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REFERENCE DATA FILE FOR NEUTRON SPECTRUM ADJUSTMENT AND RELATED RADIATION DAMAGE CALCULATIONS

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ABSTRACT

The REAL-88 interlaboratory exercise organized by IAEA resulted in a neutron metrology file (NMF-90) comprising problem dependent data for benchmark neutron fields, furthermore, nuclear data and computer programs for neutron spectrum adjustment and radiation damage parameter calculations for the service life assessment of nuclear facilities. Calculation results of some experienced laboratories are also present. This paper describes and analyses the content of the neutron metrology file and outlines the most important problems and tasks to be solved in the field of radiation damage parameter calculations.

1. INTRODUCTION

IAEA Nuclear Data Section (NDS) has organized the REAL-80, REAL-84, AND REAL-88 interlaboratory exercises (1-3) in order to improve the quality of the results of radiation damage calculations for the service life assessment of nuclear facilities. The emphasis was concentrated on radiation damage (exposure) parameters for reactor pressure vessels and related nuclear technology. The aim striven for could be achieved by using good quality input data and proper calculation methods. The common effort of the participants and evaluators of the exercises has contributed to the solution of

numerous basic mathematical and physics problems in the neutron spectrum adjustment procedure for radiation damage purposes (1,2, 4-8). The output of the exercises resulted in a neutron metrology file which is available at IAEA for distribution to interested laboratories. The neutron metrology file has been developed by a joint team from the Netherlands Energy Research Foundation, Petten (H. J. Nolthenius, W. L. Zijp), Technical University of Budapest (É. M. Zsolnay, E. J. Szondi), Argonne National Laboratory, Argonne (L. R. Greenwood), Physikalisch-Technische Bundesanstalt, Braunschweig (M. Matzke), and Oak Ridge National Laboratory (F. W. Stallmann).

The content of the neutron metrology file was discussed by a workshop at the IAEA Advisory Group Meeting on the Status and Requirements of Nuclear Data for Radiation Damage and Related Safety Aspects, held in Vienna, 19-22 September, 1989.

2. STRUCTURE OF THE NEUTRON METROLOGY FILE (NMF-90)

The structure of NMF-90 is shown by Fig. 1. It contains the following information in the form of four separate modules:

1. User's guide and help module
2. Reference data file for neutron spectrum adjustment and related radiation damage calculations (module BENCHMARK),
3. Relevant cross section libraries (module XSECLIB),
4. Software packages and utility programs.

The users have the freedom to request one or more modules from IAEA depending on their interest and task.

In the following chapters details of the different modules will be given.

2.1 Reference data file

The reference data file has been developed in order to create consistent data sets for neutron spectrum adjustment and subsequent radiation damage parameter calculations, which can be considered as benchmarks for other scientists in testing their relevant calculation procedures. Of course, the comparison is correct only in case if the complete REAL-88 input set is used in combination with the IRDF-85 cross section library.

On the other hand, certain data of the benchmark fields (eg input spectrum covariance matrices) can be used for substituting missing data in the calculations of similar environments.

The reference data file contains problem dependent input data for 6 different spectrum cases and also the solutions of some experienced laboratories for these spectra.

Fig. 1.
The structure of the NMF-90

Neutron spectra considered. The six neutron spectra (Fig. 2) considered as benchmark fields in the REAL-88 exercise are as follows:

1. AND: Pressure vessel cavity of the Arkansas Power and Light Reactor (Arkansas Nuclear One-1).
2. PS1: Oak Ridge Research Reactor, Pool Side Facility in the metallurgical irradiation experiment (position: simulated surveillance capsule).
3. PS2: Oak Ridge Research Reactor, Pool Side Facility in the metallurgical irradiation experiment (1/4T position in the simulated pressure vessel wall).
4. U35: fission spectrum of the ^{235}U .
5. CFR: Neutron spectrum in the centre of the Coupled Fast Reactivity Measurement Facility (CFRMF).
6. RTN: Fusion simulation spectrum measured at the RTNS-II, a 14 MeV neutron source at the Lawrence Livermore Laboratory.

