the new library. This report provides a roadmap for the production of the new nuclear data library which will be called the International Reactor Dosimetry and Fusion File (IRDFF). Specific actions are assigned that will lead to the creation of IRDFF by the end of 2011, using published evaluations that are available by June 2011. The file will contain evaluated cross section data up to a minimum of 60 MeV and may include higher energy data where available. Covariance data will be provided for all reactions, using evaluated data where possible, and supplemented with nuclear physics calculations where data is not available.

Presented at the Consultants' Meeting on
Improvements and Extension to the International Reactor Dosimetry File (IRDF-2002)
From 5 to 7 May, 2010

STATE OF ART OF CANDIDATE CROSS SECTIONS FOR IMPROVEMENT AND EXTENSION OF IRDF-2002

Eva M. Zsolnay[1] and Henk J. Nolthenius[2]

1. INTRODUCTION

The International Reactor Dosimetry File (IRDF-2002) was put on the web by IAEA NDS in 2005, while the final report on it was released in 2006 [Tec452]. The file contained 66 reaction cross sections for reactor dosimetry application accompanied with uncertainty information in the form of covariance matrices and characteristic nuclear data (isotopic abundances, half-lives, etc.) for the target and reaction product nuclei present in the library. There were data given also for three cover material cross sections (Cd, B and Gd). The cross section data covered the energy region from 10^{-10} to 20 MeV. The library at the time of its preparation contained the best quality data for reactor dosimetry application, nevertheless there remained several shortcomings and lack of information (especially related to the covariance information of the cross sections) in the file.

In the meantime new cross section evaluations have become available, furthermore, a request from the side of fusion application appeared to add new reactions to the library and to extend the energy limit of the cross section data up to 50 MeV. Therefore, IAEA NDS held a Consultants' Meeting at the IAEA Headquarters on 25-26 January, 2007, and an informal meeting on 23-24 July, 2009 in order to discuss the problems and the way of improving and extending the file IRDF-2002 with new cross section evaluations, applicable also in the fusion energy region. It has been decided that the primary data will be the pointwise ones, and for the reactor dosimetry reactions the cross section data will be given also in the SAND-II 640 energy group structure.

Unfortunately, in most of the cases no covariance information is available in the energy region above 20 MeV. To generate these data further efforts are needed. In order to reach the aim of improving and extending the file IRDF-2002, many efforts have been made in the last time: several new cross section evaluations have been made (e.g. [Zol08, Zol09]), the data were converted into different formats and characterized. At the last meeting it was suggested that the new, extended library should have the name "**IRDFF**: **I**nternational **R**eactor **D**osimetry and **F**usion **F**ile"

In the following parts we will summarize the way of characterization of the cross section data for inclusion in the extended library and, after having an overview on the present situation in connection with the available new cross section data, we give the State of Art of the candidate cross sections for IRDFF, together with the shortcomings and missing information still present in IRDF-2002.

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2. REQUIREMENTS AND TESTS ON THE CROSS SECTION DATA TO BE USED FOR THE INTERNATIONAL REACTOR DOSIMETRY AND FUSION FILE IRDFF (energy region from thermal upto 50 MEV)

2.1. The cross section data for the reactor dosimetry and fusion file will have to be given in more forms:

a) Complete point cross section data together with the uncertainty information will have to be given in ENDF-6 format, at a neutron temperature of 300 K (from 0 to ~ 50 MeV) (Master library);

b) For Reactor Dosimetry purposes the cross section data have to be given in 640 SAND-type energy group structure in an ENDF-6 format from 10^{-10} MeV to 20 MeV and in a "Metrology Format" (No MF=10, but everything is in MF=3; and special MT numbers are used, see Appendix 1 of [Tec452]), at a neutron temperature of 300 K. Also the material damage (induced by neutrons) cross section data (dpa) should be given in the format written in this point;

c) Complete point cross section data together with the uncertainty information in "ACE" format for calculation with the Monte Carlo codes like MCNP, are also needed.

d) The data will have to be consistent with the IAEA Standard Cross Section Library.

2.2. For reactor dosimetry purposes cross section data with complete covariance information are only accepted. In exceptional cases cross section data with diagonal covariance matrices can be used with the assumption of creating the complete covariance matrices in a short time, and substitute the diagonal matrices with them.

2.3. The cross section data together with the related uncertainty information have to be tested before releasing them:

- The data have to correspond to the above mentioned format specifications;
- The correctness of the covariance information has to be checked first from mathematics point of view (rank of the matrices, eigen-values, no negative eigen values are allowed, etc.), and corrected if necessary.
- The lower energy limits of the cross section data and the uncertainty information will have to be made equal for all libraries of interest.
- The quality of the cross section data to be used in the cross section library of interest will have to be checked and tested by comparing the integral library data with the corresponding up-to date experimental ones in the following reference (and standard) neutron fields [Gri06, Zso06, Hol03, Mug03, Man06]:
  - Spontaneous fission neutron field of ^{252}Cf (standard neutron field);
  - 1/E slowing down spectrum in a hydrogenous moderator;
  - Maxwellian thermal spectrum at a specified neutron temperature;
  - Mono-energetic 14 MeV neutron field from a deuterium-tritium source.
  - The integral cross section data above 20 MeV also will have to be compared with experimental ones (***the kind of the spectrum has to be discussed***).

