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THE NEUTRON METROLOGY FILE NMF-90

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Abstract: The Neutron Metrology File NMF-90 is an integrated database and software package for neutron spectrum adjustment and radiation damage (exposure) parameter calculations on PC. It contains 4 different neutron spectrum adjustment ("spectra unfolding") codes, the reactor dosimetry cross section library IRDF-90/NMF-G with covariance files, 6 input data sets for benchmark reactor neutron fields and a number of utility programs for processing and plotting the input and output data. The package – including manuals – is distributed on CD-ROM by the Nuclear Data Section of IAEA (free of charge). It is also available online (<http://www-nds.iaea.or.at>). About 30 MB of HDD space is needed to install the file and run a typical reactor dosimetry neutron spectrum adjustment problem.

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Introduction

The Nuclear Data Section of the International Atomic Energy Agency (IAEA NDS) organized a long term reactor dosimetry programme in order to improve the accuracy in the radiation damage characterization and hereby in the service life prediction of nuclear facilities. The emphasis was concentrated on radiation damage (exposure) parameters (derived from neutron spectrum information by an adjustment procedure) for reactor pressure vessels and related nuclear technology.

The programme was realized in frame of several interlaboratory exercises named REAL-80*, REAL-84 and REAL-88, and covered a period longer than a decade [1-4]. The improvement of the radiation damage (exposure) parameters required the use of good quality input data and proper calculation methods. The combined effort of the participants and evaluators** of the exercises contributed to the solution of numerous basic mathematical and physics problems detected in the neutron spectrum adjustment procedure for radiation damage purposes.

The final outcome of the project resulted in the Neutron Metrology File NMF-90 [4,5] comprising the following information in the form of separate modules:

1. DEMO;
2. Reference data file for the benchmark neutron fields of the REAL-88 project;
3. Tested cross section library;
4. Software packages and utility programs for neutron spectrum adjustment (“spectra unfolding”) and subsequent radiation damage (exposure) parameter calculations.

The file is distributed by the Nuclear Data Section of IAEA.

1. Module DEMO

The module DEMO contains a sample problem and performs neutron spectrum adjustment runs (including cross section processing as well) and related radiation damage calculations with all the programs involved in NMF-90. The spectrum set chosen for this purpose was derived for the reactor cavity of the Arcansas Power and Light Reactor (Arcansas Nuclear One-1), and is one of the reference spectrum sets in the neutron metrology file (see below). It is recommended to run the DEMO in order to see all the details of the calculations before using the programs of the neutron spectrum adjustment modules.

* REAL = Reaction Rate Estimates Evaluated by Adjustment Analysis in Leading Laboratories.

**The evaluators of the exercises were: Energy Research Foundation of the Netherlands (ECN) and Institute of Nuclear Techniques of the Technical University of Budapest (INT TUB).

2. Reference Data File

This module contains problem dependent input data sets for the six benchmark neutron fields of the REAL-88 exercise, furthermore, characteristic data calculated by some experienced laboratories for the spectrum sets in question. The benchmark neutron fields are:

1. ANO – Pressure vessel cavity (between the pressure vessel wall and the concrete shielding) of the Arkansas Power and Light Reactor (Arkansas Nuclear One-1).
2. PS1 – Oak Ridge Research Reactor, Poolside Facility; metallurgical irradiation experiment, simulated surveillance position.
3. PS2 – Oak Ridge Research Reactor, Poolside Facility; metallurgical irradiation experiment, simulated pressure vessel capsule position.
4. RTN – Fusion simulation spectrum measured at RTNS-11, a 14 MeV neutron source at the Lawrence Livermore Laboratory. The spectrum is a simulation of the first wall spectrum in a fusion reactor.
5. Fission neutron spectrum of ^{235}U .
6. CFR – Neutron spectrum in the centre of the coupled fast reactivity measurement facility (CFRMF).

Each input data set contains the following information:

- a) measured reaction rates and related uncertainty information (in the form of covariance matrices) in the neutron field of interest;
- b) calculated neutron spectrum for the neutron field in question, accompanied with covariance information;
- c) weighting neutron spectrum in a fine energy group structure (for cover and selfshielding calculations and cross section processing).

