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FENDL3 cross-section testing: sensitivity of the neutron flux deep in the shield of an ITER-like tokamak

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Ljubljana, February 2010

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Testiranje FENDL3 presekov: občutljivost nevtronskega fluksa globoko v ščitu tokamaka tipa ITER

KLJUČNE BESEDE:

jedrski podatki, FENDL, ENDF/B, JENDL-HE, MCNP, NJOY, tokamak

POVZETEK:

Pri nevtronskih transportnih izračunih skozi plasti sten tokamaka tipa ITER, je možno opaziti velika razhajanja med knjižnico FENDL3 in starejšo verzijo FENDL2.1, ki so v glavnem posledica različnih diferencialnih presekov za Mo in Fe. Začasna rešitev z uporabo popravka za NJOY je opisana v tem poročilu.

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FENDL3 cross-section testing: sensitivity of the neutron flux deep in the shield of an ITER-like tokamak

KEYWORDS:

nuclear data, FENDL, ENDF/B, JENDL-HE, MCNP, NJOY, tokamak

ABSTRACT:

When calculating neutron transport through the layers of an ITER-like tokamak walls, large discrepancies between the Fusion Evaluated Nuclear Data Library FENDL3 and the older version, FENDL2.1, were found, mainly due to differences in double differential Mo and Fe cross-sections. The temporary solution using an NJOY patch is presented.

Definition of Symbols, Terms and Abbreviations

ϕ_i	MCNP F4 tally neutron flux in the inner side supeconducting magnets
ϕ_o	MCNP F4 tally neutron flux in the outer side supeconducting magnets
ϕ_0	MCNP F4 tally neutron flux for FENDL2.1 library
ϕ_{th}	MCNP F4 tally neutron flux for energies below 100 keV
ϕ_f	MCNP F4 tally neutron flux for energies above 100 keV
$\Delta\phi$	$\phi - \phi_0$
$rd(\phi)$	Relative deviation of ϕ ($\Delta\phi/\phi_0$)
ENDF	Evaluated Nuclear Data File
FENDL	Fusion Evaluated Nuclear Data Library
JENDL	Japanese Evaluated Nuclear Data Library
MCNP	Monte Carlo N-Particle code
XS	Cross-section

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1 Introduction

At the first Research Co-ordination Meeting of the Nuclear Data Libraries for Advance Systems - Fusion Devices (Fusion Evaluated Nuclear Data Library - FENDL3 [1]), which was held at the IAEA Headquarters in Vienna from 2 to 5 December 2008, the task was assigned to process the starter FENDL-3 library to produce a library in ACE format for Monte Carlo codes and a library in MATXS format for deterministic codes. In testing the library M. Sawan [2] noticed an unusually large discrepancy in the flux in a simulated deep penetration problem, representative of the ITER shielding. Nuclide ^{96}Mo was identified as one of the major contributors to the discrepancy, followed by other Mo isotopes, which were all taken from the JENDL-HE library [3], truncated to 150 MeV.

Superconducting magnets used in tokamaks need to be cooled down to the temperature of liquid helium. The magnets are heated by conduction and, as relevant for this study, by irradiation (mostly by neutrons). Since the helium cooling consumes a large amount of energy, we wish to minimize the neutron flux reaching the magnets. However, calculations of the neutron flux when using different libraries (particularly FENDL2.1 [4] and FENDL3) may deviate at the position of the magnets [2]. Before reaching the magnets the neutrons, originating in the plasma, are transported through numerous layers of different materials, and obviously, differences in cross-sections of some of these materials affect the neutron transport thorough these layers. The exact source of this discrepancy is to be detected and suppressed.

2 Computational model

Our study is based on MCNP5 [5] model of a simplified ITER-like tokamak, made by Sawan and Bohm [2]. The model consists of concentric regions of different material composition (for details see Fig. 2.3). Since the emphasis of the study is on fusion nuclear data testing and not reactor parameter calculation, the model is based on cylindrical rather than toroidal geometry, for simplicity (see Figs. 2.1 and 2.2). The upper and lower boundary conditions are reflective, whereas the inner and outer boundary are surfaces of no return for neutrons. Thus, the whole model is effectively an infinite cylinder minus an infinite cylinder with a smaller radius in the middle.