2.4. The integral values of the library cross section uncertainties have to be calculated and qualified.

3. STATE OF ART OF THE CANDIDATE CROSS SECTIONS FOR IRDFF

3.1. The first set of new cross section evaluations tested and analysed for inclusion in IRDF-2002

Over the subsequent two to three years after releasing IRDF-2002, new cross section evaluations have become available (e.g. within the JEFF-3.1 [Kon06], US ENDF/B-VII [Cha06], and evaluations of K. Zolotarev [Zol08]) that were suitable to re-define the data of this library. Both the nature and the quality of these new reactions have been assessed and analysed in accordance with the requirements listed above, furthermore, inter-comparisons were made with integral measurements in order to determine whether they should be adopted to update and improve IRDF-2002. The results obtained for the analysed 14 new reaction cross sections are presented in Table 1. [Zso08].

Conclusion

1. *Slow neutron-induced reactions*: The cross section for the ^{6}Li(n,t) reaction from the ENDF/B–VII file shows somewhat poorer agreement with the experimental data than the corresponding cross sections in IRDF-2002 [Tec452], although the difference is small. Since the new ENDF/B-VII evaluation is based on the standards cross section file of IAEA, we suggest substitution of the cross section data for this reaction in IRDF-2002 with the corresponding new data of the file ENDF/B–VII. The resonance integral calculated for the ^{58}Fe(n,γ) reaction is in good agreement with the experimental data of Holden, while a large difference arises between the calculated and experimental resonance integral values when the data of Mughabghab are considered (this inconsistency needs to be resolved). Furthermore, the uncertainty of the cross section averaged over the ^{252}Cf fission spectrum is also very large [Zso08].
2. *Threshold reactions*: new evaluations of threshold reactions suitable for inclusion in IRDF-2002 are found in the various files prepared by K. Zolotarev [Zol08], and constitute 12 reactions. Better (sometimes much improved) C/E (Calculated/Experimental) values and uncertainties for the average cross sections are obtained by means of these new evaluations. ^{60}Ni(n,p) is the only reaction in which the C/E value is larger for the new data than for the original IRDF-2002 file, while the uncertainty of the new evaluation for this cross section is much smaller than in the older file (this contradiction needs to be addressed) [Zso08].

Table 1. Characteristics of analysed cross sections and their uncertainties for fission reactor dosimetry [Zso08].

Reaction	Selected evaluation	Calculated library cross section 2200 m s^{-1} σ_L (barn)	Resonance integral from library data, IR_L (barn)	Uncertainty in library data		Calculated average library cross section ^{252}Cf fission $\langle\sigma_c\rangle$ (mb)	Uncertainty in $\langle\sigma_c\rangle$ (%)	C/E
				Thermal (%)	Epithermal (%)			
^{6}Li(n,t)	ENDF/B-VII	970	425.3	0.14	0.13	311.6	1.12	thermal: 1.032 ± 0.17% (a) IR: 1.008 ± 0.91% (a)
^{58}Fe(n,γ)	JEFF-3.1	1.31	1.28	5.11	5.28	2.01	50.17	thermal: 1.01 ± 5.17% (a) 1.01 ± 5.6% (b) IR: 0.98 ± 5.40% (a) 0.75 ± 6.21% (b)
^{24}Mg(n,p)	RRDF-2007	–	–	–	–	2.105	0.80	1.055 ± 2.57% (c)
^{27}Al(n,p)	RRDF-2006	–	–	–	–	4.751	2.05	0.973 ± 2.96% (c)
^{32}S(n,p)	RRDF-2008	–	–	–	–	74.11	2.48	1.022 ± 4.28% (c)
^{47}Ti(n,p)	RRDF-2004	–	–	–	–	19.56	2.73	1.015 ± 3.19% (c)
^{60}Ni(n,p)	RRDF-2007	–	–	–	–	2.803	1.81	1.173 ± 5.73% (c) *
^{63}Cu(n,2n)	RRDF-2006	–	–	–	–	0.200	1.39	1.013 ± 4.21% (c)
^{65}Cu(n,2n)	RRDF-2006	–	–	–	–	0.656	1.89	0.996 ± 2.92% (c)
^{64}Zn(n,p)	RRDF-2006	–	–	–	–	42.70	1.69	1.052 ± 2.36% (c)
^{115}In(n,2n)	RRDF-2007	–	–	–	–	1.634	4.95	no experimental
^{127}I(n,2n)	RRDF-2007	–	–	–	–	2.108	3.03	1.019 ± 4.08% (c)
^{197}Au(n,2n)	RRDF-2006	–	–	–	–	5.531	1.87	1.005 ± 2.62% (c)
^{199}Hg(n,n')	RRDF-2006	–	–	–	–	296.2	3.65	0.993 ±4.07% (c)

