RESEARCH REPORT

VTT-R-00948-13

A Dosimetry Cross Section Library Mainly Based on IRDFF

Authors: Tom Serén

Confidentiality: Public

Report's title	
A Dosimetry Cross Section Library Mainly Based on IRDFF	
Customer, contact person, address Valtion ydinjätehuoltorahasto	Order reference 5/2012SAF
Project name CRISTAL/SAFIR 2014	Project number/Short name 73800
Author(s) Tom Serén	Pages 5/2
Keywords dosimetry, IRDFF	Report identification code VTT-R-00948-13

Summary

A dosimetry cross section library in the SAND-II 640-group format has been compiled. The library is mainly based on the newly released IRDFF library in the ENDF-6 format. A few reactions of interest in reactor dosimetry and nuclide production and not included in IRDFF have been added, however without uncertainty information. The library will be used to update the cross sections for the PREVIEW code and to produce coarse-group cross sections for the adjustment codes LSL-M2 and NSVA 3.

Confidentiality	Public

Espoo 5.2.2013

Written by	Reviewed by	Accepted by
Tom Serén, Senior Scientist	Petri Kotiluoto, Principal Scientist	Timo Vanttola, technology manager

VTT's contact address
Teknologian tutkimuskeskus VTT, PL 1000, 02044 VTT

Distribution (customer and VTT)
SAFIR2014/TR3, TK5011

Contents

1 Introduction: the IRDFF Library

A new dosimetry cross section library IRDFF [1] was released by the IAEA in May – June 2012. It supersedes the IRDF-2002 library [2], which was released in 2005. The most important changes are:

- The energy range is extended from 20 MeV to 60 MeV for fusion and accelerator-based applications,
- Nine new reactions have been included (^{235}U(n,γ) is missing in Table 4 of [1]), bringing the total number of reactions to 75 plus three cover reactions,
- The cross sections and their uncertainties for 33 reactions previously included in IRDF-2002 have been revised.

Fortunately many of the most frequently used reactions (such as ^{54}Fe(n,p), ^{58}Ni(n,p), ^{63}Cu(n,α) and ^{93}Nb(n,n')) have not undergone changes from IRDF-2002.

The cross section data and their uncertainties are given in the ENDF-6 format [3] as original pointwise data and in the extended SAND-II 640-group format with additional data above 20 MeV. The group data have been processed with the codes LINEAR and GROUPIE from the PREPRO 2010 package [4]. The NJOY code system [5] was used to convert uncertainty data in the MF=32 format to MF=33.

2 Need for a Simplified Library

For many applications the rather complex ENDF-6 data format cannot be used directly, and a simplified representation is necessary. An example is the LSL-M2 adjustment code package [6] which is in use at VTT. It uses a "Master" library in the SAND-II format (first group, last group, cross section data in ascending energy order) from which the data can be converted to a coarse group structure (e.g. the 47-group BUGLE-80 group structure) with the FLXPRO code using appropriate weighting. The BUGLE-80 group structure is also used in the PREVIEW code [7] used by VTT for VVER-440 dosimetry applications.

The rather complicated ENDF-6 formats for representing covariance information are replaced by a simplified format with relative groupwise uncertainties plus a correlation matrix multiplied by 1000 (integers, upper triangle representation). By expressing the cross sections in cm^2 reaction rates can be directly calculated by groupwise multiplication and summing since fluence rates are conventionally expressed as n/(cm^{2}s). This format is simple, straightforward and "human readable".

A "Master" library in the format described above, based on IRDF-2002, has previously been developed for internal use (IRDF2002.XSO). With the introduction of IRDFF it is now time to update this library.

3 The New Master Library

The conversion programs CVXS (cross sections) and CVCT (uncertainties) from the LSL-M2 package were the main tools in creating the new Master library. However, CVCT cannot handle the LB=8 covariance format used in some MF=33 uncertainty files. Also, for six reactions (^{55}Mn(n,γ), ^{197}Au(n,γ), ^{232}Th(n,γ), ^{235}U(n,f), ^{238}U(n,f), ^{238}U(n,γ) and ^{239}Pu(n,f)) the

uncertainty information was given in a very fine group structure. In both those cases the X333 program from the STAYNL package [8] was used (slightly modified to accommodate larger covariance matrices). In order to save space the fine-group covariances were condensed to the 47-group BUGLE-80 structure with a standard weighting spectrum (Maxwell + 1/E + fission). This required some editing work since the output format of X333 is different from that of CVCT. The editing was conveniently accomplished by importing the data to Excel and performing the necessary transformations.

Since the library is mainly intended for use with fission reactors there is no need to extend the upper energy limit beyond 20 MeV (upper limit in the SAND-II group structure). In order to reduce the volume of the covariance information the same upper energy limit was also imposed on these matrices. The truncation was performed manually as needed. An example of the data format used is given in Appendix 1 (excerpt from the file IRDFF.XSO).