3 Results

We analyzed the influence of cross-sections of different libraries on the neutron flux at the position of the superconducting magnets. In real tokamak the magnets are continuously winded around the small radius of the torus, of course. However, in Sawan's model, the magnets consist of two parts since the inner and outer vacuum vessel walls are separated. Roughly speaking (in orders-of-magnitude-precision), the

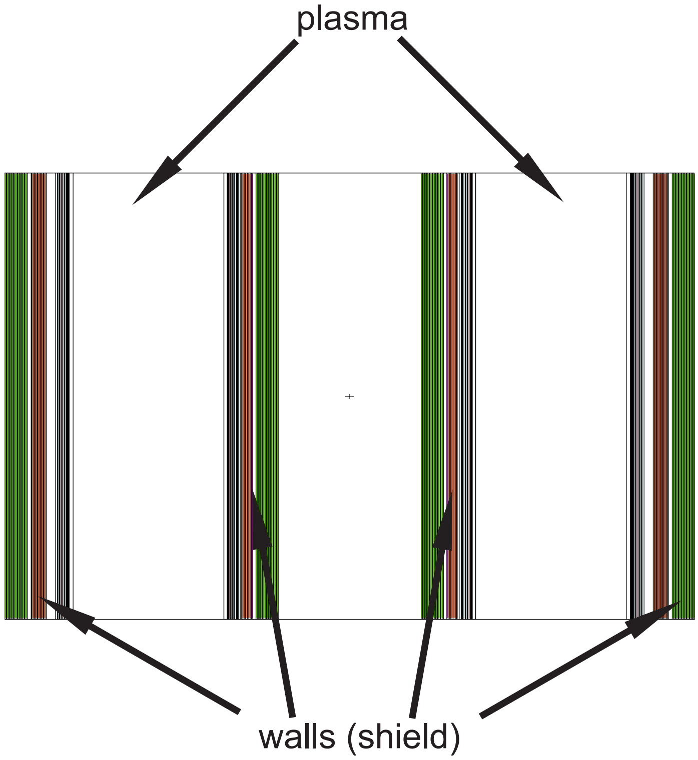

Figure 2.1: Axial cross section of the ITER-like tokamak model [2].

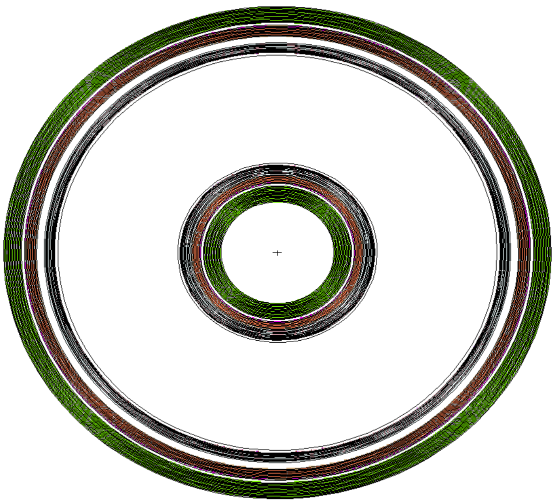

Figure 2.2: Radial cross section of the ITER-like tokamak model [2].

flux at the inner magnets (ϕ_i) could be thought as the maximum flux in the real tokamak superconducting magnets, whereas the flux at the outer magnets (ϕ_o) would represent the minimum. Since we are only interested in comparing cross-sections, we do not need any absolute values of neutron flux, fluence, or heating power. Thus, the flux is not normalized and is left in relative units, as given by the MCNP output.

