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Updating the fusion library FENDL-3.2b to FENDL-3.2c

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July 2024

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ABSTRACT

This report describes the main differences between the fusion libraries FENDL-3.2b and FENDL-3.2c. The changes are related to corrections of a few evaluated nuclear data files and to a set of updates applied to the NJOY2016.74 processing system. For incident neutrons, the main impact is in heating and damage calculations. Additionally, minor changes can be found in the probability tables and Bondarenko cross-sections in the unresolved resonance range as well as in the energy-angle distributions for several materials. For charged particles, the laboratory angle-energy representation (MF6/LAW7) is converted to LAW67 on the ACE-formatted file for all materials. Previously, it was converted to ACE/LAW61 except for some light elements taken from the Japanese Evaluated Nuclear Data Library (JENDL). Furthermore, the recent updates have also some impacts on energy-angle distributions, the scattering cross section at lowest energies and the treatment of redundant cross-sections for charged particles. FENDL-3.2c is available on https://www-nds.iaea.org/fendl/ and the updated NDS/NJOY2016 package can be found on https://github.com/IAEA-NDS/NJOY2016.

July 2024

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1. Introduction

The FENDL-3.2b library was released on February 15, 2022. Extensive verification and validation work has been performed since its release [1]. Additionally, other studies [2] have been conducted using evaluations that share similar features with FENDL-3.2b evaluations. FENDL-3.2b evaluations were processed using NJOY2016.60 plus a set of patches introduced by experts from the IAEA Nuclear Data Section (NDS). Since then, new patches have been introduced to the NJOY2016 [3] code by developers from the Los Alamos National Laboratory (LANL) and the NJOY2016.74 version was made available. Furthermore, NDS experts have also implemented new features and patches to NJOY2016.74 for the correct processing of FENDL evaluations.

Due to the feedback from FENDL users and collaborators who contributed to the verification and validation process of the FENDL library as well as the changes introduced into the NJOY2016 processing system, it was decided to update FENDL from version 3.2b to 3.2c

In this report, the changes in the evaluated nuclear data files are presented and the main patches introduced to NJOY2016 since the release of FENDL-3.2b are briefly described. Furthermore, the main differences in the processed evaluated files are discussed for a selected set of evaluations.

2. Evaluated nuclear data updates.

From FENDL-3.2b to FENDL-3.2c, the following evaluations were updated:

- Neutron incident data

  The evaluations for W-180, W-182, W-183, W-184 and W-186 were taken from ENDF/B-VIII.0 [4]. The data are the same in the fast energy region. Still, they have an updated and extended resolve resonance region compared to FENDL-3.2b data.

  The reference system flag LCT was corrected from LCT=3 to LCT=2 in MF6 for Mn-55, W-180, W-182, W-183, W- 184, W-186 and Th-232. It implies that the recoil distributions are now given in the center of the mass system (CM). Before, they were erroneously flagged in the laboratory system (LAB).

- Proton incident data

  The Li-7 evaluation was adopted from the latest revision of the JENDL-5 library [5]. Within this file, discrete gamma-ray energies emitted from MT=51 (p,n_1) and MT=601 (p,p_1) were corrected to 429.1 and 477.6 keV, respectively. Production data given in MF6/MT51 and MF6/MT601 were included in MF6/MT5 for correctly managing them using MCNP [6] and PHITS [7] Monte Carlo codes.

- Deuteron incident data

  The elastic scattering data in MF3/MT2 and MF6/MT2 were corrected removing some NaN (Not a Number) symbols for Ti-50, Ba-132, Gd-157, Er-170 and W-182. This was an undetected error in the FENDL-3.2b library.

3. NJOY2016 updates

The FENDL-3.2c evaluated nuclear data files have been processed using the NDS/NJOY2016.74+ system, which is based on the LANL/NJOY2016.74 code plus a set of updates included by the NDS for processing FENDL and other application libraries provided by the NDS.

The updates introduced by LANL/NJOY2016 developers since the release of FENDL-3.2b can be found in the NJOY2016 official GitHub repository (https://github.com/njoy/NJOY2016). A summary of the main updates, affecting processing of the FENDL-3.2c evaluated nuclear data files, is listed below:

- Correction of the Euler-Mascheroni constant, which has an influence on the Coulomb wave functions for the R-matrix formalism (MF2/LRF=7) in the resolved resonance region for charged particle channels;
- Correction of the assignment of ENDF/TAB1 record values for the generalized evaporation spectrum (MF5/LF=5) and the tabulated energy-angle distributions (MF6/LAW1/LANG=11-15). This affects energy-angle distributions;
- Correction of the implementation of the radiative capture energy distribution in the ACE-formatted file (MT102/ACE/LAW33);
- Correction of the reading and writing of large ENDF/TAB1 and ENDF/LIST records.

Moreover, the patches and new features introduced by the NDS can be found in the NDS GitHub repository (https://github.com/IAEA-NDS/NJOY2016/tree/nds-iaea-njoy2016-dev). A brief description of the main updates is given in Appendix I and a summary of them is presented here:

- Implementation of the kinematic method for estimating the total and partial KERMA factors as a new feature in HEATR. The patch was adapted from the original Japanese updates by Kazuaki Kosako and Chikara Konno. Despite recent improvements in the energy balance, heating numbers can be wrong in some evaluations. Therefore, replacing heating values from the energy balance method by the upper kinematic limits is still relevant.
- Correction of the recoil energy (ER) calculation for MT=102 (radiative capture) in module HEATR. Now the square of gamma yield is used for the recoil energy calculation. It impacts heating and damage values for incident neutrons at low energy (E<100 keV) [8].
- In the module HEATR now the particle energy is taken to be the available energy for the binary (n, particle) reactions, instead of the minimum value of the available energy and the Coulomb barrier energy for calculating the damage-energy cross section. This affects the damage calculation above the reaction threshold energy for several FENDL materials [9].
- Addition of a new feature (new input parameter *f0bin*) and procedure for managing small total cross section samples in module PURR. The minimum value of the total cross section is limited to $\sigma_{tot}^{min} = \min(\sigma_{pot}, \sigma_{tot}^{\infty})/f0bin$. This was important for processing some FENDL materials like La-139 [10] and Cd-106.
- Addition of a new input option for processing the laboratory angle-energy law (ENDF6/MF6/LAW7) to ACE format LAW=67. Important for incident charged particles, because the latest versions of NJOY2016 convert ENDF6/MF6/LAW7 to ACE format LAW=61 (newfor=1). MCNP-6.1 and 6.2 cannot correctly manage LAW=61 for charged particles. The patch was adapted from the Japanese patch to NJOY2016.65 for processing JENDL-5 materials [11].
- Correction of the reconstruction of elastic scattering cross section for incident charged particles when linearization is applied (RECONR) and the nuclear plus interference cross section (σ_{NI}) given in MF3 is negative for the first energies. This impacts the scattering cross section at lower energies if the nuclear plus interference representation is used (ENDF6/MF6/LAW5/LTP≥12).