(a) Experimental data from CRC Handbook of Chemistry and Physics, CRC Press, 2003 [Hol03].
(b) Experimental data from Mughabghab [Mug03].
(c) Experimental data in the neutron field of ^{252}Cf spontaneous fission spectrum from W. Mannhart [Man06].
* Data from single experiments which were not part of the evaluation process of W. Mannhart [Man06].

3.2. Further new cross section evaluations for IRDF-2002 extension

Several new cross section evaluations have been made later on for extension of IRDF-2002 for fission and fusion application. The majority of the new cross section data was made by K. Zolotarev in frame of a contract with IAEA NDS. The new evaluations were treated by Daniel López Aldama (Cubaenergia) [Ald010]. 29 dosimetry reactions were considered (part of them is present also in Table 1.) and thereafter, due to a comprehensive treatment on the original data, the following result were obtained [Ald010]:

- *"Pointwise linearly interpolable cross section data and the corresponding uncertainties in the form of covariance matrices were generated using the NJOY-99 code system.*
- *The covariance matrices were plotted and the eigenvalues were calculated.*
- *Multi-group cross section data are also supplied in the SAND-II energy group structure for fission applications and in 356 energy groups for fusion systems.*
- *Additionally, cross section data in ACE-format were prepared to be used in Monte Carlo codes, like MCNP."*

The treated reactions and some characteristics of the data are shown in Table 2. [Ald010].

Table 2. Characteristics of data treated by D.L. Aldama [Ald010].

No.	Dosimetry reaction	Source of data	Temperature at original evaluation [K]	Higher energy limit [MeV]	ENDF-6 MT number	Comments
1	^{24}Mg(n,p)*****	NDS/IAEA	0.	21	103	Fission
2	^{27}Al(n,p)*****	NDS/IAEA	0.	40	103	Fission+Fusion
3	^{27}Al(n,α)	NDS/IAEA	0.	40	107	Fission+Fusion
4	^{32}S(n,p)*****	NDS/IAEA	0.	21	103	Fission
5	^{47}Ti(n,p)*****	NDS/IAEA	0.	20	103	Fission
6	^{55}Mn(n,2n)	NDS/IAEA	0.	40	16	Fission+Fusion
7	^{55}Mn(n, γ)	NDS/IAEA	0.	20	102	Fission+Fusion
8	^{57}Fe(n,γ)	JEFF-3.1	0.	20	102	Fission
9	^{58}Fe(n,γ)	JEFF-3.1	0.	20	102	Fission
10	^{59}Co(n,2n)	NDS/IAEA	0.	60	16	Fission+Fusion
11	^{59}Co(n,p)	NDS/IAEA	0.	75	103	Fission+Fusion
12	^{60}Ni(n,p)*****	NDS/IAEA	0.	21	103	Fission
13	^{63}Cu(n,2n)*****	NDS/IAEA	0.	20	16	Fission
14	^{64}Zn(n,p)*****	NDS/IAEA	0.	20	103	Fission
15	^{65}Cu(n,2n)*****	NDS/IAEA	0.	20	16	Fission
16	^{90}Zr(n,2n)	NDS/IAEA	0.	40	16	Fission+Fusion
17	^{115}In(n,2n)*****	NDS/IAEA	300.	20	16	Fission+Fusion
18	^{115}In(n,n')	NDS/IAEA	300.	20	51	Fission+Fusion
19	^{115}In(n, γ)	NDS/IAEA	300.	20	102	Fission+Fusion
20	^{127}I(n,2n)*****	NDS/IAEA	0.	32	16	Fission
21	^{197}Au(n,2n)*****	NDS/IAEA	300.	40	16	Fission+Fusion
22	^{197}Au(n,γ)	NDS/IAEA	300.	30	102	Fission+Fusion
23	^{199}Hg(n,n')^{199m}Hg*****	NDS/IAEA	0.	20	57	Fission
24	^{232}Th(n,f)	NDS/IAEA	300.	60	18	Fission
25	^{232}Th(n,γ)	NDS/IAEA	300.	60	102	Fission
26	^{235}U(n,f)	NDS/IAEA	300.	200	18	Fission

No.	Dosimetry reaction	Source of data	Temperature at original evaluation [K]	Higher energy limit [MeV]	ENDF-6 MT number	Comments
27	^{238}U(n,f)	NDS/IAEA	300.	200	18	Fission
28	^{238}U(n,γ)	NDS/IAEA	300.	30	102	Fission
29	^{239}Pu(n,f)	NDS/IAEA	300.	200	18	Fission

***** - Reactions treated also before, see the results in Table 1 above.

The ***cross section data*** in the *Table above* together with the ***related uncertainty information will have to be tested*** in accordance with the requirements written in *point 2.3. above*, ***before releasing them***.