Table 1. Technical details for the input information of the REAL-88 benchmark spectra

input data	measured reaction rates	covariances for measured reaction rates	calculated input spectrum	covariances for calculated input spectrum
AND	6 reaction rates, no subcadmium response	available	16 groups	16 groups
PS1	10 reaction rates	only variances	37 groups calculated	37 groups calculated
PS2	6 reaction rates	only variances	37 groups calculated	37 groups calculated
CFR	23 reaction rates	only variances	26 groups	26 groups
U35	23 reaction rates	only variances	24 groups	24 groups
RTN	12 reaction rates	available	60 groups	good estimates 60 groups

Fig. 2.
Benchmark neutron spectra contained in the NMF-90

Problem dependent input data. In Table 1 information is given on the problem dependent input data sets (3). The collection comprises all the data (ie reaction rates and input spectra accompanied with their covariances) required for the neutron spectrum adjustment. The reaction rates can be considered to have negligible neutron self-shielding effects.

All detectors of the set PSI have been irradiated inside a gadolinium cover, therefore the gadolinium total cross section values are also incorporated in the corresponding data set to facilitate the calculation of the cover shielding.

For all the data sets a detailed weighting neutron spectrum in a continuous form or fine energy group structure has been made available.

Calculation results. A detailed discussion of the results of the REAL-88 exercise with a summary for each spectrum was prepared in the form of progress reports with restricted distribution, which were then distributed among the participants. The reference data file contains spectrum characteristic integral data (such as integral neutron fluence rate values above some specific energy limits, displacement and gas production rates in iron for the neutron spectra in question, etc), together with uncertainties as calculated by some experienced laboratories using the REAL-88 input data set. The users can then compare their output results with the ones of the reference file.

2.2 Cross section libraries

Two cross section libraries, IRDF-85 and IRDF-90, are given in the XSECLIB module of the NMF-90.

1. The International Reactor Dosimetry File IRDF-85, Version 2 (9) contains the cross sections and their uncertainty information to be used in the calculations on the REAL-88 reference spectra. The library has the ENDF-5 format.
A simplified damage characterization for steel has been introduced in the REAL-88 tasks, ie the relevant damage parameters are calculated for pure iron.
2. The International Reactor Dosimetry File IRDF-90 (10) is partly based on the ENDF/B-VI data and it contains improved information extended with several dosimetry reactions as compared with the IRDF-85. This library is written in the ENDF-6 format, which might cause difficulties in processing the data with the old computer codes interpreting the input only in the ENDF-5 format. The IRDF-90, which came available recently in restricted distribution, has not yet been widely tested by neutron metrology calculations.

2.3 Software packages and utility programs

Three software packages (STAYNL, MIEKE, and LSL-M2) recently developed by different laboratories have been made available for the users. Each of them is complete in neutron metrology calculation for radiation damage purposes: they start with cross section data processing, perform neutron spectrum adjustment by the generalized least squares method and terminate in radiation damage (exposure) parameter calculation.

For convenience of the users some utility programs independent of the software packages have also been included in the NMF-90.

The programs are available as standard FORTRAN-77 source files and they can be compiled either for running on PCs or on mainframe computers. (Syntactic extensions over the FORTRAN-77 are not present.) The distribution of executable (load) programs was avoided owing to the copyright restrictions of the runtime subroutine libraries.

The STAYNL module. This program package has been developed by the Institute of Nuclear Technics of the Technical University of Budapest (BME) and the Netherlands Energy Research Foundation (ECN) with the aim of producing an "integrated software" for neutron metrology calculations. It means that one cross section processing code, one neutron spectrum adjustment and radiation damage calculation program and one plotting program are concatenated in the module and each program is running only once for one job.

The cross section library is processed by the UNC32 (11) and X333 codes. The latter one is a significantly extended version of the code UNC33 (11). The program X333 calculates weighted, group averaged, self-shielded cross section values and their relative covariance matrix in the user's energy grid, starting from the files No. 3 and No. 33 of the ENDF-5 or ENDF-6 format data sets. It calculates the damage and gas production cross sections as well. The output of the cross section codes can directly be used by the neutron spectrum adjustment code and utility programs.