- Patched the outgoing particle energy calculation in subroutine acecp. It was estimated for continuum energy-angle distribution (LAW=1) with LANG=1 (Legendre coefficients) and LANG=11-15 (tabulated data) using the Kalbach-Mann formalism assuming isotropic angular distribution. The patch uses the actual representation.
- Removal of the double counting of redundant cross sections for incident charged particles.
- Correction of the inclusion of extra points in the unified incident energy grid for charged particles.
- Correction of the smoothing option for Kalbach-Mann formalism if histogram interpolation is used at low energies for incident neutrons (MF6/LAW1/LANG=2/ZAP=1). This affects energy angle distributions at low energies for incident neutrons.
- Correction of the values of ZA and AWR in several subroutines when the particle is not a neutron.
- Addition of checking and plotting capabilities for LAW67.

4. Main differences between the FENDL-3.2b and FENDL-3.2c processed files

The differences between the processed files from FENDL-3.2b and FENDL-3.2c are caused by the changes in evaluations and processing methods.

For incident neutrons, differences in the heating and damage calculations for most of the materials are expected. Additionally, due to the change of the default value of the new input parameter *f0bin* (see above and Appendix I) from 20 to 50 in the module PURR of the NDS/NJOY2016.74 code, differences in the unresolved resonance region are also expected for some isotopes. Using this new default value, the probability tables are closer to those obtained using the LANL/NJOY2016.74 code. For most of the FENDL evaluations, the impact is small. Differences in the energy-angle distributions are also found, but they do not significantly affect neutron transport. Furthermore, probability tables in the unresolved resonance region were included for the three isotopes Cd-106, Re-185 and Re-186. In the FENDL-3.2b library this kind of data was missing. Appendix II summarizes the main differences found for 102 selected materials for incident neutrons and Appendix III presents plots for a subset of these isotopes.

Larger differences are expected in the processed files for incident charged particles due to the changes presented in Section 3. In FENDL-3.2c, all the laboratory angle-energy distributions (MF6/LAW7) are converted to ACE/LAW67. In FENDL-3.2b, ACE/LAW61 was used, but this law cannot be correctly handled by some Monte Carlo codes, such as MCNP and PHITS, amongst others. Similarly, some differences in the partial heating numbers are expected and double counting of redundant cross sections has been eliminated for several materials. Minor changes in the scattering cross section at the lowest energies are also expected for those evaluations that use the nuclear plus interference formalism with a negative nuclear interference cross section (σ_{NI}) at lowest energies.

5. Final remarks and recommendations

An updated version of the FENDL library labelled FENDL-3.2c has been assembled and made available for fusion applications. All evaluated nuclear data files for incident neutrons and charged particles were processed using the NDS/NJOY2016.74 code system.

FENDL-3.2c is available on the https://www-nds.iaea.org/fendl/ website and the updated NDS/NJOY2016 package can be found on https://github.com/IAEA-NDS/NJOY2016. In addition, the evaluated nuclear data files are available on https://github.com/IAEA-NDS/fendl-endf and the processed (application) files at https://github.com/IAEA-NDS/fendl-processed.

It is recommended to continue the verification and validation process of the transport libraries including the incident charged particle processed files analyzing an appropriate set of benchmarks for fusion.

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APPENDIX I: LANL/NJOY2016.74 main updates for processing FENDL-3.2c

A description of the main updates is given below, by module in alphabetical order:

Module **acecm**

- Modification of *subroutine mtname* for charged particles. Correction of several reaction names.
- The Fortran integer format descriptor i6 is changed to i9 in *subroutine advance_to_locator* considering the size of array xss (more than ten million elements)

Module **acefc**

- Starting from the Japanese updates or processing incident charged particle evaluations from JENDL-5, a new input option was implemented for controlling whether the endf/mf6/law7 is converted to endf/mf6/law1 or not when the new format option is invoked (newfor=1). It is important for charged particle transport simulations using MCNP-6.1 and MCNP-6.2 where law61 is not working. Updates applied to several *subroutines* like *acetop, acelf6, topfil , acelod,* and *acelcp*.
- Checking of law67 was added in the *subroutine consis.*
- Corrections to consider incident charged particles (awi≠1) in subroutines *consis* and *topfil.*
- The *subroutine unionx* was patched to correctly include extra points for large intervals in the unionized grid for charge particles. Current implementation can skip the point before the last and never densify the last interval. This is important for high energy evaluations.
- The *subroutine unionx* was also patched to consider the values supplied on the section MF3/MT2 for the elastic scattering of charged particles when the nuclear plus interference cross section is negative at lowest energies.
- Patched *subroutine acelod* to consider the case when the reaction MT5 does not produce the incident particle but produces other particles. For example, this is the case for 1-H-2 for incident protons from JENDL-5. The code logic was therefore patched.
- NJOY2016 now issues a warning when the LAB reference system is used in MF6/LAW6, as NJOY2016 does not treat MF6/LAW6 in the LAB system and enforces the CM system. Additionally, the coding for the generation of the normalized energy distribution for MF6/LAW6 was reorganized.
- The values of ZA for incident and product particles were corrected in the call of *subroutine bachaa* for charged particles.
- A correction to the smoothing option (ismooth=1) for histograms is applied when the first secondary energy is not 0.0. It is important for some FENDL evaluations adopted from TENDL-2011.
- *Subroutine acecpe* was modified to avoid singularities and to correctly consider all the mf6/mt2/law=5 representations.
- Corrected a typo and patched the subroutine acelf6 for the case when tabulated data (mf6/law1/lang2) is converted to the Kalbach formalism (mf6/law1/lang2) for newfor=0.
- Patched the outgoing particle energy calculation in subroutine acecp. It was estimated for continuum energy-angle distribution (LAW=1) with LANG=1 (Legendre coefficients) and LANG=11-15 (tabulated data) using the Kalbach-Mann formalism assuming isotropic angular distribution. The patch uses the actual representation of the data.
- Patched *subroutine acelpp* responsible for preparing the unified energy grid part of a law1 for discrete photons.
- Modified *subroutines aplodd* and *aploxp* for plotting law67. Corrected recoil heat plotting.