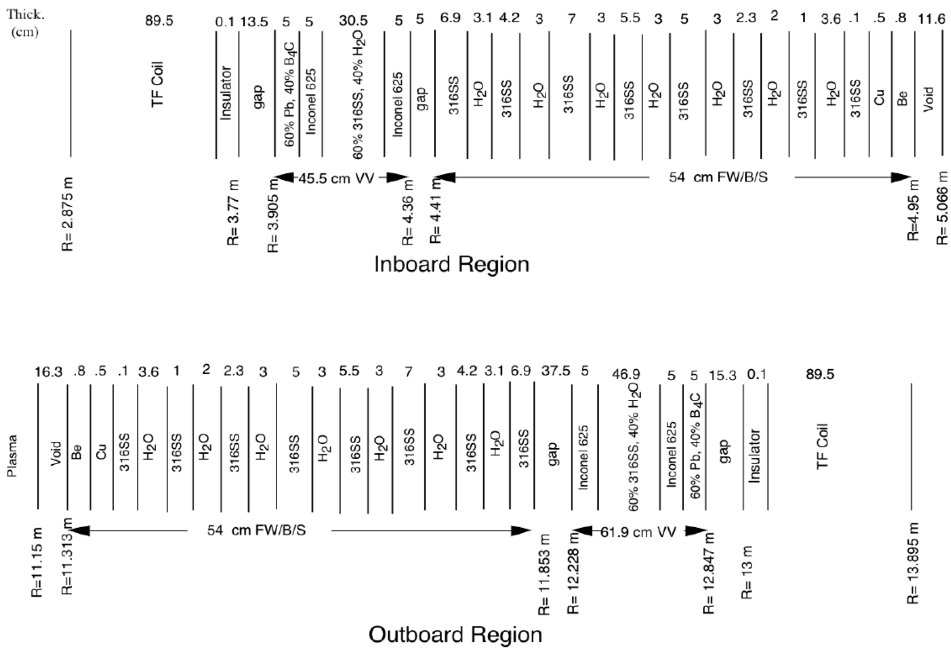

Figure 2.3: Radial profile of the ITER-like tokamak model [2].

In Tables 3.1 and 3.2 calculated neutron fluxes at the inner and outer magnets obtained using different cross-section libraries are given. First, FENDL2.1 (as a reference), ENDF/B-VII.0 [6], and the starter FENDL3 library were used. Confirming Sawan's [2] findings, we observe a large discrepancy between FENDL2.1 and original FENDL3 results, especially for energies below 100 keV (Table 3.2). On the other hand, very good agreement (within a few %) was observed between FENDL2.1 and ENDF/B-VII.0 results. A more detailed analysis (by substituting single element/isotope cross-sections only) has shown that the major contribution to the discrepancies between FENDL3 and ENDF/B-VII.0 is due to Mo (mostly isotopes ^{92}Mo and ^{96}Mo) and Fe (^{56}Fe). Although we are interested in FENDL2.1-FENDL3 comparison, cross-sections of particular elements or isotopes from FENDL3 library were substituted by ENDF/B-VII.0 cross-sections since FENDL2.1 treats some materials (e.g. Mo) as natural mixtures only. The FENDL3-ENDF/B-VII.0 substitution is justified by small FENDL2.1-ENDF/B-VII.0 discrepancies.

With corrections in FENDL3 cross-section library processing (as described in section 4) the discrepancies were significantly reduced (last rows of Tables 3.1 and 3.2).

Table 3.1: Neutron flux (in relative MCNP units) at the inner (ϕ_i) and outer (ϕ_o) magnets in a simplified model of an ITER-like tokamak. $rd()$ is relative deviation with respect to FENDL2.1.

