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Titel

Edition 2 of the MICROR Interface Code

Ersetzt
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Autor / en

S. Pelloni

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P.W.

Abstract

A new version (Edition 2) of the MICROR interface code now is available on the CRAY-2. MICROR produces cross section libraries in the FDTAPE, GARTAPE, and GGTAPE formats for the two-region spectrum code MICROX-2. MICROX-2 is an integral transport theory cell code for the efficient and rigorous preparation of broad group neutron cross sections for both fast and thermal reactor calculations.

Edition 2 of MICROR primarily has been written to enable the main sodium resonance at 2.81 keV to be considered when performing detailed pointwise slowing down calculations of fast spectra, and to allow the preparation of complete fission product MICROX-2 libraries for use in the two-dimensional, diffusion theory, burn-up code 2DB.

In this technical note we document the main differences between Edition 2 and Edition 1 of MICROR.

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	Expl.
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Reserve	10
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Seiten	10
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Visum Abt./Laborleiter:

1410014

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1 Introduction

At PSI, suitably shielded multigroup neutron cross sections for fast breeder and high temperature reactor calculations [1] are currently generated using a PSI version (Edition 14) of the two-region spectrum cell code MICROX-2 from General Atomics [2].

MICROX-2 is an integral transport theory spectrum code which solves the neutron slowing down and thermalization equations on a detailed energy grid for a two region lattice cell, using pointwise and fine group cross section libraries in the formats GARTAPE, FDTAPE, and GGTAPE.

The GARTAPE data library contains pointwise, Doppler-broadened capture, fission, fission production, and elastic scattering resonance cross sections. Fine points up to about 9 keV, the threshold energy for ^{235}U inelastic scattering, may be defined according to the criterion of either equidistant lethargy or velocity spacing, the spacing being chosen to provide an accurate self-shielding of the important resonances.

The FDTAPE data file contains 92 neutron group dilution- and temperature- dependent cross sections up to P_3 in the fast energy range.

The GGTAPE data file consists of two sections which include infinitely dilute P_0 and P_1 cross sections in the fast and thermal energy ranges (101 thermal neutron groups) respectively.

The present MICROX-2 libraries, which were prepared using NJOY (Version 89.62) in connection with Edition 1 of MICROR [3], show some fundamental limitations when used in neutronics calculations, the most important being reported here:

- To ensure a correct shielding of the unresolved resonances, the upper energy boundary for the pointwise slowing down calculation in MICROX-2 must lie below the unresolved range of any important isotope in the cell. This is necessary because the unresolved resonance cross sections prepared with Edition 1 of MICROR for the GARTAPE data libraries are energy-averaged cross sections at infinite dilution. Therefore, it is not possible to include the main sodium resonance at 2.81 keV into the pointwise slowing down calculation of a fast breeder reactor cell, because a considerable part of the unresolved resonance region of important nuclides lies below the sodium resonance and would not be shielded (the problem has already been described in a previous study [4]).

- There are no fission products and minor actinides available on the PSI libraries. Isotopes, including short lived fission products and minor actinides, must be generated as "primary nuclides" when using Edition 1 of MICROR: full scattering matrices are required, which makes the library processing time consuming and even incomplete, if either energy or angular distributions are not available (such as in activation libraries).

- The multigroup total cross section currently available in the libraries is that produced by the GROUPR module of NJOY (i.e. MF=3, MT=1 in the ENDF terminology). This cross section does not always match the sum of the partial cross sections due to the interpolation used by NJOY. Particularly affected by this inconsistency are data of actinides processed at low background cross sections and not too high temperatures, and the effect is enhanced at energies where there is an overlap between the unresolved energy range and inelastic scattering.

  The ratio between the summed partial cross sections and the total cross section is almost 1.001 for the JEF-2.2 evaluation of ^{238}U processed at a background cross section of 10 barns, room temperature, in the unresolved range and at energies between about 40 keV and 300 keV.

  The use of such slightly "unbalanced" data may either lead to a wrong prediction of the eigenvalue or even cause serious problems in the convergence of a transport-theory calculation particularly when analyzing hard spectra systems.

To remove these limitations, we decided to write a new version (Edition 2) of MICROR. In particular, this version allows to increase the upper boundary for the pointwise resonance calculation in MICROX-2 to about 8 keV.

In the next section the main differences between the two versions of MICROR are given, together with some coding details, and the new part of the input description is illustrated. Many other Edition 2 coding improvements that do not significantly affect the physics results (such as the capability to include an unlimited number of data sets) are not listed here.

2 Edition 2 of MICROR: Input Description and Coding Details

2.1 Coding Details

The input changes with respect to Edition 1 are identified with update lines "JUNE92.***". Edition 2 accepts the same input as Edition 1, provided that the new parameters are defaulted (i.e. a slash (/) must end each input line). Edition 2 is a stand-alone code with routines from the driver of NJOY (Version 89.62).

On the CRAY-2 the source of Edition 2 of MICROR is

/u0/pelloni/micror/micred2.f,

the binary executable

/u0/pelloni/micror/micred2.x,

the binary program library /u0/pelloni/micror/micred2.lib,

the compilation job /u0/pelloni/micror/micred2.compile,

and the listing file /u0/pelloni/micror/micred2.l.

The dmget utility should be used if files were migrated.
Edition 2 can be recognized looking at the banner printed at the beginning of execution:

```
****************************************
****************************************
****************************************
THIS IS EDITION 2 OF THE MICROR INTERFACE
CODE, COMPILED ON THE FIRST OF JULY 1992
BY SANDRO PELLONI AT PSI
****************************************
****************************************
****************************************
```

The main differences between Edition 2 and Edition 1 of MICROR are explained in detail below.

2.1.1 Input Card 1

Allowed unit numbers are between 20 and 30, and between 40 and 98. Unit number 99 now is reserved: it is assigned to a PENDF file on which the unresolved resonance region is shielded.

2.1.2 Input Card 3

GMATINP: an input parameter (Word 4) has been added to allow the user to supply nuclide identification numbers on the thermal part of the GGTAPE library. GMATINP has been introduced to avoid the duplication of identification numbers which can occur with the automatic identification number generation scheme, as for example, when processing carbon data from JEF-2.2 and ENDF/B-VI (with the same material number 600 in both evaluations) using different thermal scattering options such as graphite, free gas, or polyethylene.