- Increased array sizes for large evaluations in several subroutines.
- Revised some subroutines to avoid double-counting of redundant cross sections for incident charged particles.

Module **acer**

- Modified the module to consider the new input parameter no7 for converting endf/mf6/law7 to ace/law67 when newfor=1. Useful for charged particle processing.

Module **broadr**

- Implemented minor changes to keep some legacy options to avoid problems with some FORTRAN compilers.

Module **endf**

- Rewind the ENDF-6 tape before using it in subroutine tpidio. Needed when running multiple modules in sequence.

Module **errorr**

- A checking and corrective action was introduced if a negative variance is found, which is now signaled by a warning.

Module **gaspr**

- Included direct production of two alpha particles from Li-8 residual (Li-8->Be-8->2α).
- Minor changes to process reaction with MT>200 from JENDL-5.

Module **groupr**

- Slightly reordered the code and increased the size of some arrays.
- Implemented a correction to the smoothing option (ismooth=1) for histograms when the first secondary energy is not 0.0 or 0.00001 eV. It is important for some FENDL evaluations coming from TENDL-2011

Module **heatr**

- Implemented the kinematic method for estimating the total and partial KERMA factors as a new feature in HEATR. The patch was adapted from the original Japanese updates by Kazuaki Kosako and Chikara Konno. Despite recent improvements in the energy balance, heating numbers can be wrong in some evaluations. Therefore, replacing heating values from the energy balance method by the upper kinematic limits is still relevant.
- Corrected the recoil energy (ER) calculation for MT=102 (radiative capture) in the module HEATR. Now the square of gamma yield is used for the recoil energy calculation. It impacts heating and damage values for incident neutrons at low energy (E<100 keV).
- In the module HEATR now the particle energy is taken to be the available energy for the binary (n, particle) reactions, instead of the minimum value of the available energy and the Coulomb barrier energy for calculating the damage-energy cross section. It affects the damage calculation above the reaction threshold energy for several FENDL materials.

Module **matxsr**

- Corrected a FORTRAN format descriptor that produces wrong data when ASCII matxs-formatted files are produced. The group energy boundaries can be corrupted. Important for FENDL processing.

Module **plotr**

- Increased some arrays dimension for large plots. Consistency with module viewer dimensions is required.

Module **purr**

- Added a new feature (new input parameter *f0bin*) and procedure for managing small sampled total cross section in PURR. The minimum value of the total cross section is limited to $\sigma_{tot}^{min} = \min(\sigma_{pot}, \sigma_{tot}^{\infty}) / f0bin$. This was important for processing some FENDL materials, such as La-139 and Cd-106.

Module **reconr**

- Implemented the correct treatment of the elastic scattering cross section for charged particles. For mf6/law5/ltp≥12, the mf3/mt2 section should contain the values of the "nuclear plus interference" cross section σ_{NI}, which can be negative. For ltp=1 or ltp=2, the values should be 1.0 even at the threshold energy. Otherwise, the elastic scattering cross section could be incorrectly calculated in *subroutine acecpe*.
- Removed the production of redundant cross sections for incident charged particles.

Module **util**

- Now the scratch tape is closed before opening it in *subroutine openz*, if needed.
- Minor correction in *function sigfig.*

APPENDIX II: Main differences between FENDL-3.2c and FENDL-3.2b for incident neutrons for 102 selected continuous energy ACE-formatted files

Main differences between FENDL-3.2b and FENDL-3.2c for incident neutrons
(102 selected isotopes, continuous energy ACE-formatted files)

No.	Isotope	Heating & damage	Unresolved resonance range self-shielding	energy-angle distribution smoothing option for outgoing neutrons	ACE/LAW61 energy-angle distributions for outgoing non-incident particles	MT102 ACE/LAW33
1	1-H-1	x				x
2	1-H-2	x				
3	1-H-3					
4	2-He-3	x				x
5	2-He-4					
6	3-Li-6	x		x		
7	3-Li-7	x		x		
8	4-Be-9	x		x	x	
9	5-B-10	x				
10	5-B-11	x		x		
11	6-C-12	x			x	
13	7-N-14	x			x	
14	7-N-15	x		x		
15	8-O-16	x		x		
16	9-F-19	x			x	
17	10-Ne-20	x		x		
18	11-Na-23	x			x	
19	12-Mg-24	x			x	
20	13-Al-27	x		x		
21	14-Si-28	x		x		
22	14-Si-29	x		x		
23	14-Si-30	x		x		
24	15-P-31	x		x		
25	16-S-32	x				
26	19-K-39	x	x	x		
27	20-Ca-40	x			x	
28	20-Ca-42	x			x	
29	20-Ca-43	x			x	
30	20-Ca-44	x			x	
31	20-Ca-46	x			x	
32	20-Ca-48	x			x	
33	22-Ti-46	x			x	
34	22-Ti-47	x			x	
35	22-Ti-48	x			x	
36	22-Ti-49	x			x	
37	22-Ti-50	x			x	
38	23-V-50	x		x		
39	23-V-51				x	
40	24-Cr-50	x				

No.	Isotope	Heating & damage	Unresolved resonance range self-shielding	energy-angle distribution smoothing option for outgoing neutrons	ACE/LAW61 energy-angle distributions for outgoing non-incident particles	MT102 ACE/LAW33
41	24-Cr-52	x				
42	24-Cr-53	x				
43	24-Cr-54	x				
44	25-Mn-55	x	x			
45	26-Fe-54	x				
46	26-Fe-56	x				
47	26-Fe-57	x				
48	26-Fe-58	x	x			
49	27-Co-59	x			x	
50	28-Ni-58	x		x		
51	28-Ni-60	x		x		
52	28-Ni-61	x		x		
53	28-Ni-62	x	x	x		
54	28-Ni-64	x		x		
55	29-Cu-63	x		x		
56	29-Cu-65	x		x		
57	30-Zn-64	x	x		x	
58	40-Zr-90	x	x		x	
59	40-Zr-91	x	x		x	
60	40-Zr-92	x	x		x	
61	40-Zr-94	x	x		x	
62	40-Zr-96	x	x		x	
63	41-Nb-93	x	x		x	
64	42-Mo-92	x	x		x	
65	42-Mo-94	x	x		x	
66	42-Mo-95	x	x		x	
67	42-Mo-96	x	x		x	
68	42-Mo-97	x				
69	42-Mo-98	x	x		x	
70	42-Mo-100	x	x		x	
71	47-Ag-107	x				
72	47-Ag-109	x				
73	48-Cd-106	x	x	x		
74	50-Sn-112	x	x			
75	50-Sn-114	x	x			
76	50-Sn-115	x	x			
77	50-Sn-116	x	x			x
78	50-Sn-117	x	x			x
79	50-Sn-118	x	x			x
80	50-Sn-119	x	x			
81	50-Sn-120	x	x			
82	50-Sn-122	x	x			
83	50-Sn-124	x	x			
84	51-Sb-121	x				
85	51-Sb-123	x				