The file has been developed in order to create consistent data sets for neutron spectrum adjustment and related radiation damage (exposure) parameter calculations, which can be considered as benchmarks for interested scientists in testing their relevant calculation procedures. At the same time, certain data of the benchmark fields can be used for substituting missing data (eg input neutron spectrum covariance matrix) of the neutron spectrum adjustment calculations in similar environments. Nevertheless, this method can be applied only in case if it is justified by physics based information.

3. Tested cross section library (IRDF-90)

The cross section library (named IRDF-90/NMF-G [6]) involved in NMF-90 is based on the second version of IRDF-90 [7-9]. Some corrections have been introduced to the numerical values, furthermore, the files in ENDF-5 format of the second version have been converted into ENDF-6 format. The cross sections are available in 640 groups (extended SAND II) histogram format.

The library contains 53 dosimetry reactions together with uncertainty information in the form of covariance matrices.* Besides these data, cross sections for detector cover materials and radiation damage calculations (eg dpa) are also present. Some results on testing of the library data can be found in [6,8,9].

4. Software packages and utility programs

Three software packages (STAYNL, MIEKE and LSL [5,11-14]) developed by different laboratories and running on PC-s have been made available for the users. Each package can provide a complete neutron metrology calculation for radiation damage purposes. They start with cross section processing from ENDF-6 format data (except LSL, which contains a master library), perform neutron spectrum adjustment by the generalized LSQ method and terminate in radiation damage (exposure) parameter calculation.

The modules STAYNL and LSL have been written in standard FORTRAN77. The module MIEKE applies Microsoft Fortran77 compiler specific extensions, therefore, it can run only in case if Microsoft runtime libraries are available. A mathematical processor is strongly recommended for older PCs.

4.1. Module STAYNL

The module STAYNL – developed by the Institute of Nuclear Techniques of the Technical University of Budapest and by the Energy Research Foundation of the Netherlands – comprises two computer codes: X333 and STAYNL [11,12,15].

X333 – The code X333 is the cross section processing code of the module. It calculates group cross section values and their covariance matrices from the data given in MF=3 and MF=33 of preprocessed cross section libraries in ENDF-6 format like IRDF-90. The cross section data present in file MF=3 are given in histogram form, in the 640 group SAND II energy group structure. The code performs simple self- and cover-shielding calculations as well. The input requires the list of the reactions, the cross sections of which will have to be processed, the detector and cover geometry and material data (optional), the requested output energy group structure, and a weighting neutron spectrum for the neutron field of interest (based on reactor physics information) in a fine energy group structure. The output of the code is a problem dependent cross section and cross section covariance library.

* The content of the files MF=32 present in Ver. 2. of IRDF-90 has been converted into form MF=33 during the preparatory work of IRDF-90/NMF-G

STAYNL – The code solves the neutron spectrum adjustment problem by the generalized least squares method (GLSQM). The spectrum normalization before adjustment is performed also by the GLSQM, and the cross covariance terms in the calculation of the covariance matrix of the reaction rates are also taken into consideration. The user's input consists of the measured reaction rates and their covariance matrix, and of the calculated neutron spectrum in the neutron field of interest, also accompanied by its covariance information. The problem dependent cross section library can be generated using the code X333. The output of the code is the adjusted neutron spectrum (together with its covariance information) that minimizes the χ^2 value for the problem.

XSSPPP – This utility program converts the I/O files of the codes X333 and STAYNL into a form similar to file MF=3 in ENDF-6. The output of the utility can be used as input for the plotting programs EVALPLOT and COMPLIT* of the ENDF pre-processing code package PREPRO96 [16].

COVPLOT – This utility program plots the covariance matrices obtained from the jobs of X333 and STAYNL both in 3D and color coded 2D forms.

XSL&OUT – This utility program calculates the radiation damage (exposure) parameters based on the outputs of the codes X333 and STAYNL.

XSLXTRCT – This utility program converts the (direct access, binary) cross section library generated by the code X333 into card-image ASCII form (eg for the purpose of further manual editing).

X333SCR – This utility program converts the content of the scratch files of the job X333 into character form to help the user in the debugging procedure of the cross section processing.