2.1.3 Input Card 4

IS0, ITIG, MATINP: three additional input parameters (Words 6-8) in the GAR section.

IS0 (Word 6) is the sigma zero sequence number on the PENDF file for shielding GAR data in the unresolved energy range. IS0 corresponds to a single, problem dependent, energy-averaged input background cross section (a value between 10 and 50 barns is recommended for U-238 in fast breeders). The default value (IS0=1) corresponds to 10^{10} barns.

If IS0 is not defaulted, the new subroutine NURP of MICROR checks whether the unresolved region has been shielded on the PENDF file, and whether IS0 is either smaller or equal to the maximum number of dilution cross sections available. If IS0 is too big, a warning is printed, and the unresolved GAR data is not shielded (MICROR does not quit).

Otherwise, subroutine NURP prints out upper and lower energy limits of the unresolved energy range, reads in from PENDF File 2 self-shielded cross sections at the corresponding input dilution cross section (MF=2, MT=152 in the ENDF terminology), shields total, elastic, fission, and capture cross sections on File 3 (MF=3, MT=1, 2, 18, 19, 102 in ENDF terminology), and writes a new PENDF file on unit 99 using NJOY specific routines. If the total cross section does not match the sum of the partial cross sections on File 2 (i.e. MT=2, plus either 18 or 19, plus 102), a warning is printed and the total, shielded cross section is reset to the sum of the partial cross sections.

If LGPRNT=1 (see Card 2, Word 1) the resulting, energy dependent shielding factors are printed.

If the energy grids on File 2 and File 3 are not the same, the unresolved resonance cross sections on File 3 are interpolated for those energy points which do not belong to File 2. If LGPRNT=1 (see Card 2, Word 1) those energies are printed. Linear interpolation was found to be accurate enough, because the energy grid on File 2 is fine, the cross section quite smooth, and the neutron balance is not destroyed.

ITIG (Word 7): a new input parameter to allow the user to supply identification labels (see new Input Card 1G) on the GARTAPE data file. This additional parameter has been introduced to be able to better characterize and describe the origin of library nuclides.

MATINP (Word 8): an additional input parameter to allow the user to supply nuclide identification numbers on the GARTAPE data file. MATINP has been introduced to avoid identification number duplication when processing data from JEF-2.2 and ENDF/B-VI into the same library.

A consistency check has been introduced when new GAR data is added to an existing library. If either the top or bottom velocity, the velocity spacing, the number of points, or the number of points per record would not match, a fatal error with the following message would occur:

```
INCOSISTENCIES DETECTED BETWEEN NEW AND OLD GAR DATA
CHECK EITHER INPUT VELOCITY SPACING
                  TOP VELOCITY
                  LOWEST VELOCITY
           NUMBER OF POINTS ON TAPE
    OR  NUMBER OF POINTS PER RECORD
```

2.1.4 Input Card 1B

ITIF, FMATINP: two additional input parameters (Words 5-6) in the FDTAPE and fast GGTAPE sections.

ITIF (Word 5): a new input parameter to allow identification labels to be supplied (see new Input Card 1F) on the FDTAPE and on the fast part of the GGTAPE data libraries. This parameter has been introduced to be able to better characterize and describe the origin of library nuclides.

FMATINP (Word 6): an additional input parameter to allow the user to supply nuclide identification numbers on the FDTAPE and fast part of the GGTAPE data file. FMATINP has been introduced to avoid identification number duplication when processing dilution-dependent data from JEF-2.2 and ENDF/B-VI into the same library. If FMATINP is not defaulted, the second dilution cross section processed will be identified by FMATINP+0.00001, the third dilution cross section by FMATINP+0.00002, and so on.

2.2 Secondary Nuclides

Input parameter LTYPE (see Card 2C, Word 1) is still not active, because it is not needed. LTYPE has not been removed from the input for the sake of consistency with Edition 1. The misleading identification print "-1" for a secondary, "0" for a primary nuclide at the beginning of the fast GGTAPE session has been removed (nuclides were always primary in Edition 1 of MICROR).

A secondary nuclide (minor fission product or actinide) originates when only vector cross sections were processed into GENDF format. The number of neutrons per fission (ν) for a minor actinide is taken from MT=452 (ENDF terminology), because of missing fission matrices. If MT=452 is not available on the GENDF file, the fatal error

"***ERROR IN GAMXS***INCORRECT NUMBER OF ITEMS IN GAM-II RECORD 15."

appears.

The thermal section of the GGTAPE has been corrected to account for the possibility that scattering matrices are not available on the GENDF file.

The total cross section for secondary nuclides in the FDTAPE and fast GGTAPE sections were set equal to the absorption cross section (subroutine FASTM). In this way the total cross section becomes the sum of the partial cross sections, because of missing scattering matrices. This approximation seems to be reasonable for treating minor fission products.

If a secondary nuclide is processed, following message is printed (subroutine FASTM):

```
***   WARNING FROM FASTM:     ***
***   NUCLIDE IS SECONDARY.   ***
***   NO SCATTERING MATRICES  ***
***   AVAILABLE. ABSORPTION   ***
***   IS USED INSTEAD OF      ***
***   TOTAL XS (BALANCE).     ***
```

2.3 Total Cross Section

The multigroup total cross section available on the GENDF file (i.e. MF=3, MT=1 in the ENDF terminology) does not always match the sum of the partial cross sections due to the interpolation used by NJOY.

To avoid subsequent numerical problems, Edition 2 of MICROR calculates in subroutine GAMXSM an effective total cross section as the sum of absorption cross section (expressed as fission plus "capture" cross section, the "capture" cross section includes in addition to the (n,γ), (n,α), (n,p) and other cross sections), total inelastic (computed from the inelastic scattering matrices), total elastic (computed from the elastic scattering matrix), and total (n,xn) cross section (computed as the sum of (n,2n), (n,3n) , and (n,4n) vector cross sections).