cross-sections	ϕ_i	ϕ_o	$rd(\phi_i)[\%]$	$rd(\phi_o)[\%]$
FENDL2.1	$1.00 \cdot 10^{17}(1 \pm 0.02)$	$1.47 \cdot 10^{16}(1 \pm 0.02)$	0	0
ENDF/B-VII.0	$1.05 \cdot 10^{17}(1 \pm 0.02)$	$1.47 \cdot 10^{16}(1 \pm 0.02)$	5 ± 3	0 ± 3
FENDL3	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.17 \cdot 10^{16}(1 \pm 0.02)$	15 ± 3	48 ± 3
Mo*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$1.65 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 - 36 \pm 3$
^{92}Mo*	$1.13 \cdot 10^{17}(1 \pm 0.02)$	$1.99 \cdot 10^{16}(1 \pm 0.02)$	$15 - 2 \pm 3$	$48 - 13 \pm 3$
^{94}Mo*	$1.13 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 2 \pm 3$	$48 + 1 \pm 3$
^{95}Mo*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.12 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 4 \pm 3$
^{96}Mo*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$1.88 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 20 \pm 3$
^{97}Mo*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 - 0 \pm 3$
^{98}Mo*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$2.17 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 - 1 \pm 3$
^{100}Mo*	$1.17 \cdot 10^{17}(1 \pm 0.02)$	$2.17 \cdot 10^{16}(1 \pm 0.02)$	$15 + 2 \pm 3$	$48 - 1 \pm 3$
Fe*	$1.10 \cdot 10^{17}(1 \pm 0.02)$	$2.05 \cdot 10^{16}(1 \pm 0.02)$	$15 - 5 \pm 3$	$48 - 8 \pm 3$
^{54}Fe*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.17 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 1 \pm 3$
^{56}Fe*	$1.09 \cdot 10^{17}(1 \pm 0.02)$	$2.06 \cdot 10^{16}(1 \pm 0.02)$	$15 - 6 \pm 3$	$48 - 8 \pm 3$
^{57}Fe*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
^{58}Fe*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
H*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 + 1 \pm 3$
O*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$2.17 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 - 0 \pm 3$
OH*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 + 1 \pm 3$
$H_2O^\star$	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.10 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 5 \pm 3$
OHFe*	$1.09 \cdot 10^{17}(1 \pm 0.02)$	$2.08 \cdot 10^{16}(1 \pm 0.02)$	$15 - 6 \pm 3$	$48 - 7 \pm 3$
OHFeMo*	$1.12 \cdot 10^{17}(1 \pm 0.02)$	$1.60 \cdot 10^{16}(1 \pm 0.02)$	$15 - 3 \pm 3$	$48 - 40 \pm 3$
H_2OFeMo*	$1.09 \cdot 10^{17}(1 \pm 0.02)$	$1.60 \cdot 10^{16}(1 \pm 0.02)$	$15 - 6 \pm 3$	$48 - 40 \pm 3$
Cr*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.20 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 + 1 \pm 3$
Ni*	$1.14 \cdot 10^{17}(1 \pm 0.02)$	$2.23 \cdot 10^{16}(1 \pm 0.02)$	$15 - 1 \pm 3$	$48 + 4 \pm 3$
B*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
Be*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
Pb*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
Cu*	$1.15 \cdot 10^{17}(1 \pm 0.02)$	$2.18 \cdot 10^{16}(1 \pm 0.02)$	$15 - 0 \pm 3$	$48 - 0 \pm 3$
C*	$1.13 \cdot 10^{17}(1 \pm 0.02)$	$2.20 \cdot 10^{16}(1 \pm 0.02)$	$15 - 2 \pm 3$	$48 + 1 \pm 3$
FENDL3†	$1.11 \cdot 10^{17}(1 \pm 0.02)$	$1.63 \cdot 10^{16}(1 \pm 0.02)$	**11 ± 3**	**11 ± 3**

* cross-section for labelled isotope/element(s) from ENDF/B-VII.0, other materials from FENDL3
† corrected version

Table 3.2: 'Thermal' (below 100 keV) and fast neutron flux (in relative MCNP units) at the inner and outer magnets in a simplified model of an ITER-like tokamak. Relative statistical standard uncertainty is 2% unless stated otherwise. $rd()$ is relative deviation with respect to FENDL2.1.

XS	$\phi_{th,i}[10^{16}]$	$\phi_{f,i}[10^{16}]$	$\phi_{th,o}[10^{15}]$	$\phi_{f,o}[10^{15}]$	$rd(\phi_{th,i})$	$rd(\phi_{f,i})$	$rd(\phi_{th,i})$	$rd(\phi_{f,i})$
FENDL2.1	4.21	5.83	6.14	8.53	0	0	0	0
FENDL3	5.02	6.51	11.2$^{\diamond}$	9.54	19%	12%	82%	12%
ENDF7	4.40	6.17	6.07	8.63	5%	6%	-1%	1%
Mo*	4.82	6.62	7.32	9.21	14%	14%	19%	8%
^{92}Mo*	4.86	6.46	10.4$^{\diamond}$	9.51	15%	11%	69%	11%
^{96}Mo*	4.90	6.58	9.30$^{\diamond}$	9.56	16%	13%	51%	12%
^{56}Fe*	4.74	6.17	11.5$^{\diamond}$	9.06	13%	6%	87%	6%
H_2OFeMo*	4.58	6.31	7.09	8.90	9%	8%	15%	4%
FENDL3†	4.64	6.51	6.74	9.62	**10%**	**12%**	**10%**	**11%**

* cross-section for labelled isotope/element(s) from ENDF/B-VII.0, other materials from FENDL3

† corrected version

$^{\diamond}$ relative statistical standard uncertainty is 4%

4 Nuclear data analysis

The greatest difference in calculated neutron flux is due to differences in FENDL3 and ENDF/B-VII.0 ^{96}Mo data. The ^{96}Mo FENDL3 cross-sections are taken from the JENDL-HE (Japanese Evaluated Nuclear Data Library - High Energy File) [3] library.