All the programs of the module have been written in a user friendly form, ie no manual editing is needed between the neutron spectrum adjustment, plotting and radiation damage parameter calculations. Furthermore, the same input is possible for the codes X333 and STAYNL.

4.2. Module MIEKE

The module MIEKE [13] – developed by the Physikalische Technische Bundesanstalt (PTB) Braunschweig (BRD), contains a cross section processing code (UNC33M) and three neutron spectrum adjustment codes (MSITER, MSANDB, MIEKEB), accompanied by several utility programs.

1) The cross section processing in this module is performed by the application of the code UNC33M and 3 utility programs.

UNC33M – Cross section covariance processing code converting ENDF-6 format covariance data in the file MF=33 to the user's energy group structure.

MCROBI – This utility program converts the ENDF-6 formatted data into a formatted SAND II 640 energy group library.

* Also these programs are recorded on the NMF-90 CD-ROM.

UMSBIB – This utility program converts the formatted SAND II library into binary form needed as input for UNC33M.

MFITIB – This utility program converts cross section and neutron fluence rate data given in SAND II energy grid to coarse energy groups, and performs simple neutron self-shielding calculations for cross sections needed as input for MSITER.

XSC32M90 – The module MIEKE can process data from the cross section library IRDF-85 in case, if the covariance information on the resonance parameters (MF=32 files) of the target materials ^{23}Na , ^{237}Np , and ^{58}Fe has been pre-processed and attached to the library in a special format. Then the utility program XSC32M90 selects the one of the 3 materials requested by the user for further processing by the code UNC33M. (Neither the pre-processing code nor the pre-processed data are present in the module MIEKE.)

2) Neutron spectrum adjustment codes:

MSITER – This code solves the neutron spectrum adjustment problem also by the GLSQ method, but the neutron spectrum modification is performed in iterative way. The number of iterations to be performed by the program can be given either in the input, or it is determined by the convergency of the results obtained in the subsequent iteration steps. The normalization of the input neutron spectrum can be performed in three different ways:

- a) the normalization factor can be a constant defined in the input;
- b) the normalization can be performed by the GLSQM before the spectrum modification;
- c) the normalization and the spectrum modification can be performed in one step by the GLSQM.

Selection of the procedure to be carried out is done by the user in the input.

MSANDB – The algorithm of this adjustment code is taken from the code SAND II [17], however, the uncertainties of the reaction rates (ie the elements along the main diagonal of the covariance matrix of the reaction rates) can be taken into account in the adjustment procedure.

MIEKEB– It is a neutron spectrum adjustment code for use in cases when there is a lack of *a priori* information on the neutron spectrum. The code is using Monte-Carlo algorithm for solving the problem. (It is not a GLSQM code.)

Running the codes of the module MIEKE requires some editing work. Several utility programs are given to prepare the input for the codes and to plot the results of the spectrum adjustment runs and radiation damage (exposure) parameter calculations.

MSPECT – This utility program creates neutron fluence rate values in the required energy group structure for: Watt fission spectrum, NBS-Uranium fission spectrum, NBS-Californium fission spectrum or for a neutron spectrum defined by the user, to be used as input for the code MSITER.

UMSDAT – This utility program converts the data of the reference data file to the format needed in this (MIEKE) module.

PLOT – This utility program prepares plots for a HP-plotter or LASER JET printer.

PLOF – This utility program plots cross section data from IRDF-90 or from a formatted or unformatted SAND II type cross section library.

4.3. Module LSL

The module – developed by the ORNL, Oak Ridge, USA – contains the neutron spectrum adjustment code LSL-M2 [14] and a MASTER cross section library (based on IRDF-85 data). For using data of ENDF-6 type in the neutron spectrum adjustment by this program one has to run the code X333 from the module STAYNL (and a small utility program for format conversion), thus producing the cross section data for the sample problem. The code LSL-M2 is based on the GLSQM and it is working in the logarithmic space. The spectrum normalization before adjustment is based on the ratio of measured and calculated reaction rates of the detector(s) selected by the user. The calculations require several editing steps.

The code LSL-M2 is not distributed in this package, it can be obtained from RSSIC, Oak Ridge, TN, USA.