This cross section replaces the NJOY total cross section in the FDTAPE and fast GGTAPE libraries. If its relative difference with the total cross section from NJOY exceeds 0.01%, a corresponding warning is printed:

```
960 FORMAT(/,' WARNING FROM GAMXSM',/,
   1         ' -------------------',/,
   1         ' IN GROUP                          ',6X,I6,/,
   1         ' TOTAL XS (MT=1) IS                ',1PE12.5,/,
   2         ' TOTAL XS (SUM OF THE PARTIALS) IS',1PE12.5,/,
   3         ' THEIR RELATIVE DIFFERENCE (%) IS ',1PE12.5,/,
   4         ' SUM OF THE PARTIALS IS RETAINED  ')
```

2.4 Scattering Matrices

An error leading in Edition 1 to an unexpected truncation of the inelastic and (n,2n) outscatter vectors particularly affecting ^{238}U ENDF/B-VI fast data has been eliminated and corrected as follows:

```
*DELETE FDTAPE.3100
      MM = ISTOP - MMM + IST
```

2.5 Additional Fast Reactions

Edition 2 of MICROR treats most ENDF neutron reactions.

The following reactions which were ignored by Edition 1 of MICROR are now added to both the vector and matrix inelastic scattering cross sections (some of these appear in the modern evaluations of sodium):

MT=22: (n,n'α) cross section;
MT=23: (n,n'3α) cross section;
MT=28: (n,n'p) cross section;
MT=29: (n,n'2α) cross section;
MT=32: (n,n'd) cross section;
MT=33: (n,n't) cross section;
MT=34: (n,n'^{3}He) cross section;

MT=35: (n,n'd2α) cross section;
MT=36: (n,n't2α) cross section.

The following reactions which were ignored by Edition 1 are now added to both the vector and matrix (n,2n) cross sections:

MT=24: (n,2nα) cross section;
MT=26: (n,2n) isomeric state cross section.

The following reaction which was ignored by Edition 1 is now added to both the vector and matrix (n,3n) cross sections:

MT=25: (n,3nα) cross section.

