New comments on data below 20 MeV in FENDL-3.1d

Japan Atomic Energy Agency
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Consultants' Meeting on the FENDL Library for fusion neutronics calculations
15-18 October 2018
IAEA Headquarters, Vienna, Austria

We have found out new problems on FENDL-3.1d since the last FENDL meeting in 2016.

We would like to divide my presentation to the following five presentations.

1. **Problems on KERMA and damage energy of ^{39}K and ^{40}K in FENDL-3.1d**
2. **Problem on p-table in ACE file of FENDL-3.1d**
3. **Problem on MATXS file of FENDL-3.1d due to NJOY unresolved resonance processing**
4. **IAEA patch effects for TRANSX**
5. **Comments on TENDL-2017**

Problems on KERMA and damage energy of ^{39}K and ^{40}K in FENDL-3.1d

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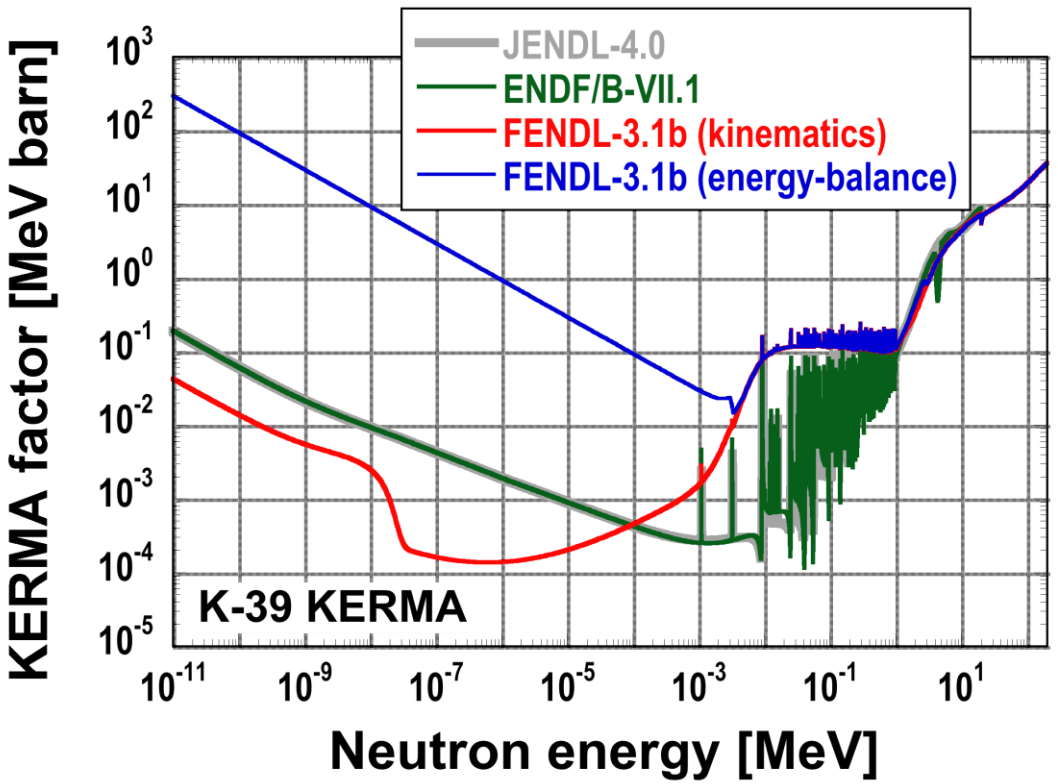
Introduction -(1)