Comparison of the total (Fig. 4.4) and partial reaction ^{96}Mo cross-sections indicates that the differences between FENDL3 and ENDF/B-VII.0 libraries are insignificant for incident neutron energies below 20 MeV. The main difference is that the JENDL-HE cross-sections are extended up to 150 MeV, but this should not affect the neutron transport in the walls of a fusion reactor since the neutron source (DT fusion reaction) has a relatively narrow (width $<$ 1 MeV) Doppler-broadened spectrum with peak around 14.1 MeV.

However, there are major differences in neutron emission spectra of continuum inelastic scattering reaction (compare Figs. 4.5 and 4.6), (n,2n), (n,3n), etc., plotted with the ACER module of NJOY [7]. The FENDL3 emission spectra are rather strange and unphysical. The discrepancies might originate from error in the plotting, processing of the ACE library, or the interpolation of the data in MCNP. These emission spectra discrepancies seem to be the main cause of the differences in neutron transport calculations.

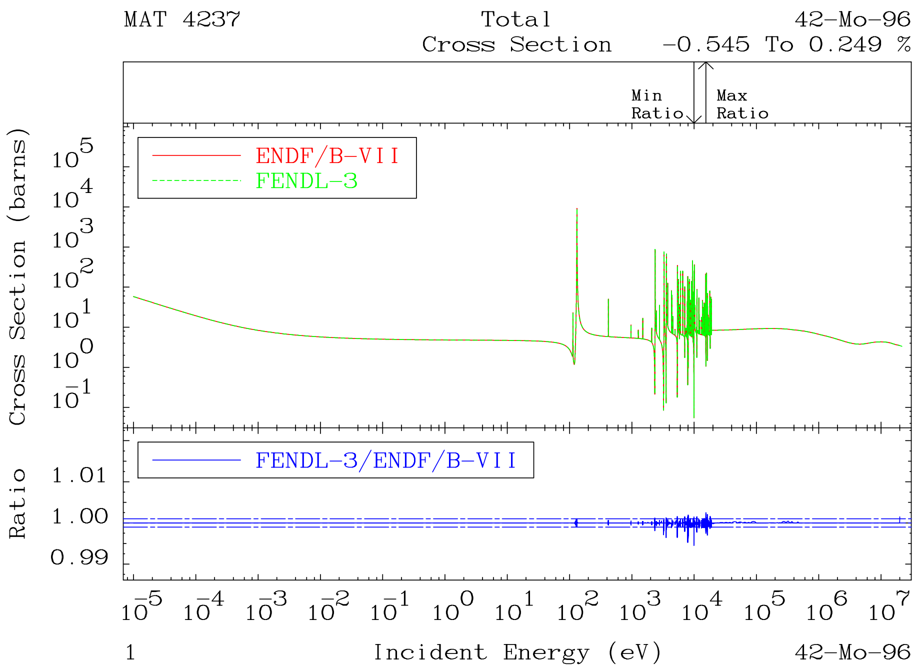

Figure 4.4: Comparison of the FENDL3 and ENDF/B-VII.0 total ^{96}Mo cross-sections.