5 Revised Part of the Input Description

```
EDITION 2 OF MICROR: INPUT DESCRIPTION CHANGES
----------------------------------------------

C     * CARD 1 UNITS                                                    *  MICROR.16
C     *   NPENDF     INPUT UNIT FOR PENDF TAPE                          *  MICROR.17
C     *   NGEN1      INPUT DATA FOR UNIT FROM GROUPR                    *  MICROR.18
C     *   NGEN2      INPUT UNIT FOR DATA FROM GAMINR                    *  MICROR.19
C     *   NFDIN      INPUT UNIT FOR OLD FD DATA                         *  MICROR.20
C     *   NGARIN     INPUT UNIT FOR OLD GAR DATA                        *  MICROR.21
C     *   NGGIN      INPUT UNIT FOR OLD GG DATA                         *  MICROR.22
C     *   NFD        OUTPUT UNIT FOR NEW FD DATA                        *  MICROR.23
C     *   NGAR       OUTPUT UNIT FOR NEW GAR DATA                       *  MICROR.24
C     *   NGG        OUTPUT UNIT FOR NEW GG DATA                        *  MICROR.25
C     *                                                                 *  MICROR.26
C     * WARNING: IF CREATION OF NEW GAR DATA IS DESIRED                 *  MICROR.27
C     * (NGAR.NE.0.AND.LIB.NE.0) ONE AS TO DEFINE THE GENDF FILE AS     *  MICROR.28
C     * WELL (NGEN1.NE.0)                                               *  MICROR.29
C     *                                                                 *  MICROR.30
C     * ALLOWED UNIT NUMBERS BETWEEN 20 AND 30, AND BETWEEN 40 AND 98.  *  JUNE92.1
C     *                                                                 *  MICROR.32
C     * CARD 2 USER IDENTIFICATION                                      *  MICROR.33
C     *   LGPRNT     0/1 MEANS GAR SUMMARY PRINT/FULL PRINT             *  JUNE92.2
C     *   LFPRNT     0/1/2/3 MEANS DIFFERENT FD PRINT OPTIONS           *  JUNE92.3
C     *   LTPRNT     0/1/2/3 MEANS DIFFERENT GG PRINT OPTIONS           *  JUNE92.4
C     *              0: HEADING                                         *  MICROR.37
C     *              1: HEADING,FLUXES AND GROUP BOUNDARIES             *  MICROR.38
C     *              2: HEADING,FLUXES,GROUP BOUNDARIES AND RESPONSE    *  MICROR.39
C     *                 FUNCTIONS                                       *  MICROR.40
C     *              3: FULL PRINT                                      *  MICROR.41
C     *                                                                 *  MICROR.42
C     *                                                                 *  MICROR.43
C     *   LIB         LIBRARY OPTION (0=EDIT OR DELETE GIVEN DATA ON     *  MICROR.44
C     *                NEW UNITS NGAR,NFD,OR NGG. 1=FD,2=GG,3=BOTH,     *  MICROR.45
C     *                4=FAST GG)                                       *  MICROR.46
C     *   IOPT        =0 PROCESS FOR EACH OF THE NMATN MATERIALS GIVEN   *  MICROR.47
C     *                  NTEMP TEMPERATURES AND NSIGZ DILUTIONS         *  MICROR.48
C     *                  (CARDS 4-5. FIRST TEMPERATURE AND FIRST        *  MICROR.49
C     *                  DILUTION,FIRST TEMPERATURE AND SECOND DILUTION *  MICROR.50
C     *                  ..... ARE FIRST PROCESSED                      *  MICROR.51
C     *              =1 PROCESS FOR EACH OF THE NMATN MATERIALS EVERY   *  MICROR.52
C     *                  TEMPERATURE AND DILUTION ON THE GENDF FILE     *  MICROR.53
C     *                                                                 *  MICROR.54
C     *                                                                 *  MICROR.55
C     *   NTEMP       NUMBER OF TEMPERATURES TO PROCESS                  *  MICROR.56
C     *               (MEANINGFUL ONLY FOR IOPT.EQ.0)                    *  MICROR.57
C     *   NSIGZ       NUMBER OF SIGMA ZEROES TO PROCESS                  *  MICROR.58
C     *               (MEANINGFUL ONLY FOR IOPT.EQ.0)                    *  MICROR.59
C     *   NMATN       NUMBER OF MATERIAL NAMES TO BE READ                *  MICROR.60
```

```
C     *              IN EDITION 2 OF MICROR: NMATN MUST BE 1.          *  JUNE92.5

C     ------------------------------------------------------------------------

C     * SUPPLY CARD 3 NMATN TIMES (MATERIAL DATA)                       *  MICROR.85
C     * CARD 3                                                          *  MICROR.86
C     *   HMATR      HOLLERITH MATERIAL IDENTIFIER (6 CHARACTERS        *  MICROR.87
C     *              DELIMITED BY  *)                                   *  MICROR.88
C     *   MATR       INTEGER MATERIAL IDENTIFIER                        *  MICROR.89
C     *   NTHER      INELASTIC THERMAL SCATTERING MT NUMBER             *  MICROR.90
C     *              (DEFAULT=0 MEANS ELASTIC SCATTERING)               *  MICROR.91
C     *   GMATINP    0./GMATINP THERMAL GG IDENTIFICATION NUMBER IS     *  JUNE92.6
C     *              GENERATED BY THE CODE/IS EQUAL TO GMATINP          *  JUNE92.7
C     *              (DEFAULT=0.)                                       *  JUNE92.8

C     ------------------------------------------------------------------------

C     *---INPUT-SPECIFICATIONS-FOR-GAR-TAPE-----------------------------*  MICROR.99
C     *                                                                 *  MICROR.100
C     * SUPPLY CARDS 1A-5A IF NGAR.GT.0                                 *  MICROR.101
C     *                                                                 *  MICROR.102
C     * SUPPLY CARD 1A ONLY IF LIB.NE.0                                 *  MICROR.103
C     * CARD 1A                                                         *  MICROR.104
C     *   NPT        NUMBER OF RESONANCE CROSS SECTION POINTS TO BE     *  MICROR.105
C     *              RECONSTRUCTED ON GAR FILE                          *  MICROR.106
C     *   EO         TOP ENERGY OF RESONANCE RANGE (EV)                 *  MICROR.107
C     *   EL         LOWEST ENERGY OF RESONANCE RANGE (EV)              *  MICROR.108
C     *   NPRK       NUMBER OF POINTS/RECORD (DEFAULT=10)               *  MICROR.109
C     *   ILOG       0/1=EQUIDISTANT VELOCITY/LETHARGY SPACING          *  MICROR.110
C     *   ISO        SIGMA ZERO SEQUENCE NUMBER FOR SHIELDING THE       *  JUNE92.9
C     *              UNRESOLVED ENERGY RANGE (DEFAULT=1,I.E. S0=10**10)*  JUNE92.10
C     *   ITIG       0/1 DO NOT/DO SUPPLY LABEL CARD 1G. IF ITIG=0,     *  JUNE92.11
C     *              THEN THE LABEL CARD IS WRITTEN BY THE CODE.        *  JUNE92.12
C     *              (DEFAULT=0)                                        *  JUNE92.13
C     *   MATINP     0/MATINP LIBRARY MATERIAL NUMBER IS GENERATED      *  JUNE92.14
C     *              IN THE CODE/IS EQUAL TO INPUT INTEGER NUMBER       *  JUNE92.15
C     *              MATINP (DEFAULT=0).                                *  JUNE92.16
C     *                                                                 *  JUNE92.17
C     * SUPPLY CARD 1G ONLY IF ITIG.EQ.1                                *  JUNE92.18
C     * CARD 1G                                                         *  JUNE92.19
C     *   (OUT(I),I=1,13)                                               *  JUNE92.20
C     *              GAR INPUT ISOTOPE LABEL:                           *  JUNE92.21
C     *              MAXIMUM OF 52 CHARACTERS DELIMITED WITH *.         *  JUNE92.22
C     *                                                                 *  JUNE92.23

C     ------------------------------------------------------------------------

C     * SUPPLY FOLLOWING CARDS ONLY IF NFD.GT.0.OR.NGG.GT.0             *  MICROR.145
C     * INPUT AND OUTPUT UNIT NUMBERS HAVE TO BE DIFFERENT              *  MICROR.146
C     *---FOR LIB.EQ.1.OR.LIB.EQ.3-(FD TAPE OUTPUT)--------------------*  MICROR.147
C     *---(NFD.GT.0)---------------------------------------------------*  MICROR.148
C     *                                                                 *  MICROR.149
```

```
C     * CARD1B                                                          *  MICROR.150
C     *   NCARDS       NUMBER OF 72 CHARACTER CARD IMAGES TO USE TO     *  MICROR.151
C     *                DESCRIBE NEW FD TAPE                             *  MICROR.152
C     *   ICSPEC       NUMBER OF FISSION SPECTRA TO INPUT               *  MICROR.153
C     *                FROM CARDS 6B AND 7B                             *  MICROR.154
C     * AT THE PRESENT ONLY ICSPEC.EQ.0 IS ALLOWED                      *  MICROR.155
C     *   IFSWTH       0 = BOUND AND NORMALIZE NEW FISSION SPECTRA      *  MICROR.156
C     *                1 = NORMALIZE ONLY                               *  MICROR.157
C     *                2 = NEITHER                                      *  MICROR.158
C     * AT THE PRESENT ONLY IFSWTH.EQ.0 IS ALLOWED                      *  MICROR.159
C     *   ISQUEZ       0 = COMPRESS TRANSFER MATRICES                   *  MICROR.160
C     *                1 = DO NOT COMPRESS TRANSFER MATRICES            *  MICROR.161
C     *   ITIF         0/1 INPUT ISOTOPE LABEL IS NOT/IS WISHED         *  JUNE92.24
C     *                (DEFAULT=0)                                      *  JUNE92.25
C     *   FMATINP      0./FMATINP MATERIAL ID. NUMBER IS GENERATED BY   *  JUNE92.26
C     *                THE CODE/IS EQUAL TO FMATINP (DEFAULT=0.).       *  JUNE92.27
C     *                                                                 *  JUNE92.28
C     * CARD 1F (TO BE SUPPLIED IF ITIF=1)                              *  JUNE92.29
C     *   (SS(I),I=1,18)                                                *  JUNE92.30
C     *                ISOTOPE INPUT LABEL. MAXIMUM OF 72 CHARACTERS    *  JUNE92.31
C     *                DELIMITED WITH *.                                *  JUNE92.32
C     *                                                                 *  JUNE92.33
C     * NOTE: FOR LIB.EQ.3 FMATINP IS THE NUCLIDE ID. NUMBER AND SS(I)  *  JUNE92.34
C     *       THE NUCLIDE LABEL ON THE FAST GG FILE (SEE CARDS 1C-8C)   *  JUNE92.35
C     *       AS WELL. ID NUMBER FOR THE SECOND DILUTION XS IS          *  JUNE92.36
C     *       FMATINP+0.00001, FOR THE THIRD DILUTION FMATINP+0.00002,  *  JUNE92.37
C     *       .....,IF THESE ARE GENERATED.                             *  JUNE92.38
C     *                                                                 *  JUNE92.39
```