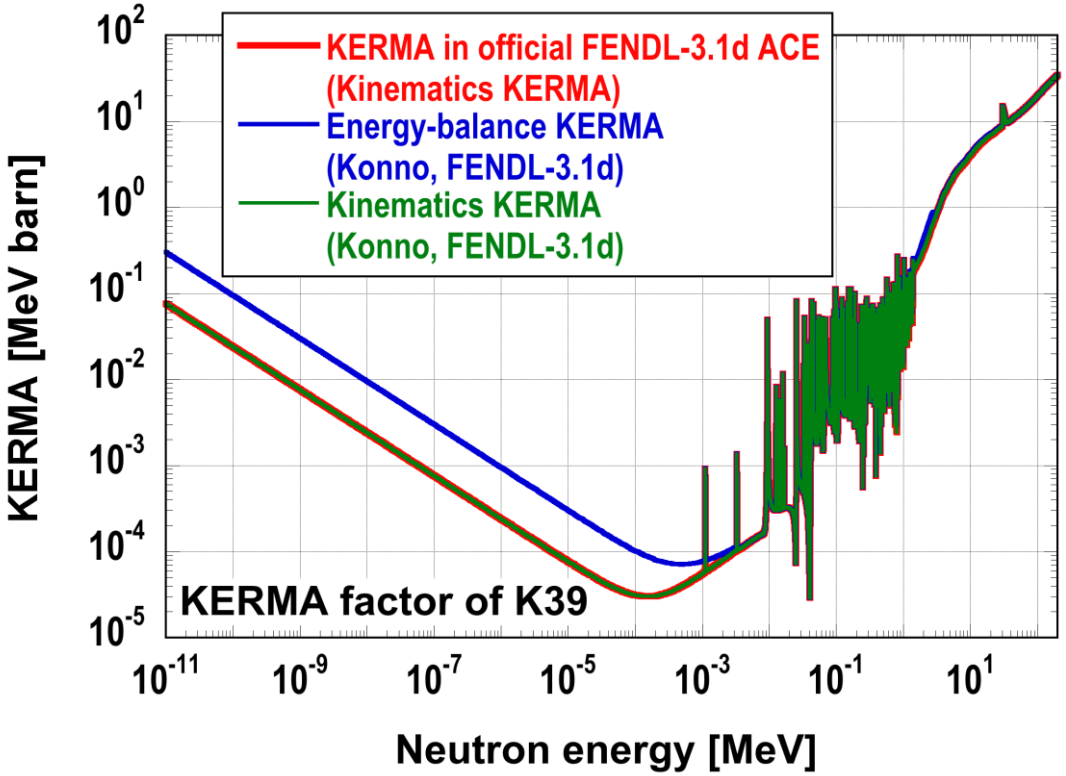
- We pointed out the following problem at Consultants' Meeting on FENDL in 2016.
  - The kinematics and energy-balance KERMA factors and damage energy of ^{39}K and ^{40}K in FENDL-3.1b (TENDL-2012) were very different in neutron energy below a few keV.
  - NJOY may not include the contribution of secondary charged particles in kinematics KERMA and damage energy, when file6 mt=600-899 data do not exist, though file6 mt=103-117 data exist.

    → *Not correct!*



Introduction -(2)

- The ^{39}K and ^{40}K data have been revised in FENDL-3.1d (TENDL-2015).
- However the problem still remains though the effect is smaller than in FENDL-3.1b.



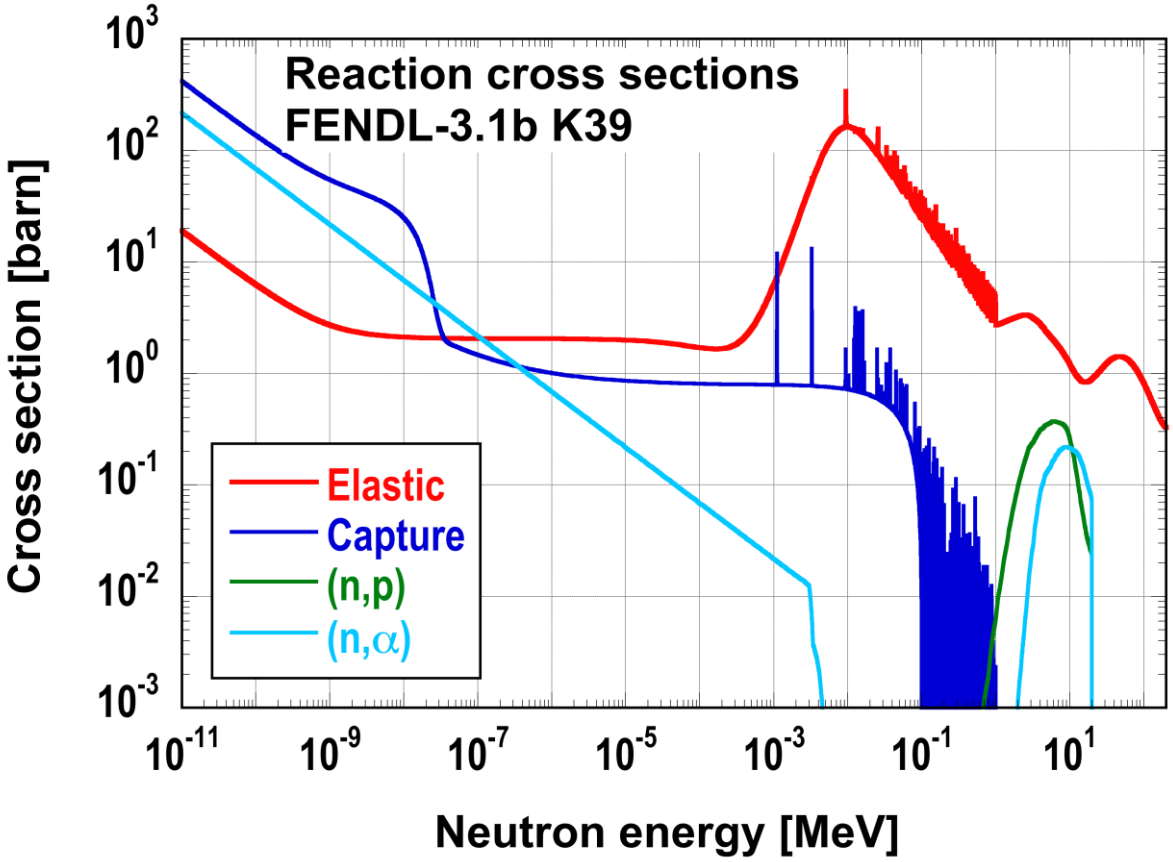
- We re-investigate this issue for ^{39}K.