Some reactions of interest in dosimetry as well as isotope production, but not included in IRDFF, have been added to the library, however without uncertainty information. These are listed in Table 1. The cross section for the reaction ^{67}Zn(n,p) was grossly erroneous in IRDFF and has been replaced (K. Zolotarev, private communication). A few reactions (mainly Ti) producing the same reaction product have also been combined as weighted sums (weights according to isotopic composition).

Table 1. Additional reactions not included in IRDFF

Reaction	Source	Comment
^{37}Cl(n,γ)	ENDF/B-VII	
^{58}Ni(n,X)^{57}Co	ENDF/B-VII	Sum of (n,2n) and (n,np)
^{75}As(n,γ)	ENDF/B-VII	
^{81}Br(n,γ)	JENDL 4.0	Commercial nuclide production
^{117}Sn(n,n')	JEFF 3.1/A + JENDL 4.0	Special interest for research reactors
^{152}Sm(n,γ)	ENDF/B-VII	Medical isotope production
^{164}Dy(n,γ)	ENDF/B-VII	Medical, sensitive to thermal neutrons

4 Future Actions

The PREVIEW code uses spectrum-weighted 47-group cross sections for calculating reaction rates, activities etc. [7]. The same cross sections in combination with input spectra and reaction rates calculated with PREVIEW can be used with the LSL-M2 adjustment code [6]. An important task for the near future is thus to update the dosimetry cross sections in PREVIEW to conform to the new fine-group library. This also provides an opportunity to check all the other basic nuclear data such as decay constants and fission yields.

Time and resources permitting, an updated cross section library should also be compiled in the 89-group structure used by the MATLAB-based NSVA-3 adjustment code [9], preferably in MATLAB's own .mat data format.

References

1. E. M. Zsolnay et al., Summary Description of the New International Reactor Dosimetry and Fusion File (IRDFF release 1.0), INDC(NDS)-0616, IAEA, Vienna, May 2012. http://www-nds.iaea.org/IRDFF.
2. International Reactor Dosimetry File 2002 (IRDF-2002), IAEA Technical Reports Series No. 452, Vienna 2006, http://www-nds.iaea.org/irdf2002/docs/irdf-2002.pdf.
3. A. Trkov, M. Herman and D. A. Brown (ed.), ENDF-6 Formats Manual, Report BNL-90365-2009 Rev. 2, Brookhaven National Laboratory, Upton, New York, December 2011.
4. D. E. Cullen, PREPRO 2010, ENDF/B Pre-processing Codes, IAEA, Vienna, November 2010, http://www-nds.iaea.org/ndspub/endf/prepro/.
5. R. E. MacFarlane and D. M. Muir, NJOY-99.0: Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data, Technical Report PSR-480, Los Alamos National Laboratory, 2000.
6. F. W. Stallmann, LSL-M2: A Computer Program for Least-Squares Logarithmic Adjustment of Neutron Spectra, NUREG/CR-4349, ORNL/TM-9933, Oak Ridge 1986. Additional instructions for version 2.0 dated 1994.
7. T. Serén, An Optimised Adjustment Library for the Kernel-Based PREVIEW Program, Licentiate's Thesis, Helsinki University of Technology, November 2001.
8. E. J. Szondi, H. J. Nolthenius, User's Guide to the Cross Section Processing Code X333, BME-NTI 222/95, Institute of Nuclear Techniques, Technical University of Budapest, May 1995.
9. J. G. Williams, A. P. Ribaric and T.Schnauber, NSVA-3: A Computer Code for Least-Squares Adjustment of Neutron Spectra and Measured Dosimeter Responses, Proceedings of the 13th International Symposium on Reactor Dosimetry, Akersloot, the Netherlands, 25-30 May 2008, World Scientific, Singapore 2009.

APPENDIX 1 (Report VTT-R-00948-13)