References

[1] S. Pelloni, " New Data Libraries for Fast Breeder Calculations ", Seminar on NJOY91 and THEMIS for the Processing of Evaluated Nuclear Data Files (April 7-8, 1992, Saclay, France)

[2] D. R. Mathews, P. Koch, " MICROX-2. An Improved Two-Region Flux Spectrum Code for the Efficient Calculation of Group Cross Sections, " Genaral Atomics Report, GA-A15009, Vol.1 (1979)

[3] D. R. Mathews, J. Stepanek, S. Pelloni, C. E. Higgs, " The NJOY Nuclear Data Processing System: the MICROR Module, " Paul Scherrer Institute Report, EIR Report 539 (December 1984)

[4] S. Pelloni, " Comparison Calculation of a Large Sodium-Cooled Fast Breeder Reactor Using the Cell Code MICROX-2 in Connection with ENDF/B-VI and JEF-1.1 Neutron Data, " Paul Scherrer Institute Report, PSI Report 118 (February 1992)

PAUL SCHERRER INSTITUT
Labor für Reaktorphysik und Systemtechnik

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Titel

Neutronics Calculations of the SCHERZO Fast Experiments

Ersetzt
—

Autor / en
S. Pelloni

Erstellt
26 Aug. 1992/PS41

Abstract

We have analyzed the SCHERZO fast spectrum experiments using three evaluations, JEF-2.2, ENDF/B-VI (Revision 1), and JEF-1.1, and compared the results with the measurements. The experiments simulate fuel assemblies consisting of either 5.56 % enriched uranium (SCHERZO-556) or 7.40 % enriched uranium oxide (SCHERZO-740) in infinite geometry.

The cross sections were generated using the NJOY code system (Version 89.62), and further processed with a new version (Edition 2) of the coupling code MICROR for later use in PSI-Edition 14 of the spectrum cell code MICROX-2. The eigenvalue k_∞ and reaction rates were calculated using the one-dimensional, discrete-ordinates transport-theory code ONEDANT.

It is shown that the results for SCHERZO-740 obtained using JEF-2.2 data agree well, generally within one standard deviation, with the experimental values. The calculated eigenvalue of SCHERZO-556 (1.016) is significantly too high.

These results seem to be consistent with those obtained in Cadarache using the European Cell Code ECCO.

Verteiler

Abt.	Empfänger	Expl.	Abt.	Empfänger	Expl.
4000	W. Kroeger	1	41	J. Hammer	1
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4122	J. Kallfelz	1			

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1 Introduction

In the frame of the JEF project we have been asked by CEA (CEN Cadarache) to analyze the fast spectrum experiments SCHERZO using the newest nuclear data files released, JEF-2.2, ENDF/B-VI (Revision 1), and JEF-1.1. The SCHERZO experiments, which simulate fuel assemblies consisting of either 5.56 % enriched uranium metal (SCHERZO-556) or 7.40 % enriched uranium oxide (SCHERZO-740) in infinite geometry, are very simple but difficult to be properly calculated [1].

The main objectives were the testing of the new PSI codes for simple, fast reactor like experiments, the identification of eventual deficiencies of these codes when comparing with calculations using the European Cell Code ECCO, and the identification of relevant discrepancies coming from the use of different, modern nuclear data sources for uranium.

In Section 2 the computational model used is described, whereas Section 3 is devoted to the main results and conclusions.

2 Computational Model

The nuclear data used in the calculations was either from the JEF-2.2, the ENDF/B-VI (Revision 1), or the JEF-1.1 evaluation. The cross sections were generated using the NJOY code system (Version 89.62) and further processed with a new version (Edition 2) of the coupling code MICROR [2], for later use in PSI-Edition 14 of the spectrum cell code MICROX-2 from General Atomics [3]. 24362 points, equally spaced in velocity, building a very fine energy grid between 8 keV and 2 eV were used in the MICROX-2 spectrum calculations. The Bondarenko formalism was used to shield resonance cross sections of uranium and oxygen above 8 keV, where 60 fine fast groups, equally spaced in lethargy, were considered. The detailed slowing down calculation is not required when analyzing SCHERZO-556 (uranium metal), because the spectrum is very hard.

Eigenvalues and reaction rates were calculated using the one-dimensional, discrete-ordinates transport-theory code ONEDANT from Los Alamos, using spectrum-averaged 33 neutron broad group cross sections, a fission spectrum calculated in the usual way from the total, nuclide dependent, fission production rates [4], and a simple, single zone, infinite spherical model. The use of more broad groups in the ONEDANT calculations did not change the results presented in this report.

Edition 2 of MICROR has the advantage that 8 keV (which is about the maximum energy where neutron scattering is always elastic) can be used systematically as the upper boundary for the pointwise resonance slowing down calculation. Indeed, the MICROX-2 libraries, which were generated using Edition 1 of MICROR [5], were found to have the following important limitations when used in the neutronics calculations of the SCHERZO experiments.

- To be able to correctly shield the unresolved resonance cross sections (Bondarenko formalism), the upper energy boundary for the pointwise slowing down calculation in MICROX-2 had to be smaller than the lower limit of the unresolved range for any important isotope [4]. This condition was needed because the pointwise unresolved resonance cross sections from the UNRESR module of NJOY, prepared with Edition 1 of MICROR, were energy-averaged cross sections given at infinite dilution.