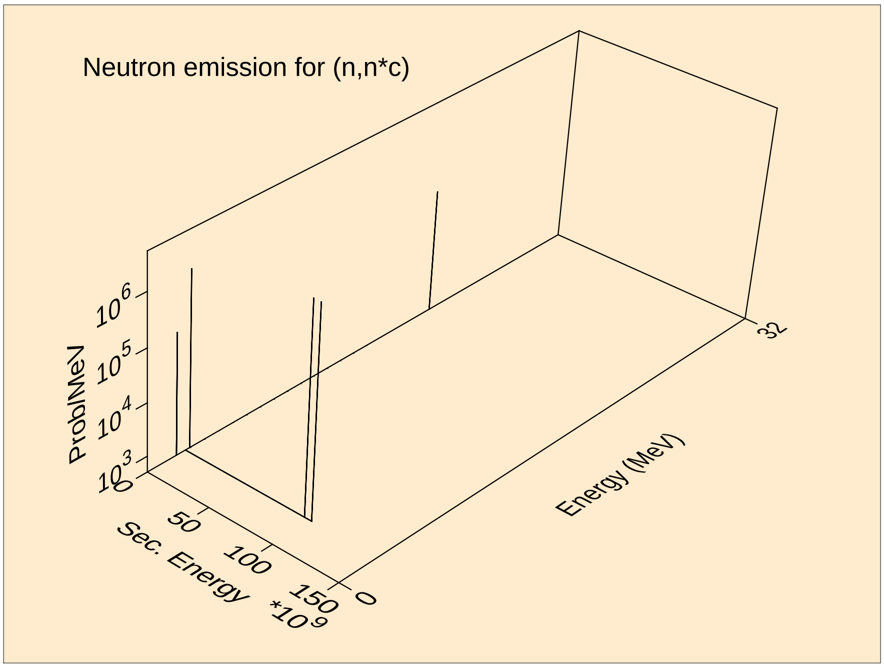

Figure 4.5: FENDL3 ^{96}Mo continuum inelastic scattering neutron emission spectrum.

4.1 Summary

The evaluated nuclear data files and the processing methods were analysed closely. The following observations were made:

- The ENDF checking codes did not identify any problems with the files originating from the JENDL-HE library.
- The differences between the cross sections of ^{96}Mo in JENDL-HE and ENDF/B-VII.0 are minimal below 20 MeV (Fig. 4.4).
- The QA procedure (developed at the IAEA, document INDC(SEC)-0107 [8]) of generating the ACE file did not reveal any problems in the ACE files.
- By carefully analysing the plots generated by the ACER module of NJOY, an anomaly was noticed in the plots of the neutron emission spectra. An example of the neutron emission spectrum of ^{96}Mo for the reaction of continuum inelastic scattering is shown in Fig. 4.5.
- By systematically checking all files originating from JENDL-HE it was found that all nuclides with double-differential data in MF-6 have the same problem, namely the nuclides of Na, Ca, Ti, V, Mn, Zr, Nb and Mo. The nuclides C, N, Mg, Ga and Ta seem to be processed correctly; they only use MF6 for MT5.
- In addition a similar problem was found in ^{19}F and ^{58}Fe from ENDF/B-VII.0.

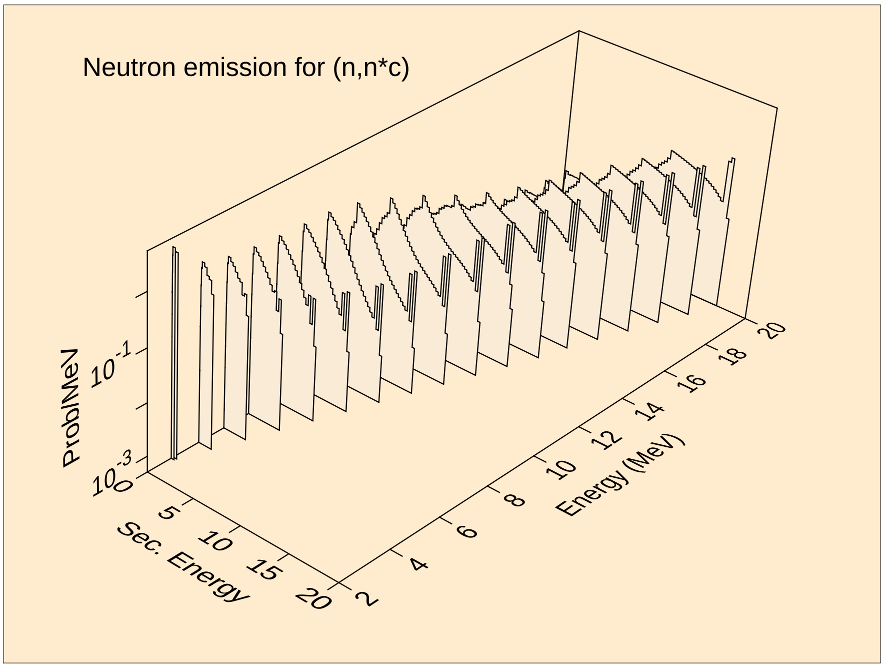

Figure 4.6: ENDF/B-VII.0 ^{96}Mo continuum inelastic scattering neutron emission spectrum.

- The symptoms suggest that it is likely an NJOY processing problem, which is very specific for the combination of data representation in the relevant files. The following manual modifications to the files were tested:
  - LEP=1 implying histogram interpolation in energy of Legendre coefficients,
  - NR=2 implying different interpolation laws from threshold to 20 MeV and above 20 MeV.