3.3. Problems to be solved in connection with preparing the same cross section library for reactor dosimetry and fusion application.

a) *Extending the cross section data up to 50 MeV in pointwise format is not a problem*, but there are *several problems related to the group format of the high neutron energy library*:

- In the high (E>20 MeV) neutron energy region no uncertainty information (especially in the form of covariance matrices) is available for the majority of the reactions of interest. If we try to extend the group format of IRDF-2002 to the high neutron energy region (where the corresponding uncertainty information is missing) then the new library will not be consistent. Therefore, it is better to make a separate group format library with limited uncertainty information for the fusion application. This has already been done by D. Aldama as shown in the previous point 3.2. At the same time, the uncertainty information in the high (E>20 MeV) neutron energy region will have to be generated. This problem will have to be discussed in detail. Perhaps no group format library should be given at all for the high neutron energy region.

b) In the high neutron energy region not enough experimental data for reference neutron spectra are present to validate the evaluated cross section data. Therefore, for several reactions needed for the dosimetry in this range no comparison with experimental data will be possible. The required experimental data will have to be measured.

3.4. Further problems to be solved in connection with IRDF-2002

The shortcomings and problems to be solved in the future in connection with IRDF-2002 (future IRDFF) have been written in the Report [TEC452], in the conclusions of Chapters 3. and 6.

Considering what has been said there and adding the results of actions presented above, the following most important problems remain to be solved:

a) The reactions ^{197}Au(n,γ) and ^{235}U(n,f) based on the IAEA NDS standards will have to be tested in comparison with experimental data (see also in point 3.2. above) before releasing them.
b) New evaluations are present for the dosimetry reactions ^{55}Mn(n,γ) and ^{58}Fe(n,γ) (see in Table 2. above), but the integral data of the cross sections have to be compared with

the corresponding experimental ones, with a special emphasis on the resonance integral.

c) At the same time, the resonance integral should be improved for the important dosimetry reaction ^{93}Nb(n,γ).
d) Only diagonal covariance matrices are available for a number of reactions: ^{23}Na(n,γ), ^{93}Nb(n,γ), ^{181}Ta(n,γ). New evaluations with complete covariance information would be needed for as many of these reactions as possible. For the reactions ^{115}In(n,γ) (leading to ^{116m}In) and ^{232}Th(n,γ) new evaluations are present (see Table 2. above), but these data will have to be analysed.
e) The Nuclear Data part (isotopic abundance, decay data of the reaction products, etc.) of IRDF-2002 is not complete at the moment: the data are missing for the fission reactions present in the cross section library, namely for the targets ^{232}Th, ^{235}U, ^{238}U, ^{237}Np, ^{239}Pu, ^{241}Am. The mentioned nuclear data will have to be inserted in the library also for the new reactions. These data should be made available in order to make the file consistent.
f) The total cross section of the important cover material Cd is not available yet.

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Appendix 1

Consultants' Meeting on

"Improvements and Extensions to IRDF"

IAEA Headquarters, Vienna, Austria
5 – 7 May 2010

Meeting Room B1115

AGENDA

Wednesday, 5 May

08:30 - 09:30	**Registration** (IAEA Registration desk, Gate 1)
09:30 - 10:15	**Opening Session** Welcoming address Introductory Remarks Election of Chairman and Rapporteur Adoption of Agenda
10:15 - 11:00	*Administrative and Financial Matters related to participants, Coffee break*
11:00 - 12:30	**Session 1:** Presentations by participants and expectations
12:30 – 14:00	**Lunch**
14:00 – 18:00	**Session 2:** Review of newly available evaluations *Coffee break as needed*

Thursday, 6 May

09:30 - 12:30	**Session 3:** Completeness of IRDF-2002+ and evaluation requirements *Coffee break as needed*
12:30 - 14:00	**Lunch**
14:00 – 18:00	**Session 4:** Discussion on future library release: fission and fusion applications *Coffee break as needed*

Friday, 7 May

09:30 - 12:30	**Session 5:** Drafting of the Summary Report of the Meeting *Coffee break as needed*
12:30 - 14:00	**Lunch**
14:00 – 17:00	**Session 5 (cont'd):** Review and Approval of the Summary Report **Closing of the Meeting** *Coffee break as needed*

International Atomic Energy Agency

Consultants' Meeting on
"Improvements and Extensions to IRDF"

IAEA Headquarters, Vienna, Austria
5 to 7 May 2010

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