Therefore, it was not possible to increase the range of the slowing down calculation to energies higher than 2.25 keV (82 eV) when using JEF-2.2 (JEF-1.1) data. This shortcoming resulted in a significant overprediction of the capture of ^{238}U and in a corresponding underprediction of the eigenvalue of SCHERZO-740 by about 1 %.

In Edition 2 of MICROR, a constant, energy-averaged input background cross section can be used for approximately shielding the pointwise portion of the unresolved resonance range. A value of 100 barns was systematically taken for ^{235}U, in addition to 20 barns for ^{238}U in the JEF-1.1 calculations, because the unresolved range of ^{238}U starts at 4 keV in the JEF-1.1 evaluation.

- The multigroup total cross section available was that processed with the GROUPR module of NJOY. This cross section did not always match the sum of the partial cross sections due to the interpolation used in NJOY. Particularly affected by this inconsistency were data of actinides processed at low background cross sections and not too high temperatures, at energies where there is an overlap between unresolved energy range and inelastic scattering.

  The maximum ratio between the effective multigroup total cross section derived from the partial multigroup cross sections (sum of the vector absorption cross sections and the scattering cross sections derived from the scattering matrices) and the total cross section generated by NJOY is 1.0009 for the JEF-2.2 evaluation of ^{238}U processed at 10 barns dilution cross sections, room temperature, in the unresolved range and at energies between 40 keV and 300 keV.

  The use of such slightly "unbalanced" data of ^{238}U led to a too high prediction of the eigenvalue (the maximum overestimate was 1 % in the case of SCHERZO-556), and to an additional, big discrepancy (of about 1.5 %) between the eigenvalues k_∞ calculated with MICROX-2 and ONEDANT (the ONEDANT eigenvalue was always larger than the MICROX-2 eigenvalue).

  Edition 2 of MICROR uses the effective total cross section instead of the total cross section from NJOY. In this way, the above mentionned eigenvalue discrepancies dropped to a few per mille.

	JEF-2.2	JEF-1.1	ENDF/B-VI (Revision 1)	Relative Exp. Error
k_∞	1.0162	0.9997	1.0172	0.
F8/F5	1.0749	1.0812	1.0861	± 0.0088
C8/F5	1.0059	1.0373	0.9998	± 0.01473

Table 1: Ratio between Calculated and Measured (C/E) Eigenvalue k_∞, and Reaction Rate Ratios for SCHERZO-556, Otained Using Data from JEF-2.2, JEF-1.1, and ENDF/B-VI (Rev. 1), and Relative Experimental Errors

3 Results and Conclusions

Tables 1-2 show the main results for SCHERZO-556 and SCHERZO-740, expressed as ratios (C/E) between calculated and measured values, and the relative experimental errors.

In Tables 1-2 F8 is the fission rate of ^{238}U,
F5 the fission rate of ^{235}U,
C8 the capture rate of ^{238}U, and
F9 the fission rate (as a spectral index) of ^{239}Pu per atom of fuel.

Main points from these tables are:

- The use of cross sections from JEF-2.2 and ENDF/B-VI (Revision 1) leads to qualitatively similar results, and improves their accuracy when compared with JEF-1.1.
- The calculation of SCHERZO-740 using either JEF-2.2 or Revison 1 of ENDF/B-VI cross sections reproduces well, generally within one standard deviation, the measurement. Both the resolved and unresolved resonance regions play an important role (see Table 3). F8/F5 deviates by about 1.5 σ. However, the relative experimental error of this reaction rate ratio is very small.
- The calculation of SCHERZO-740 using JEF-1.1 cross sections overpredicts C8/F5 by 2.5 %, and correspondingly underpredicts k_∞ by 1.2 %.

  This is probably because the unresolved resonance region of ^{238}U prematurely terminates at 50 keV in the JEF-1.1 evaluation, resulting in the use of unshielded, therefore too high ^{238}U cross sections above 50 keV, where the spectrum peaks (the corresponding upper boundaries of the unresolved resonance region are 300 keV and 149 keV in the JEF-2.2 and in Revision 1 of the ENDF/B-VI evaluation respectively).
- When using either JEF-2.2 or ENDF/B-VI cross sections k_∞ of SCHERZO-556 is overpredicted by about 1.5 %; F8/F5 is overpredicted by as much as about 8 %. Surprisingly, the prediction of C8/F5 is very accurate. The good prediction of k_∞ achieved using JEF-1.1 cross sections is obviously due to compensating effects.

The JEF-2.2 results are consistent with those obtained in Cadarache using the European Cell Code ECCO [1]. Therefore the new PSI codes seem to be adequate for analyzing "clean" fast systems [4].

	JEF-2.2	JEF-1.1	ENDF/B-VI (Revision 1)	Relative Exp. Error
k_∞	1.0009	0.9880	1.0031	0.
F8/F5	1.0143	1.0348	1.0121	± 0.0082
C8/F5	0.9976	1.0253	0.9891	± 0.0130
F9/F5	1.0021	1.0103	0.9897	± 0.0126

Table 2: Ratio between Calculated and Measured (C/E) Eigenvalue k_∞, and Reaction Rate Ratios for SCHERZO-740, Otained Using Data from JEF-2.2, JEF-1.1, and ENDF/B-VI (Rev. 1), and Relative Experimental Errors

Energy (eV)	k_∞
8000	1.0009
5531	0.9992
3355	0.9966
1234	0.9918
0.	0.9890

Table 3: Calculated Eigenvalue k_∞ for SCHERZO-740, Otained Using Data from JEF-2.2, as a Function of the Upper Energy Limit for the Detailed Pointwise Slowing Down Calculation (Above This Energy the Bondarenko Method is Used)

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PAUL SCHERRER INSTITUT
Labor für Reaktorphysik und Systemtechnik

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Titel

Comparison Calculation of a Large Sodium-Cooled Fast Breeder Reactor Using Modern Neutron Data

Ersetzt
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Autor / en

S. Pelloni

Erstellt
14 Sept. 1992/PS41

Abstract

This technical note includes our paper to be presented at the "Symposium on Nuclear Data Evaluation Methodology" to be held on October 12-16 at the Brookhaven National Laboratory, Upton, New York, USA.