  As an example, the heading information of the (n,2n) double-differential data (MF6, MT16 in ENDF terminology) for ^{100}Mo is shown in the Appendix.
- Using LEP=2 (linear interpolation) AND forcing the same interpolation (linear, unit base) over the entire energy range removed the plotting problems.
- Restoring LEP=1 but forcing the same interpolation over the entire energy range also removes the problem.

4.2 Temporary solution

It seems there is a processing problem in NJOY [7] when more than one interpolation range between incident energies are specified. In all of the problematic cases the change of the interpolation law occurs at the 20 MeV breakpoint, where the change of representation takes place. Above this energy the particle yields are zero and the actual data are lumped into MT5. Therefore, forcing a single interpolation law over the entire energy range has no impact on the data.

Rather than modifying the data, a temporary patch to NJOY was made. While copying the data to a scratch file the multiple interpolation range information was suppressed. With this patch the plots of the double differential data seem correct, as evident from Fig. 4.8.

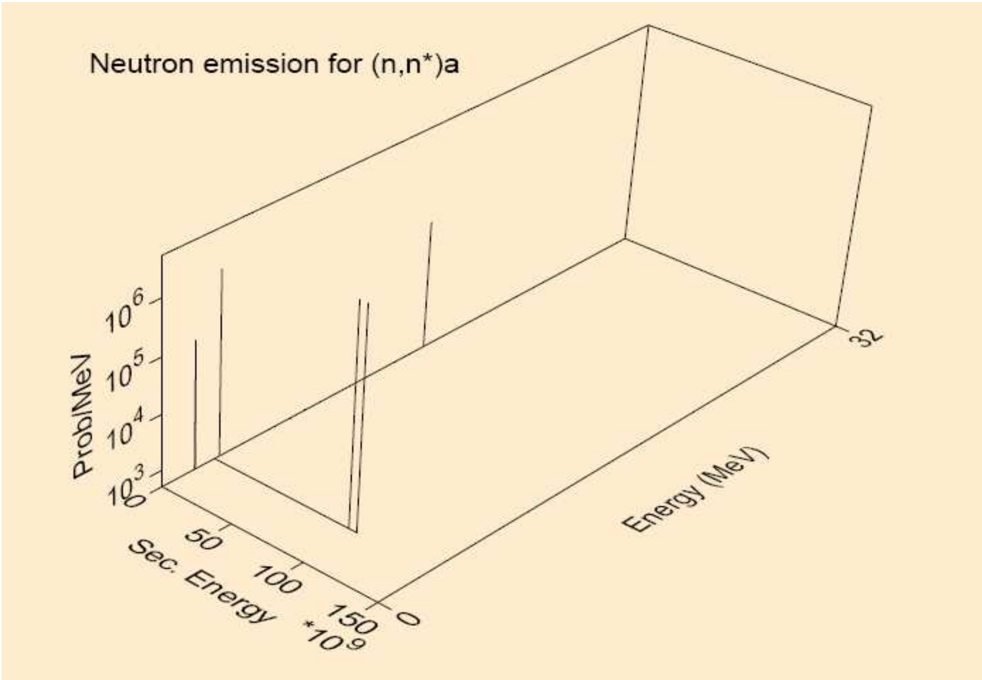

Figure 4.7: FENDL3 neutron emission spectrum from ^{100}Mo(n,na) reaction before correction.

5 Conclusion

A temporary patch to NJOY is proposed that solves processing problems for all materials (27 from JENDL-HE and two from ENDF/B-VII). The patch has no influence on the data in the ENDF files. The plots of double differential data seem to be correct after the implementation of the patch. Calculations have shown that most of the observed discrepancies disappear when the corrected files are used.

The proposed NJOY patch is not the final solution to the problem. Further testing is needed to make sure that the ACE files are generated correctly when multiple interpolation ranges are specified and that the MCNP code can interpret such data correctly.