For neutron spectrum adjustment and damage parameter calculation an updated version of the code STAYNL is used. It is a version of Perey's STAYSL code (12) extended in its algorithm and modified in the input and output organization. The code STAYNL calculates the normalization factor in the least squares procedure (4), and it takes into consideration the cross-product [nonlinear = NL (5)] terms in derivation of the covariance matrix of the calculated reaction rates. The program calculates the requested damage

(exposure) parameters related to the adjusted spectrum, and supplies them in the output together with other spectrum characteristic data. The whole set of the results is available for further computerized processing. As a sample problem, the AND task is evaluated.

The MIEKE module. This module has been developed at the Physikalisch-Technische Bundesanstalt, Braunschweig (13). The program package is not an integrated software in its construction, it consists of several small programs which have to be operated one after one by the user.

The cross section data processing is done by a PTB modified version of the codes UNC32 and UNC33 (UNC33PTB), followed by numerous utility programs. Sometimes manual editing is necessary. The shielding effect of detector covers is taken into consideration by the utility program MFITIB. Radiation damage and gas production cross sections are also calculated. This program collection can handle only ENDF-5 format data at the moment, therefore, parts of the cross section library IRDF-90 containing ENDF-6 format data sections cannot yet be processed by it.

The neutron spectrum adjustment is done by the code MSITER (13). This program is a STAY'SL type code, performing the normalization in frame of a non-linear least squares procedure. Radiation damage parameters together with other spectrum characteristic data are also given in the output.

The programs of the module generate special data files for plotting using compiler specific program elements. Therefore the plotting programs can run only in the case where the compilation of the module has been done by the suitable FORTRAN compiler. As a sample problem, the PSI task is evaluated.

The LSL-M2 module. This program package has been developed at the Oak Ridge National Laboratory (14). It consists of a cross section processing code, a neutron spectrum adjustment program, and several utility programs.

The cross section processing code starts from a 640 group structure library, the format of which deviates from the ENDF-5 and ENDF-6 standards. The data of the cross section library have been collected from sources other than IRDF-85 or IRDF-90. The processing code converts this information into the energy group structure requested by the user. The neutron spectrum is adjusted by the code LSL-M2 (14). This program performs a least squares adjustment in a logarithmic space. The main advantage of this code is that neutron spectra at several different locations can be processed simultaneously. The output contains spectrum characteristic integral data and damage parameters as well. The sample problem of the module is taken from the ORNL PSF HSST experiments.

The utility programs. The BLOW UP program (8) makes it possible for the user to generate a physics based fine group structure weighting spectrum from poor (few groups) spectrum information if the physics characteristics of the neutron field to be investigated are known.

The program XSSPLOT accomplishes the plotting of cross section data, neutron spectra, their ratios, and covariance information on CGA, EGA or HERCULES display, or on HP 7475A plotter. The plotting program uses Calcomp or Calcomp-like subroutine libraries. A collection of the necessary subroutines is given in the separate PROFIT file.

The content of the IRDF-85 and IRDF-90 cross section libraries, and the input/output data sets of the BME-ECN program package can directly be plotted by the XSSPLOT, while the corresponding files of the other (PTB and ORNL) modules require manual editing before plotting by this program.

3. CONCLUSIONS

1. The NMF-90 will contribute to the improvement of the accuracy of radiation damage calculations. It will supply good quality, consistent input data and proper calculation methods to the interested laboratories for testing and improving their neutron metrology procedures.
2. Regular updating of the content of NMF-90 will be needed.
3. It is recommended that the data of the IRDF-90 cross section library should be tested by calculations in benchmark neutron fields before distributing them for routine neutron metrology applications.
4. Unfortunately, not all the problems of the radiation damage calculations could be solved by developing the reference file NMF-90. A detailed study is still required on a number of topics:
 - generation of input spectrum covariances
 - interpretation and elimination of inconsistencies
 - neutron self-shielding in activation detectors
 - shielding effects of detector covers
 - interpolation and extrapolation procedures for neutron spectra measured at different locations (eg within a surveillance capsule, reactor pressure vessel wall, etc)
 - improved damage characterization