No.	Isotope	Heating & damage	Unresolved resonance range self-shielding	energy-angle distribution smoothing option for outgoing neutrons	ACE/LAW61 energy-angle distributions for outgoing non-incident particles	MT102 ACE/LAW33
86	73-Ta-180m	x			x	
87	73-Ta-181	x			x	
88	74-W-180	x				
89	74-W-182	x	x			
90	74-W-183	x	x			
91	74-W-184	x	x			
92	74-W-186	x	x			
93	75-Re-185	x	x	x		
94	75-Re-187	x	x	x		
95	79-Au-197	x			x	
96	82-Pb-204	x				
97	82-Pb-206	x				
98	82-Pb-207	x		x		
99	82-Pb-208	x				
100	90-Th-232	x	x			
101	92-U-235	x			x	
102	92-U-238	x	x		x	

APPENDIX III: Comparison of FENDL-3.2 vs FENDL-3.2c for selected isotopes

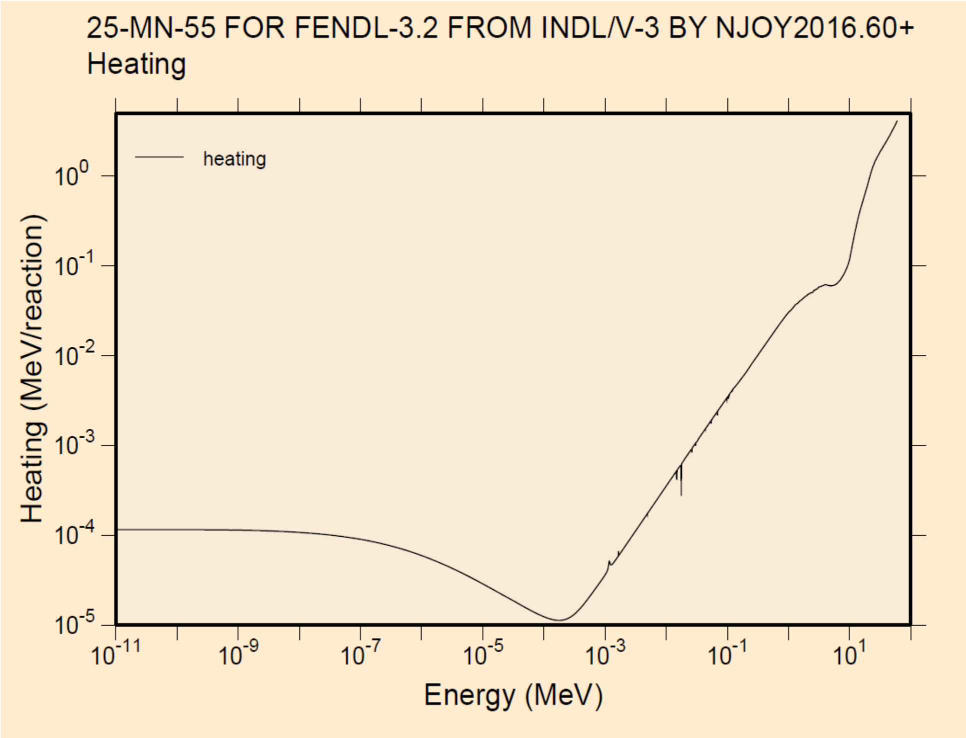

FIG. III.1. Mn-55 heating for incident neutrons from FENDL-3.2b

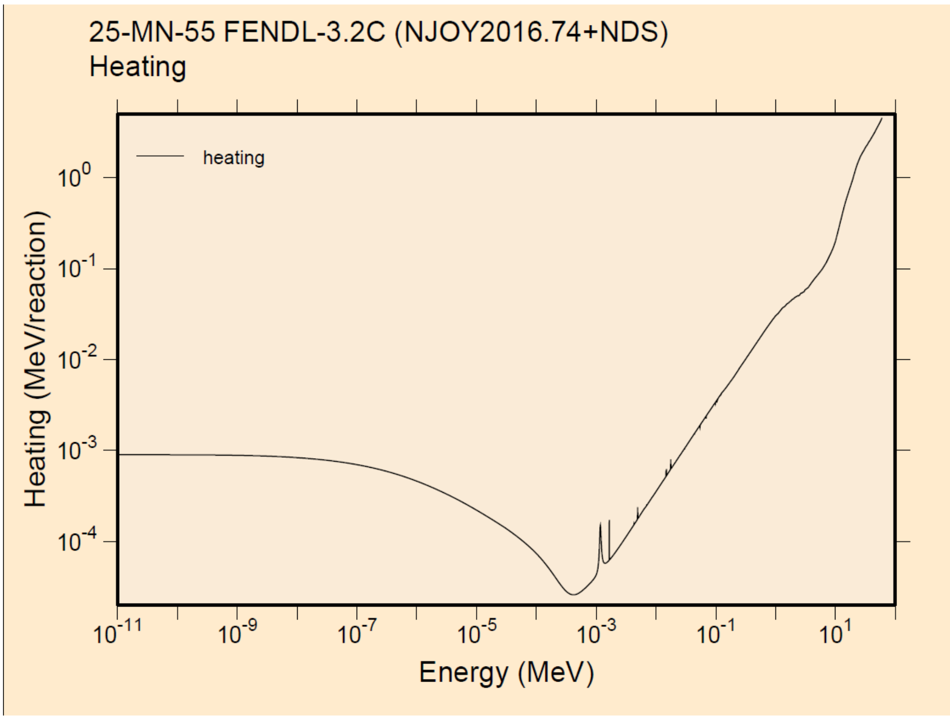