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				P. Grimm	1
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COMPARISON CALCULATION OF A LARGE SODIUM-COOLED FAST BREEDER REACTOR USING MODERN NEUTRON DATA

by

Sandro Pelloni, Shahid Ahmed

Advanced Systems, Paul Scherrer Institute,
5232 Villigen PSI, Switzerland

ABSTRACT

We have obtained results for a large sodium-cooled fast breeder reactor benchmark using data from JEF-1.1, JEF-2.2, and ENDF/B-VI (Revision 1).

The observed (relatively small) differences between the new results and the average values of sixteen published benchmark solutions lie generally within one standard deviation.

Comparing JEF-2.2 relative to JEF-1.1 predictions, the eigenvalue k_{eff} for the reference configuration is slightly (0.21 %) higher. The isothermal core fuel Doppler reactivity is up to 12.8 % higher, and the sodium void reactivity worth is up to 10.5 % smaller.

The eigenvalue predicted with ENDF/B-VI cross sections is 0.53 % larger than that calculated with JEF-2.2 cross sections, whereas Doppler and sodium void reactivity agree generally within 5 %.

The main contributions to these differences are from the fission production cross section of ^{239}Pu and from the inelastic scattering cross section of ^{238}U and ^{23}Na below 1 MeV.

1 Introduction

Results of an international calculation of a large (1250 MWe) sodium-cooled fast breeder reactor benchmark model (LMFBR benchmark) were presented and discussed at a specialist's meeting at Argonne National Laboratory (ANL) in February 1978. Sixteen solutions from ten different participating countries were analyzed and published in a ANL report[1]. The purpose of that exercise, the first detailed comparison for a large commercial sized LMFBR system, was to evaluate and document the agreement and differences of calculations of key LMFBR physics and safety parameters based on different data sets and processing codes.

The main objectives of the recalculation of the LMFBR benchmark were the identification of relevant discrepancies coming from the use of the most modern nuclear data sources available in Europe and in the USA, namely the Joint European File (JEF-1.1 and JEF-2.2)[2,3] and Revision 1 of ENDF/B-VI[4].

Section 2 of this paper reports on the main results, and Section 3 gives conclusions and recommendations.

2 Results and Discussion

Tables 1-2 summarize the relative deviations of the JEF-1.1 results from the mean benchmark values, and the variation of the JEF-2.2 and ENDF/B-VI results relative to the JEF-1.1 values.

The tables show that the new results generally lie within one standard deviation of the average benchmark values.

Specific differences are:

- The eigenvalue k_{eff} for Configuration 1 (reference configuration) predicted with JEF-2.2 is slightly (0.21 %) larger than that calculated with JEF-1.1. Comparing ENDF/B-VI relative to JEF-2.2 predictions, k_{eff} is 0.53 % higher.

- Breeding and conversion ratios predicted with JEF-2.2 and JEF-1.1 agree well within 1 %. Comparing ENDF/B-VI relative to JEF-2.2 predictions, the maximum, 4.30 % increase (i.e. 0.417 versus 0.399) of the breeding ratio is in the blanket region.

- The sodium void reactivity worths for the inner core and whole reactor calculated with JEF-2.2 are significantly (i.e. about 10 %) smaller than the corresponding JEF-1.1 values. The ENDF/B-VI and JEF-2.2 predictions differ by a maximum of 5 %.

- The reactivity worths of the central control rod with sodium calculated with JEF-2.2 increases by 5.5 % when compared with JEF-1.1. The ENDF/B-VI and JEF-2.2 predictions agree well within 2 %.

- The JEF-2.2 isothermal core fuel Doppler-reactivity coefficient exceeds the JEF-1.1 value by 3.87 % for Configuration 1 (i.e. -0.00751 versus -0.00723), and by as much as 12.77 % for the voided Configuration 3 (i.e. -0.00452 versus -0.00401). The ENDF/B-VI and JEF-2.2 predictions agree within 4 %.

- The effective delayed neutron fraction and the inhour of reactivity for Configuration 1 calculated with JEF-2.2 are about 7 % larger than the respective JEF-1.1 values. The ENDF/B-VI values for these parameters are significantly (4.61 % and 11.2 %) lower than the JEF-2.2 values. These differences are primarily due to the different delayed neutron yields of ^{238}U and ^{239}Pu (see Table 2).

- There is a significant difference in the central sodium void reactivity worth. The rather big sodium void worth in Configuration 1, calculated with JEF-1.1 data (about 1.3 standard deviations larger than the mean benchmark value), decreases by about 0.65 standard deviations when using JEF-2.2 cross sections, and by about 0.25 standard deviations when using ENDF/B-VI cross sections.

Table 3, which is indicative for the above differences, shows the relative variation of the JEF-2.2 eigenvalue k_∞ for the inner core of Configuration 1 when substituting data for individual isotopes with data from ENDF/B-VI and JEF-1.1. The main contributions to this variation are ^{239}Pu from ENDF/B-VI (-0.66 %), ^{238}U from ENDF/B-VI (+0.71 %), and ^{23}Na from JEF-1.1 (-0.553 %).

The decrease of k_∞ due to ^{239}Pu from ENDF/B-VI comes primarily from the fission production cross section. However, there are two opposite effects, a strong decrease coming from the fission cross section itself, and an increase coming from nubar and from the capture cross section[5]. The increase of k_∞ due to ^{238}U from ENDF/B-VI, and the decrease due to ^{23}Na from JEF-1.1 are from the inelastic scattering data.

The fast fission and fission production cross sections of ^{239}Pu between 10 keV and 1 MeV are up to 6 % larger in JEF-1.1 than in ENDF/B-VI. The maximum differences occur at about 50 keV (1.6 versus 1.5, respectively 4.7 versus 4.4 barns). The JEF-2.2 cross section is even larger than the JEF-1.1 cross sections at energies below 50 keV.

The inelastic scattering ENDF/B-VI cross section for ^{238}U is up to 15 % larger than the JEF-1.1 cross section at energies between 200 and 400 keV (i.e. 1.24 versus 1.07 barns at about 240 keV). The JEF-2.2 cross section is slightly smaller than the JEF-1.1 cross section in this energy range.

There is a considerable discrepancy between JEF-1.1 and ENDF/B-VI inelastic scattering cross section for ^{23}Na at energies below 400 keV. The JEF-2.2 cross section is rather similar to the ENDF/B-VI cross section.