Example of the data format in IRDFF.XSO with additional comments (in **bold**).

```
CU63 (N,A) CO60                          Unchanged from IRDF-2002
   463   640   ; First and last group followed by group cross sections (cm²)
   5.597E-32   4.477E-31   8.954E-31   1.189E-30   1.518E-30   2.346E-30
   3.943E-30   6.626E-30   1.077E-29   1.683E-29   2.531E-29   3.680E-29
   5.201E-29   7.172E-29   9.683E-29   1.284E-28   1.675E-28   2.155E-28
   2.738E-28   3.439E-28   4.277E-28   5.269E-28   6.434E-28   7.794E-28
   9.369E-28   1.118E-27   1.325E-27   1.560E-27   1.824E-27   2.120E-27
   2.448E-27   2.810E-27   3.206E-27   3.636E-27   4.099E-27   4.594E-27
   5.120E-27   5.674E-27   6.253E-27   6.856E-27   7.478E-27   8.116E-27
   8.767E-27   9.427E-27   1.009E-26   1.076E-26   1.143E-26   1.210E-26
   1.277E-26   1.343E-26   1.409E-26   1.474E-26   1.539E-26   1.603E-26
   1.666E-26   1.729E-26   1.791E-26   1.853E-26   1.914E-26   1.975E-26
   2.036E-26   2.097E-26   2.158E-26   2.219E-26   2.280E-26   2.341E-26
   2.403E-26   2.465E-26   2.527E-26   2.590E-26   2.654E-26   2.718E-26
   2.782E-26   2.847E-26   2.913E-26   2.979E-26   3.046E-26   3.114E-26
   3.182E-26   3.250E-26   3.319E-26   3.388E-26   3.457E-26   3.527E-26
   3.596E-26   3.666E-26   3.735E-26   3.803E-26   3.871E-26   3.939E-26
   4.005E-26   4.070E-26   4.134E-26   4.196E-26   4.256E-26   4.314E-26
   4.369E-26   4.422E-26   4.472E-26   4.519E-26   4.562E-26   4.601E-26
   4.637E-26   4.669E-26   4.696E-26   4.718E-26   4.736E-26   4.749E-26
   4.758E-26   4.761E-26   4.759E-26   4.752E-26   4.740E-26   4.723E-26
   4.701E-26   4.674E-26   4.643E-26   4.607E-26   4.567E-26   4.522E-26
   4.474E-26   4.422E-26   4.366E-26   4.308E-26   4.246E-26   4.182E-26
   4.116E-26   4.048E-26   3.977E-26   3.906E-26   3.833E-26   3.759E-26
   3.684E-26   3.609E-26   3.534E-26   3.458E-26   3.383E-26   3.307E-26
   3.232E-26   3.158E-26   3.084E-26   3.011E-26   2.939E-26   2.868E-26
   2.798E-26   2.729E-26   2.662E-26   2.595E-26   2.530E-26   2.466E-26
   2.403E-26   2.342E-26   2.282E-26   2.224E-26   2.167E-26   2.111E-26
   2.056E-26   2.003E-26   1.952E-26   1.901E-26   1.852E-26   1.804E-26
   1.758E-26   1.712E-26   1.668E-26   1.625E-26   1.584E-26   1.543E-26
   1.503E-26   1.465E-26   1.428E-26   1.391E-26   1.356E-26   1.321E-26
   1.288E-26   1.256E-26   1.224E-26   1.193E-26
  27 ; Number of group limits for uncertainties, group limits (eV)
   1.000E-05   2.250E+06   4.500E+06   5.000E+06   6.000E+06   7.000E+06
   8.000E+06   9.000E+06   1.000E+07   1.100E+07   1.200E+07   1.250E+07
   1.300E+07   1.350E+07   1.400E+07   1.450E+07   1.500E+07   1.550E+07
   1.600E+07   1.650E+07   1.700E+07   1.750E+07   1.800E+07   1.850E+07
   1.900E+07   1.950E+07   2.000E+07
   0.000E+00   2.878E-01   5.176E-02   3.821E-02   3.792E-02   3.512E-02
   3.420E-02   3.398E-02   3.194E-02   2.868E-02   2.575E-02   2.320E-02
   2.042E-02   1.801E-02   1.679E-02   1.723E-02   1.894E-02   2.124E-02
   2.381E-02   2.684E-02   3.077E-02   3.613E-02   4.325E-02   5.229E-02
   6.329E-02   7.622E-02 ; Relative group uncertainties, corr. mat. x 1000
 1000    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0    0    0    0    0    0    0    0    0
 1000   61   46   10   13   32   41   36   21    6   -2   -9  -11   -7    0
    8   14   15   14    9    2   -4  -10  -16  -21
 1000  570  259  178  242  290  279  202  115   55    4  -27  -28    0   37
   68   85   85   68   41    8  -24  -54  -81
 1000  778  567  406  336  323  311  282  250  206  146   75   14  -18  -23
   -9   14   42   67   87  101  109  113
```

```
 1000  877  615  429  359  346  337  321  289  227  135   35  -33  -62  -59
  -32    9   57  101  138  167  189
 1000  887  721  594  477  383  319  252  179  103   42    9    2   12   31
   51   69   83   91   96   97
 1000  945  830  649  477  359  246  143   66   30   33   57   84  105  114
  111   97   79   58   39
 1000  953  801  622  486  345  206   89   24   16   43   83  120  145  154
  149  135  115   95
 1000  937  805  684  538  367  188   50  -10   -8   30   85  140  184  211
  224  226  221
 1000  958  883  764  587  357  137    0  -46  -27   31  109  185  248  294
  324  343
 1000  978  905  757  522  261   70  -21  -32   10   85  170  246  307  353
  385
 1000  971  864  654  389  174   52   12   33   90  163  234  294  340  375
 1000  955  800  561  338  191  120  106  131  176  224  268  304  333
 1000  936  763  564  408  307  251  227  223  230  240  251  261
 1000  936  801  664  550  457  380  316  265  226  198  177
 1000  955  868  768  661  548  436  335  249  182  130
 1000  970  906  812  694  562  434  320  227  152
 1000  975  913  812  687  555  433  328  241
 1000  975  908  807  689  573  469  380
 1000  974  909  818  720  627  544
 1000  976  920  848  773  703
 1000  980  938  886  832
 1000  985  956  920
 1000  989  970
 1000  993
 1000
```