FIG. III.2. Mn-55 heating for incident neutrons from FENDL-3.2c

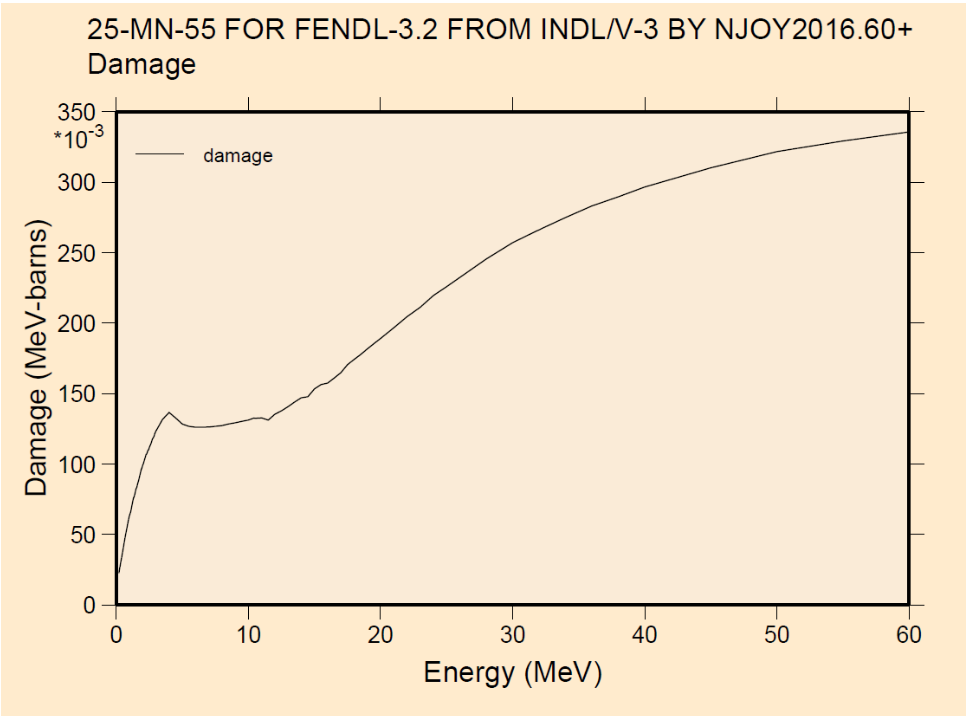

FIG. III.3. Mn-55 damage for incident neutrons from FENDL-3.2b

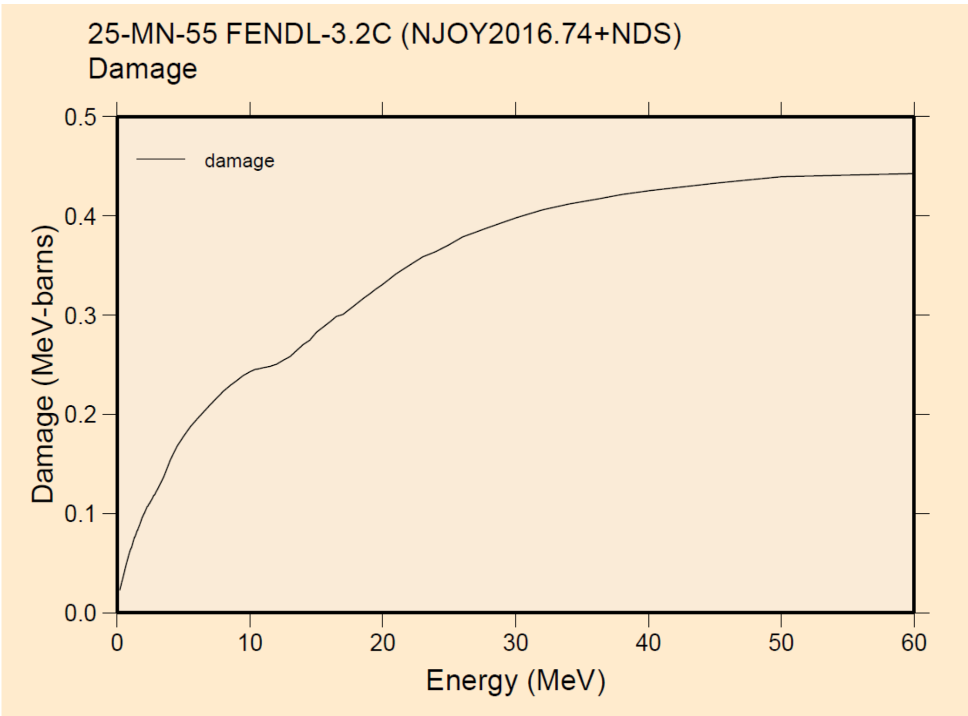

FIG. III.4. Mn-55 damage for incident neutrons from FENDL-3.2c

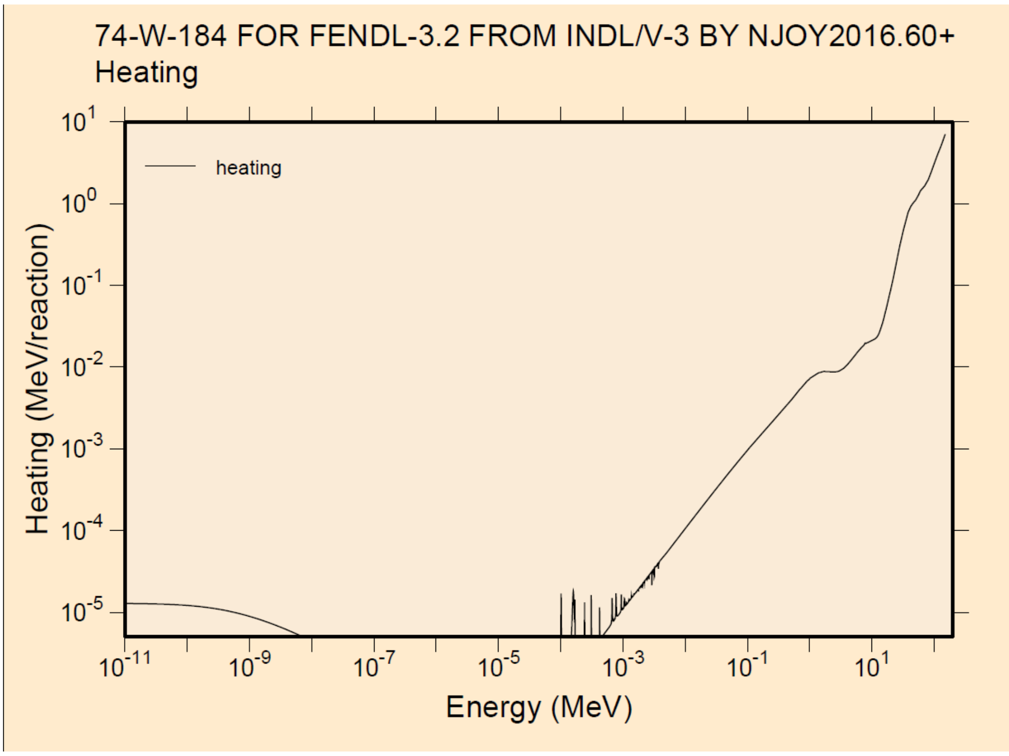

FIG. III.5. W-184 heating for incident neutrons from FENDL-3.2b

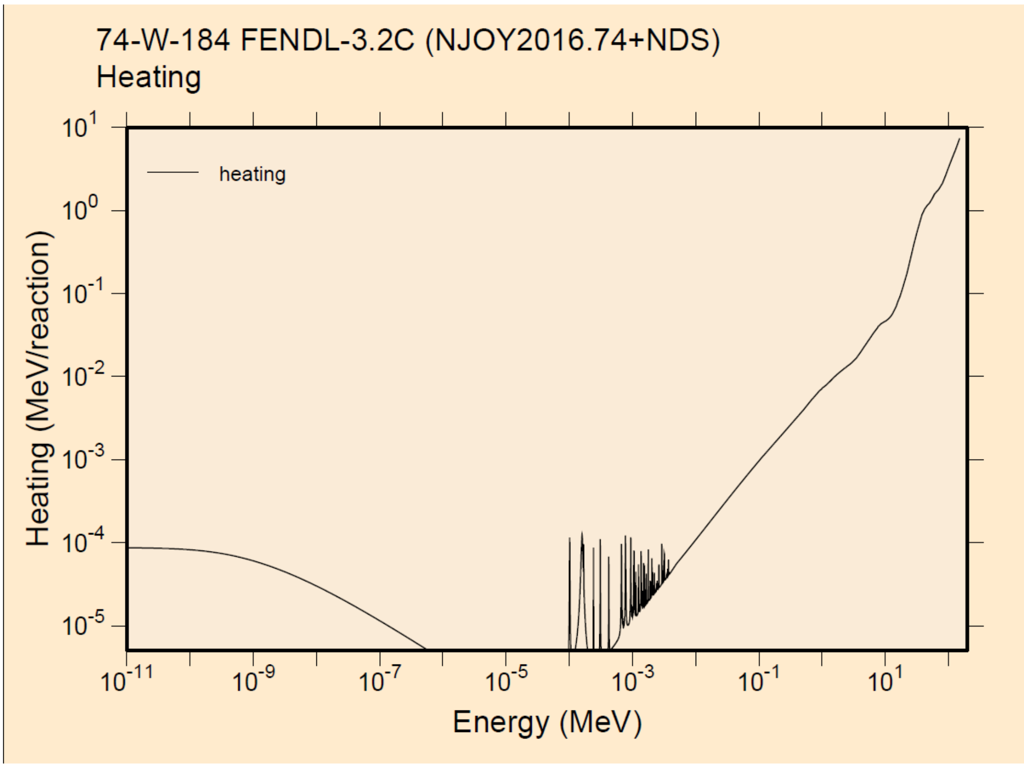