	Configuration 1		Conversion Ratio		Breeding Ratio		
	k_{∞} Inner Core	k_{eff}	Inner Core	Outer Core	Core	Blanket	Reactor Total
BENCHMARK Mean (of 16 Solutions)	1.12428	1.00509	1.09262	0.82144	0.98984	0.40227	1.39211
Std. Deviation (%)	1.8	1.3	4.2	4.4	4.2	2.4	3.5
JEF-1.1	1.12791	1.01103	1.06431	0.79834	0.96323	0.39536	1.35858
Deviation from mean in (%)	0.32	0.59	-2.59	-2.81	-2.68	-1.72	-2.41
JEF-2.2	1.13320	1.01316	1.06152	0.79563	0.96111	0.39933	1.36044
% Diff. Compared to JEF-1.1	0.46	0.21	-0.26	-0.34	-0.22	1.00	0.13
ENDF/B-VI	1.14352	1.01852	1.08005	0.80904	0.98438	0.41652	1.40091
% Diff. Compared to JEF-1.1	1.38	0.74	1.48	1.34	2.19	5.35	3.11
	Central Control Rod Worth			Na-Void Worth		Fuel Doppler Reactivities	
	$(k_{rod}-k_{ref})/k_{ref}$			$(k_{void}-k_{ref})/k_{ref}$		$(k_{2200}-k_{1100})/k_{1100}$	
	Na-In Relative to Fuel	Na-In Relative to Na	Na-Void Relative to Fuel	Na-Void Inner Core	Na-Void Outer Axial Blanket	Na-In Conf.1	Na-Void Conf.3
BENCHMARK Mean (of 16 Solutions)	-0.00355	-0.00298	-0.00460	0.02116	0.02098	-0.00729	-0.00433
Std. Deviation (%)	13.2	14.4	10.2	12.1	16.8	10.8	14.3
JEF-1.1	-0.00336	-0.00282	-0.00445	0.02471	0.02592	-0.00723	-0.00401
Deviation from mean in (%)	-5.35	-5.37	-3.26	16.77	23.54	-0.82	-7.39
JEF-2.2	-0.00354	-0.00298	-0.00456	0.02230	0.02320	-0.00751	-0.00452
% Diff. Compared to JEF-1.1	5.35	5.67	2.47	-9.75	-10.49	3.87	12.77
ENDF/B-VI	-0.00362	-0.00304	-0.00461	0.02336	0.02463	-0.00734	-0.00435
% Diff. Compared to JEF-1.1	7.73	7.80	3.59	-5.46	-4.97	1.52	8.48

Table 1: Results for the LMFBR Benchmark Obtained Using JEF-1.1, JEF-2.2, and ENDF/B-VI (Rev. 1) Cross Sections

	JEF-1.1	JEF-2.2	ENDF/B-VI	Std. Dev. (%)	JEF-1.1 Dev. Mean Value (%)	JEF-2.2 % Incr. Compared to JEF-1.1	ENDF/B-VI % Incr. Compared to JEF-1.1
β_{eff}	0.003823	0.004113	0.003924	2.62	-1.16	7.59	2.65
Inh. Reac.	1.1398	1.2193	1.0823	1.62	-1.02	6.97	-5.04
^{238}U D. N. Y.	0.0460	0.0481	0.0440	/	/	/	/
^{239}Pu D. N. Y.	0.0061	0.0065	0.00645	/	/	/	/
^{23}Na R. W.	-7.7156	-7.2150	-7.5303	9.75	11.69	-6.49	-2.40

Table 2: Effective Delayed Neutron Fraction β_{eff}, Inhour of Reactivity ($x10^5$), and Central Sodium Reactivity Worth Expressed in $\delta k_{eff}/k_{eff}/(10^{31}$ Atoms)for Configuration 1, and Their Deviations from the Mean Benchmark Values, and Delayed Neutron Yields for ^{238}U and ^{239}Pu

Evaluation	Isotope	Eigenvalue k_∞	% Diff. Compared to (Pure) JEF-2.2
ENDF/B-VI	^{16}O	1.13320	0.000
	^{23}Na	1.13506	0.164
	Natural Iron	1.13638	0.281
	^{235}U	1.13315	-0.004
	^{238}U	1.14126	0.711
	^{239}Pu	1.12575	-0.657
	^{240}Pu	1.13575	0.225
	^{241}Pu	1.13421	0.089
	^{242}Pu	1.13332	0.011
JEF-1.1	^{23}Na (JEF-1.1)	1.12694	-0.553
	^{238}U (JEF-1.1)	1.12915	-0.357
	^{239}Pu (JEF-1.1)	1.13418	0.086

Table 3: Eigenvalues k_∞ for the Inner Core (Configuration 1), Calculated Using JEF-2.2 Data, and Their Percent Increase Due to the Use of ENDF/B-VI and JEF-1.1 Data for Individual Nuclides

3 Conclusions and Recommendations

The present analyses dealt with neutronics calculations of a large sodium-cooled fast breeder reactor performed using various nuclear data.

From this study the following conclusions can be reached, and some recommendations can be made.

- Good agreement, generally within one standard deviation, was achieved between the new results and the average values over the sixteen benchmark solutions obtained in the past. However, comparing JEF-2.2 with JEF-1.1 predictions, the isothermal core fuel Doppler reactivity is significantly, up to 12.8 % higher, and the region sodium void reactivity worth is up to 10.5 % smaller.

  The eigenvalues predicted with ENDF/B-VI are about 0.5 % larger than those calculated with JEF-2.2 cross sections.

  There are additionally large discrepancies up to 10 % in the delayed neutron fractions and sodium reactivity worths predictions.

- The k_∞ deviations are mostly coming from the different fission production cross sections of ^{239}Pu, from the different inelastic scattering cross section of ^{238}U and ^{23}Na between 10 keV and 1 MeV, and from the different delayed neutron yields of ^{238}U and ^{239}Pu. Particularly, it is found that ^{238}U and ^{239}Pu from JEF-2.2 and JEF-1.1 behave neutronically in a similar way, whereas ^{23}Na from JEF-2.2 behaves rather like ^{23}Na from ENDF/B-VI.

- Therefore, we recommend to further analyze this data in order to improve the accuracy of fast breeder calculations.

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