Method

- At first we check ^{39}K in FENDL-3.1b.
  - Reaction cross sections
  - Energy balance
  - Kinematics and energy-balance KERMAs
  - Data of the secondary alpha particle, residual nucleus and secondary gamma of the (n,α) reaction
  - Damage energy
- Next we check ^{39}K in FENDL-3.1d.
- My calculation condition is the followings.
  - PSYCHE code for energy balance check
  - NJOY2016 code for KERMA, damage energy, etc.
  - Temporarily modified ^{39}K data in FENDL-3.1b and -3.1d

^{39}K in FENDL-3.1b (TENDL-2012)

Cross section check of ^{39}K in FENDL-3.1b



- Cross section of the (n,α) reaction is large in low energy neutrons. Thus KERMA and damage energy of the (n,α) reaction seem to be large.
- We examine the (n,α) reaction data in detail.

Energy balance check of ^{39}K in FENDL-3.1b #9

ENERGY BALANCE SUMMARY: Q = 1.36126E+06

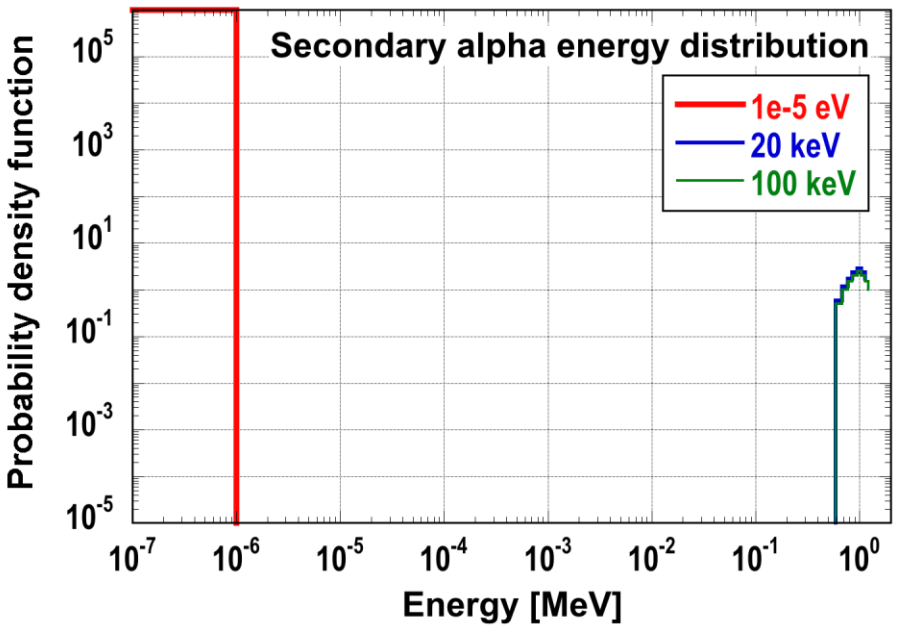
TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