FIG. III.6. W-184 heating for incident neutrons from FENDL-3.2c

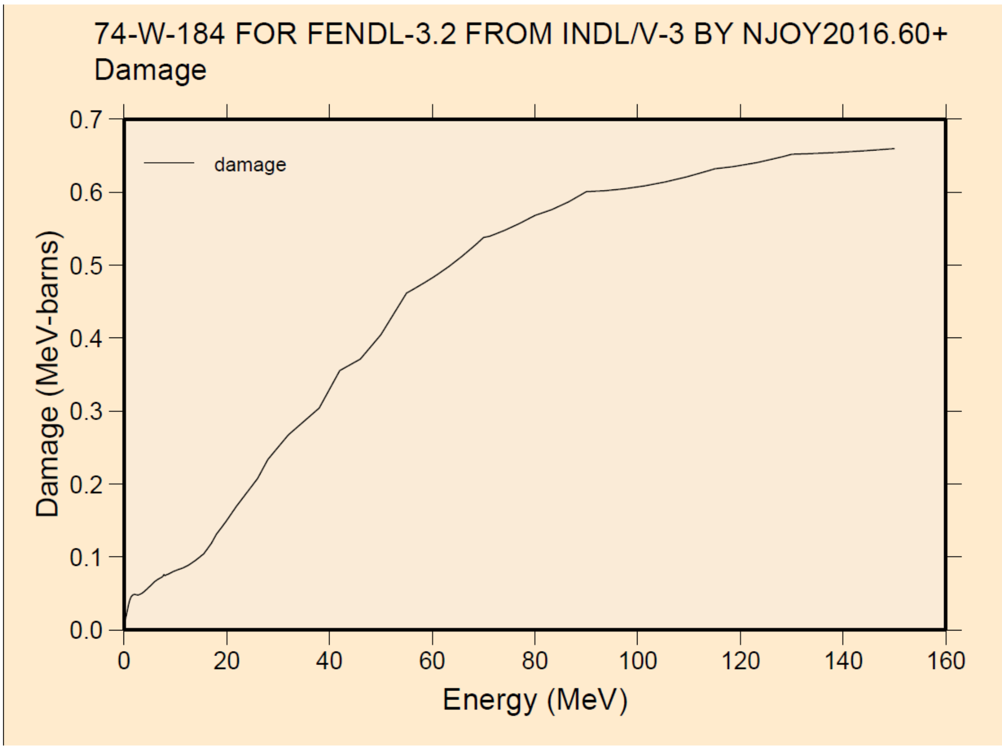

FIG. III.7. W-184 damage for incident neutrons from FENDL-3.2b

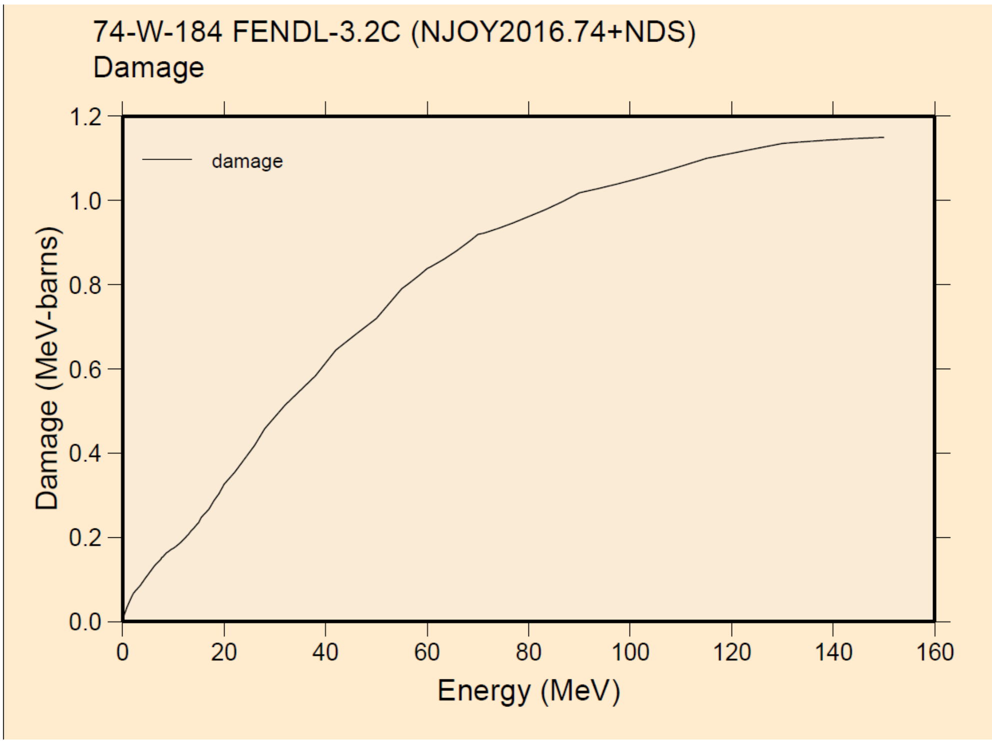

FIG. III.8. W-184 damage for incident neutrons from FENDL-3.2c

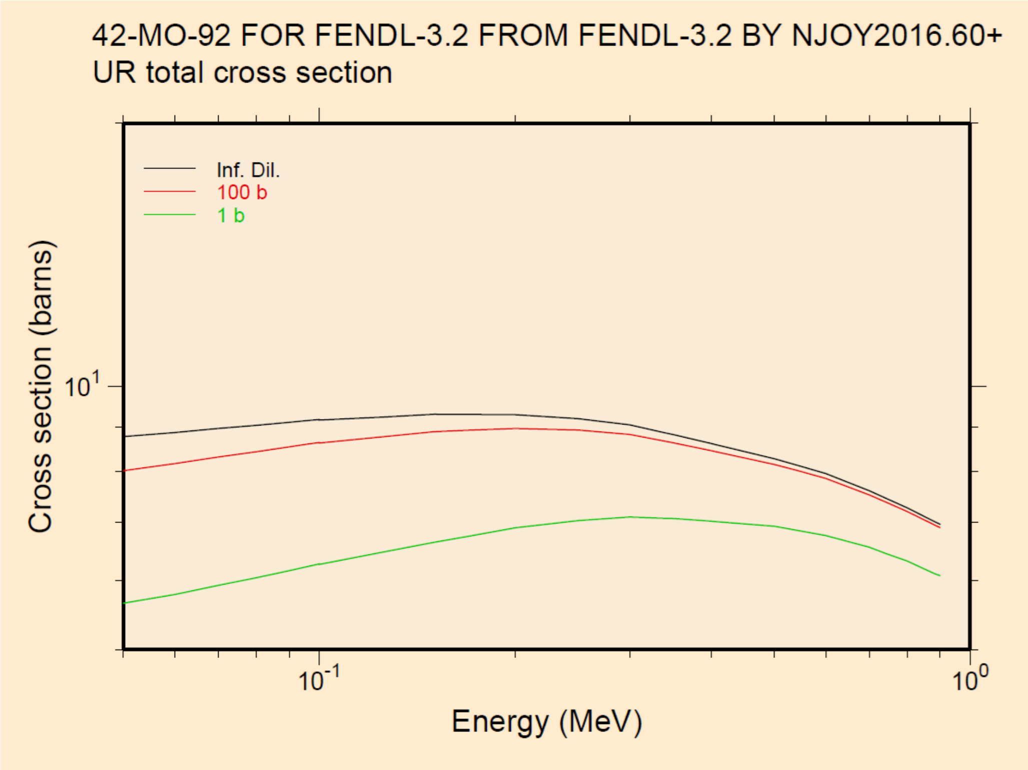

FIG. III.9. Mo-92 self-shielded total cross section in the URR from FENDL-3.2b