5. Hardware and software requirements

The NMF-90 has been developed for running on PC. Depending on the HDD addressing system, about 23–29 MB of disk space is needed to install the file, and about 2–5 MB is needed for the solution of a typical reactor dosimetry neutron spectrum adjustment problem.

The codes available in executable form (.EXE files) run under MS-DOS operating system Ver. 3.2 or above, furthermore in full screen DOS window of Windows 3.1x or Windows 95. The programs of the module STAYNL can be compiled for other platforms than PC + MS-DOS as well, while the programs of the modules DEMO and MIEKE can run only on PC.

The file NMF-90 is distributed on CD-ROM.

The manuals on the CD-ROM are given in their original format (extended ASCII, Microsoft Word 2.0, Microsoft Word 6.0, and WordPerfect).

The installation procedure is described on the CD-ROM in the file \SUMMARY.TXT.

6. References

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List of files contained on the CD-ROM

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FLUX48.MI1	04-04-91	MRESBI.48 04-04-91
FLUX48.MI2	04-04-91	MRESBI.PR1 04-04-91
FLUX48.MS	04-04-91	MSANDB.PR1 04-04-91
FLUX48.SAN	04-04-91	MSITER.PR1 04-04-91
FLUXC48.MI1	04-04-91	MSPECT.OUT 03-21-91
FLUXC48.MI2	02-02-95	MSPECT.PR 02-02-95
FLUXC48.MS	04-04-91	PACKLIST.TXT 07-29-98
MIEKEB.PR1	04-04-91	RESP48.BIN 04-04-91
MIEKEB.PR2	04-04-91	RESP48.FMT 04-04-91
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PACKLIST.TXT	07-29-98	README.DOC 02-23-95
READ1.DOC	06-29-95	
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ENDF.FOR	01-24-95	MSPECT.FOR 03-07-91
MCROBI.FOR	03-29-91	PACKLIST.TXT 07-29-98
MFITIB.FOR	04-03-91	UMSBIB.FOR 01-18-90
MIEKEB.FOR	03-19-91	UMSDAT.FOR 03-29-91
MRESBI.FOR	03-08-91	UNC33M.FOR 03-29-91
MSANDB.FOR	03-07-91	XSC32M90.FOR 03-07-91
MSITER.FOR	04-03-91	
Directory of \NMF-90\MIEKE\INPUT		
MCROBI.DAT	03-22-91	MSPECT.INP 03-06-91
MCROBI.INP	03-07-91	PACKLIST.TXT 07-29-98
Directory of \NMF-90\MIEKE\INPUTANO		
ACT.ANO	03-15-91	MSITERIN.ANO 03-19-91
MFITIBIN.ANO	03-14-91	PACKLIST.TXT 07-29-98
MIEKEBI2.ANO	03-24-91	UMSDATIN.ANO 03-14-91
MIEKEBIN.ANO	03-24-91	UNC33MIN.ANO 03-14-91
MSANDBIN.ANO	03-19-91	