4. REFERENCES

1. W. L. Zijp, E. M. Zsolnay, H. J. Nolthenius, E. J. Szondi, G.C. H. M. Verhaag, D. E. Cullen, C. Ertek: Final report on the REA-80 exercise. Report ECN 128; INDC(NED)-7; BME-TR-RES 6/82. Netherlands Energy Research Foundation, Petten, February 1983

2. W. L. Zijp, É. M. Zsolnay, H. J. Nolthenius, E. J. Szondi: Final report on the REAL-84 exercise. Report ECN-212; BME-TR-RES-18/88; IAEA-NDS-212. Netherlands Energy Research Foundation, Petten, November 1988.
3. H. J. Nolthenius: Information for the REAL-88 exercise. Report ECN-88-023. Netherlands Energy Research Foundation, Petten, January 1988.
4. É. M. Zsolnay, W. L. Zijp, H. J. Nolthenius: Effect of normalization on the neutron spectrum adjustment procedure. Report ECN-139. Netherlands Energy Research Foundation, Petten, Oct. 1983.
5. É. M. Zsolnay, H. J. Nolthenius, E. J. Szondi, W. L. Zijp: "New aspects in least squares adjustment methods." In: J. P. Genthon, H. Röttger (Ed.-s): Reactor dosimetry. Proceedings of the Fifth ASTM-EURATOM Symposium on Reactor Dosimetry, GKSS Research Centre, Geesthacht, F. R. G., September 24-28, 1984. D. Reidel Publishing Company, Dordrecht, 1985.
6. H. J. Nolthenius, É. M. Zsolnay, W. L. Zijp, E. J. Szondi: "Nuclear data aspects encountered in the REAL80 and REAL84 intercomparisons." In: V. Piksaikin (Ed.): Nuclear data for radiation damage estimates for reactor structural materials. Proceedings of an IAEA Consultants' Meeting, Santa Fe, NM, USA, 20-22 May 1985. Report INDC(NDS)-179/G. p. 95-105. International Atomic Energy Agency, Vienna, June 1986.
7. W. L. Zijp, É. M. Zsolnay, H. J. Nolthenius: "Improvement of accuracy assessment in radiation damage predictions." In: Proceedings of the 1986 International Symposium on the Effects of Radiation on Materials, Seattle, June 23-25, 1986.
8. E. J. Szondi, A. P. Bosznay: "Physically based weighting spectrum generation for cross section calculations." Publication in progress as an IAEA Technical Report on the IAEA Advisory Group Meeting on the Status and Requirements of Nuclear Data for Radiation Damage and Related Safety Aspects. Vienna, 19-22 September, 1989.
9. D. E. Cullen, P. K. McLaughlin: The International Reactor Dosimetry File (IRDF-85). Report IAEA-NDS-41, Rev. 1. International Atomic Energy Agency, Vienna, April 1985.
10. The International Reactor Dosimetry File IRDF-90. Publication in progress by the Nuclear Data Section of the International Atomic Energy Agency.
11. H. J. Nolthenius: Computer programs for calculating group crosssection covariances from uncertainty parameters in the ENDF/B-V format, UNC 32/33. Report ECN-202. Netherlands Energy Research Foundation, Petten, Oct. 1987.
12. F.G. Perey: Least-squares dosimetry unfolding: the program STAY'SL. Report ORNL/TM-6062, ENDF-254. Oak Ridge National Laboratory, October 1977.
13. M. Matzke, publication in progress as a PTB report
14. F. W. Stallmann: LSL-M2: A computer program for least-squares logarithmic adjustment of neutron spectra. Report NUREG/OR-4349, ORNL/TM-9933. Oak Ridge National Laboratory, Oak Ridge, TN, March, 1986.

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