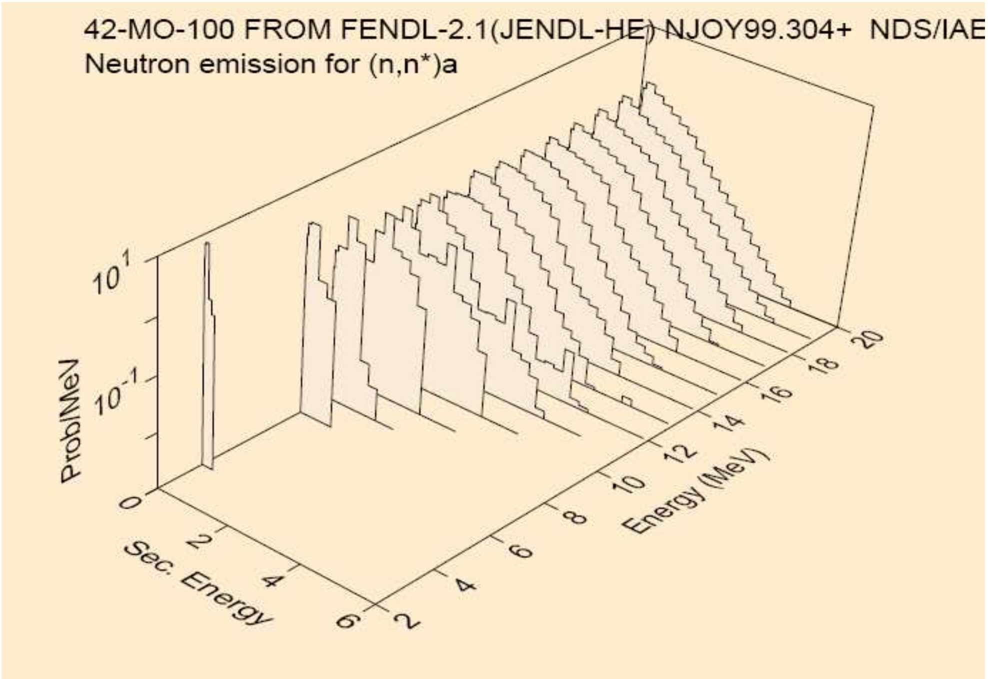

Figure 4.8: FENDL3 neutron emission spectrum from ^{100}Mo(n,na) reaction after correction.

6 References

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7 Appendix

A

Heading information of the (n,2n) double-differential data (MF6, MT16 in ENDF terminology) for ^{100}Mo is shown. Line 6 specifies that the data are tabulated at 15 energy points. Linear unit-base interpolation (flag 22) is used up to the 14-th point and plain linear interpolation is used above. The 14-th point is at 20 MeV. Above this energy the particle yield is zero, as seen from the TAB1 record at line 4 (see ENDF-6 manual for details).

```
 4.210000+4 9.904920+1          0          2          1          04249 6 16    1
 1.000000+0 1.000000+0          0          1          1          44249 6 16    2
          4          2                                            4249 6 16    3
 8.384590+6 2.000000+0 2.000000+7 2.000000+0 2.000000+7 0.000000+04249 6 16    4
 1.500000+8 0.000000+0                                            4249 6 16    5
 0.000000+0 0.000000+0          1          1          2         154249 6 16    6
         14         22         15          2                      4249 6 16    7
          .
          .
          .
```

B

```
*/
*ident upnea064
*/ acer A. Trkov, February 2010
*/    Particle emission spectra are corrupted for MF6 Law 1 LANG 1
*/    when more than one interpolation range is specified
*/    for the distributions on incident particle energies.
*/    The fix is done when writing the data to a temporary file.
*/    The multiple ranges are suppressed.  The first interpolation
*/    law is prescribed over the entire incident energy range
*/    and a message is printed.
*/    WARNING:
*/    This is a temporary patch before a proper solution is found.
*/    The true error probably occurs somewhere near acer.6651
*/    or later.
*/    Implications:
*/    JENDL-HE files (proposed for FENDL-3) were not processed
*/    correctly.  The assumption in the patch has no influence
*/    on the evaluation because the interpolation law changes
*/    above 20 MeV where the yield drops to zero because the
```

```
*/     reaction is represented by MT5.
*d acer.2373,2374
           call tab2io(nin,0,0,b,nb,nw)
           nr=n1h
           ne=nint(b(6))
           if(nr.gt.1) then
             write(string,'(a,i3)')
   &           'multiple interp.  ranges for mf6, mt',mt
             call mess('topfil',string
   &           ,'first law applied everywhere')
             nr=1
             b(5)=nr
             b(7)=ne
           end if
           call tab2io(0,nout,0,b,nb,nw)
*/
```