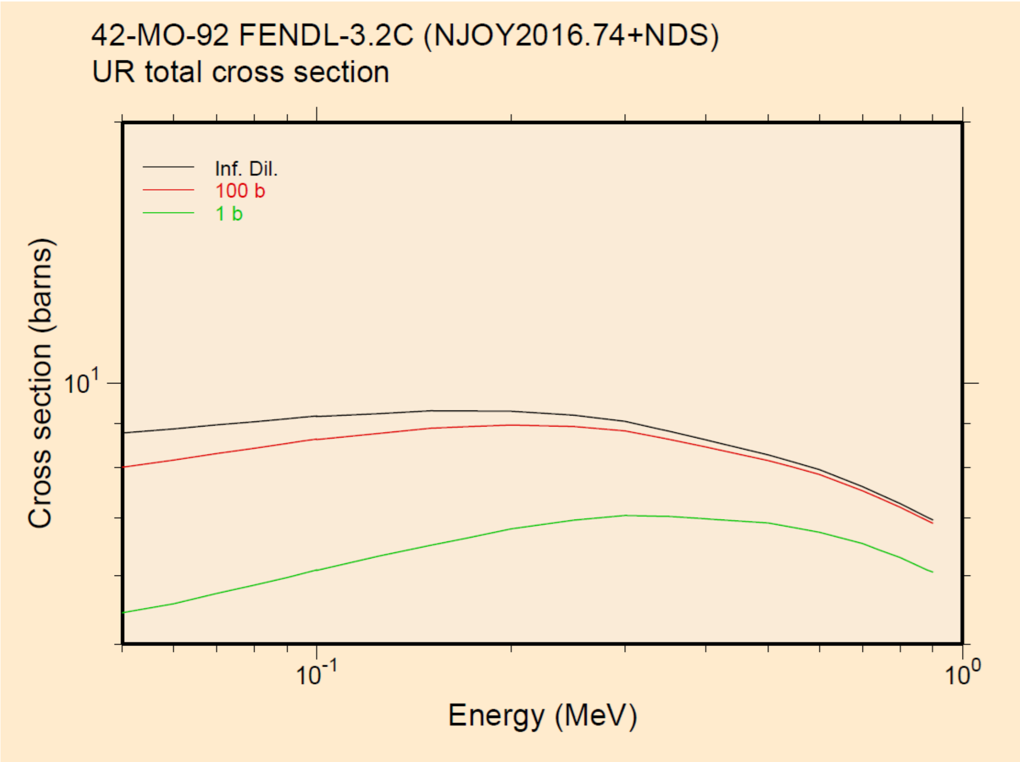

FIG. III.10. Mo-92 self-shielded total cross section in the URR from FENDL-3.2c

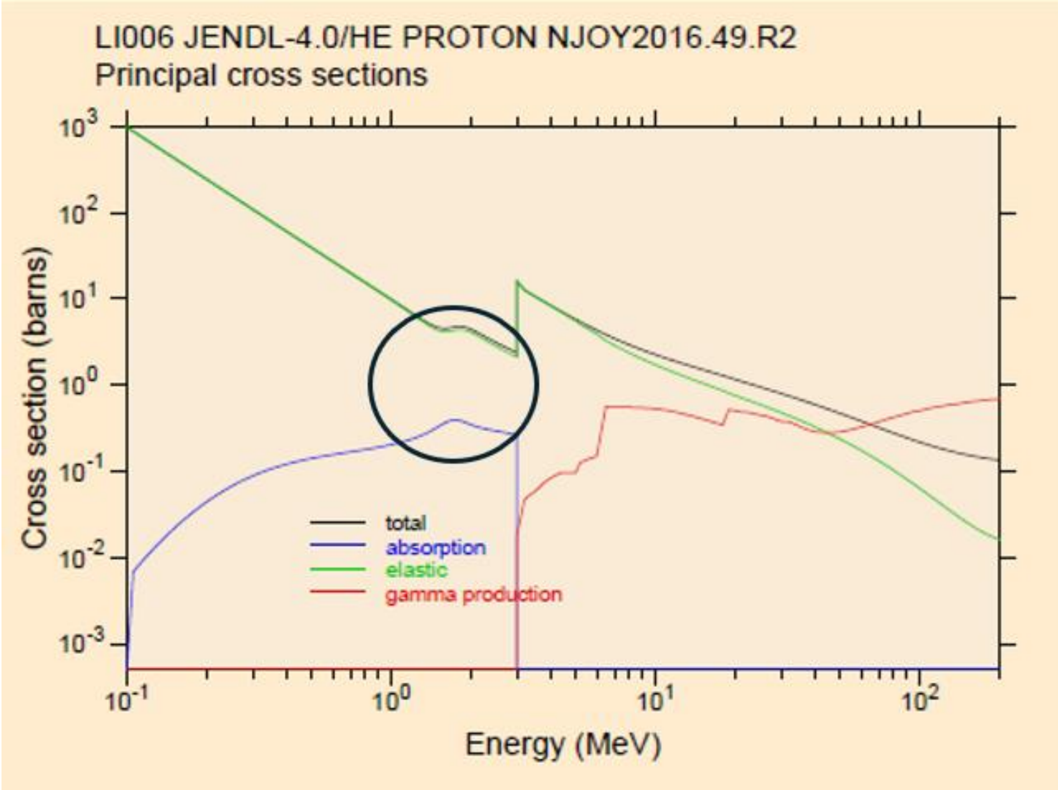

FIG. III.11. Li-6 principal cross sections for incident protons from FENDL-3.2b

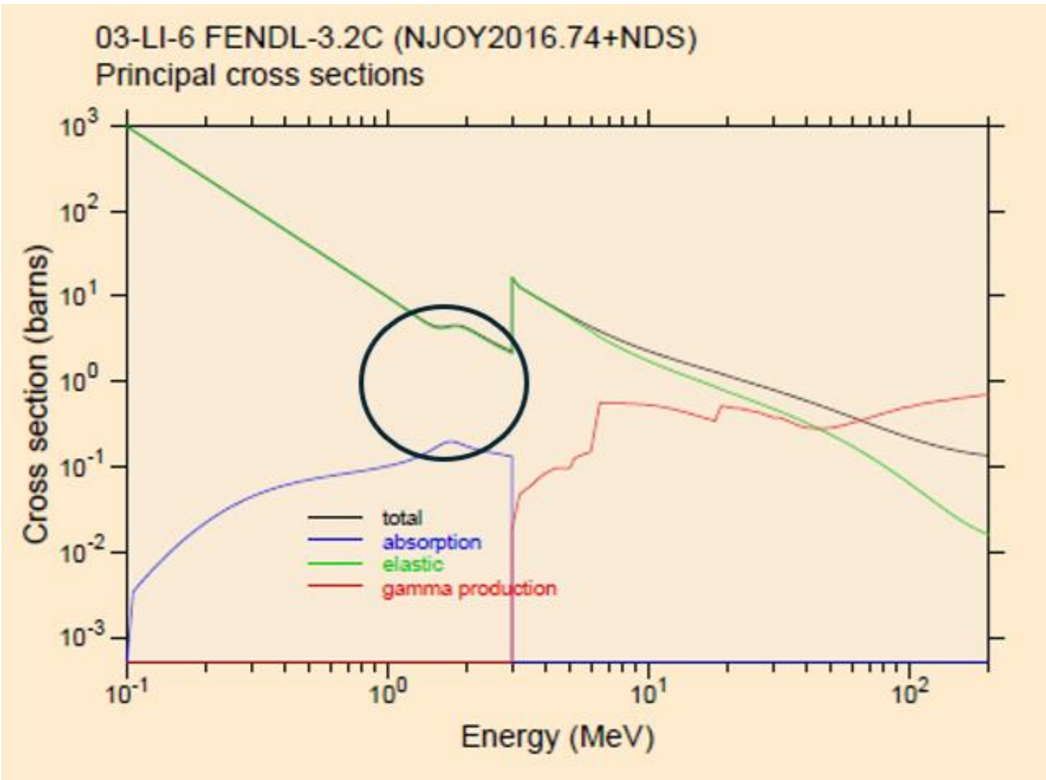

FIG. III.12. Li-6 principal cross sections for incident protons from FENDL-3.2c

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