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ACT.CFR	03-15-91	MSITERIN.CFR 03-15-91
MFITIBIN.CFR	03-14-91	PACKLIST.TXT 07-29-98
MIEKEBI2.CFR	03-24-91	UMSDATIN.CFR 03-14-91
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MSANDBIN.CFR	03-14-91	
Directory of \NMF-90\MIEKE\INPUTPS1		
ACT.PS1	03-21-91	MSITERIN.PS1 03-15-91
MFITIBIN.PS1	03-07-91	PACKLIST.TXT 07-29-98
MIEKEBI2.PS1	04-06-91	UMSDATIN.PS1 03-07-91
MIEKEBIN.PS1	03-24-91	UNC33MIN.PS1 03-07-91
MSANDBIN.PS1	01-23-90	
Directory of \NMF-90\MIEKE\INPUTPS2		
ACT.PS2	03-14-91	MSITERIN.PS2 03-15-91
MFITIBIN.PS2	03-14-91	PACKLIST.TXT 07-29-98
MIEKEBI2.PS2	04-06-91	UMSDATIN.PS2 03-14-91
MIEKEBIN.PS2	03-24-91	UNC33MIN.PS2 03-14-91
MSANDBIN.PS2	03-14-91	
Directory of \NMF-90\MIEKE\INPUTRTN		
ACT.RTN	03-21-91	MSITERIN.RTN 03-15-91
MFITIBIN.RTN	03-14-91	PACKLIST.TXT 07-29-98
MIEKEBI2.RTN	03-24-91	UMSDATIN.RTN 03-14-91
MIEKEBIN.RTN	03-24-91	UNC33MIN.RTN 03-14-91
MSANDBIN.RTN	03-14-91	
Directory of \NMF-90\MIEKE\INPUTU35		
ACT.U35	03-14-91	MSITERIN.U35 03-15-91
MFITIBIN.U35	03-14-91	PACKLIST.TXT 07-29-98
MIEKEBI2.U35	04-06-91	UMSDATIN.U35 03-14-91
MIEKEBIN.U35	03-24-91	UNC33MIN.U35 03-14-91
MSANDBIN.U35	03-14-91	
Directory of \NMF-90\MIEKE\IRDF1		
COMPNEPT.EXE	01-27-95	IRDFDAM 09-28-93
COMPXSC1.EXE	01-27-95	PACKLIST.TXT 07-29-98
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IRDF.BIN	03-22-91	PACKLIST.TXT 07-29-98
IRDF.FMT	03-22-91	
Directory of \NMF-90\MIEKE\PLOT		
ERZFON.EXE	04-05-91	PLOF.EXE 04-12-91
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MCROBI.EXE	03-21-91	MSPECT.EXE 03-21-91
MFITIB.EXE	03-21-91	PACKLIST.TXT 07-29-98
MIEKEB.EXE	04-04-91	UMSBIB.EXE 04-05-91
MRESBI.EXE	04-04-91	UMSDAT.EXE 03-21-91
MSANDB.EXE	03-21-91	UNC33M.EXE 03-29-91
MSITER.EXE	03-21-91	XSC32M90.EXE 04-05-91

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ACT.PS1	03-21-91	FMIEKE1.PS1	03-23-91
ACT2.PS1	03-22-91	FMIEKE2.PS1	04-12-91
CF.PS1	03-22-91	FSAND.PS1	03-22-91
CFMIEKE1.PS1	03-23-91	FSITER.PS1	03-22-91
CFMIEKE2.PS1	04-12-91	MFITIBPR.PS1	03-22-91
CFSITER.PS1	03-22-91	MIEKEBP2.PS1	04-12-91
COV.PS1	03-22-91	MIEKEBPR.PS1	03-23-91
COVACT.PS1	03-22-91	MSANDBPR.PS1	03-22-91
CROSS.PS1	03-22-91	MSITERPR.PS1	03-22-91
CROSS1.PS1	03-22-91	PACKLIST.TXT	07-29-98
CROSS1BI.PS1	03-22-91	UMSDATPR.PS1	03-22-91
CROSSBI.PS1	03-22-91	UNC33MPR.PS1	03-22-91
F1.PS1	03-22-91	W1.PS1	03-22-91
FF1.PS1	03-22-91		

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DOCU.TXT	07-29-98	PACKLIST.TXT	07-29-98
ENDFIO.FOR	11-08-96	PLOT.CHR	11-19-96
HARDSAVE.FOR	11-19-96	PLOT.SYM	11-19-96
HARSEND.FOR	11-19-96	SCRATCH1.FOR	10-10-96
INSTALL.BAT	07-29-98	SCREEN.FOR	11-12-96
MT.DAT	11-19-96	TIMER.FOR	10-10-96

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AAREADME	12-05-96	COMPSAVE.EXE	12-05-96
COMPLLOT.EXE	11-19-96	COMPSEND.EXE	12-05-96
COMPLLOT.FOR	11-08-96	MAKEFILE	10-10-96
COMPLLOT.INP	10-01-96	PACKLIST.TXT	07-29-98
COMPLLOT.LST	12-05-96	SEND.BAT	11-25-96

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AAREADME	12-05-96	EVALSAVE.EXE	12-05-96
EVALPLOT.EXE	11-19-96	EVALSEND.EXE	12-05-96
EVALPLOT.FOR	11-08-96	MAKEFILE	10-10-96
EVALPLOT.INP	11-19-96	PACKLIST.TXT	07-29-98
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