E	AVAIL	%DIFF	SUM	02004	17036	00000
1.00E-05	1.36E+06	-100.00	1.00E+00	5.00E-01	5.00E-01	0.00E+00
2.00E+04	1.38E+06	-24.83	1.04E+06	9.20E+05	1.17E+05	2.58E-09
5.00E+04	1.41E+06	-23.63	1.08E+06	9.56E+05	1.21E+05	6.44E-09
1.00E+05	1.46E+06	-25.83	1.08E+06	9.56E+05	1.26E+05	1.29E-08
2.00E+05	1.56E+06	-27.94	1.12E+06	9.82E+05	1.40E+05	2.58E-08
4.00E+05	1.75E+06	-23.83	1.33E+06	1.17E+06	1.64E+05	5.15E-08
6.00E+05	1.95E+06	-30.95	1.34E+06	1.16E+06	1.88E+05	7.73E-08
8.00E+05	2.14E+06	-34.79	1.40E+06	1.18E+06	2.11E+05	1.03E-07
1.00E+06	2.34E+06	-35.51	1.51E+06	1.27E+06	2.35E+05	1.29E-07
1.40E+06	2.73E+06	-33.47	1.81E+06	1.53E+06	2.83E+05	1.80E-07
1.80E+06	3.12E+06	-29.94	2.18E+06	1.85E+06	3.29E+05	2.32E-07
2.20E+06	3.51E+06	0.00	3.51E+06	2.21E+06	3.76E+05	9.18E+05
2.60E+06	3.90E+06	0.00	3.90E+06	2.58E+06	4.22E+05	8.96E+05
3.00E+06	4.29E+06	0.00	4.29E+06	2.86E+06	4.68E+05	9.59E+05

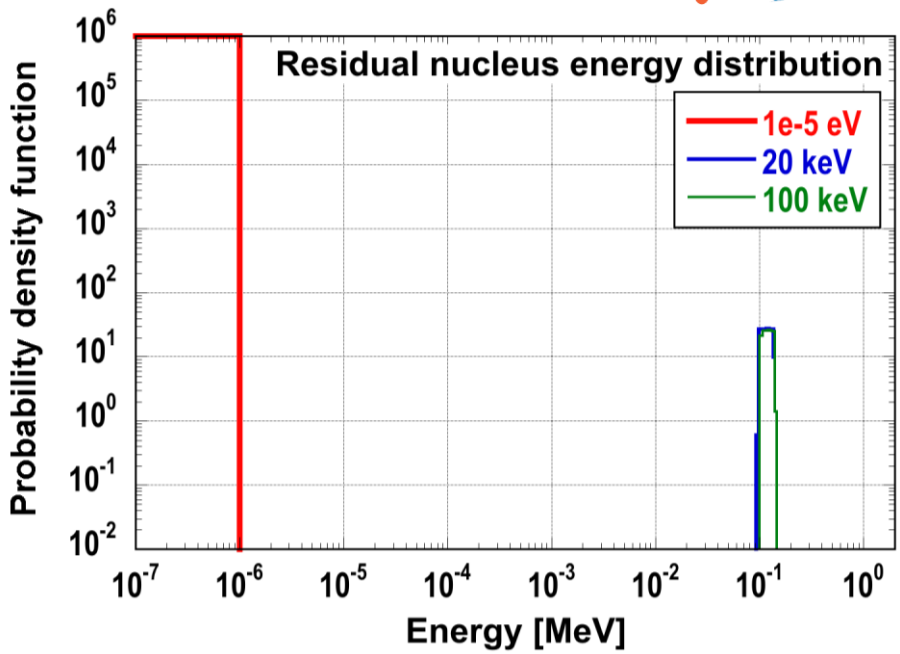
PSYCHE output for (n,α) reaction (unit : eV)

- For neutrons of 10^{-5} eV, energies of secondary alpha, residual nucleus and secondary gamma are too small.
- For neutrons up to 2.2 MeV, energies of secondary gamma are too small.

Charged particle data check of ^{39}K in FENDL-3.1b



Probability density function (energy distribution) of secondary alpha in (n,α) reaction

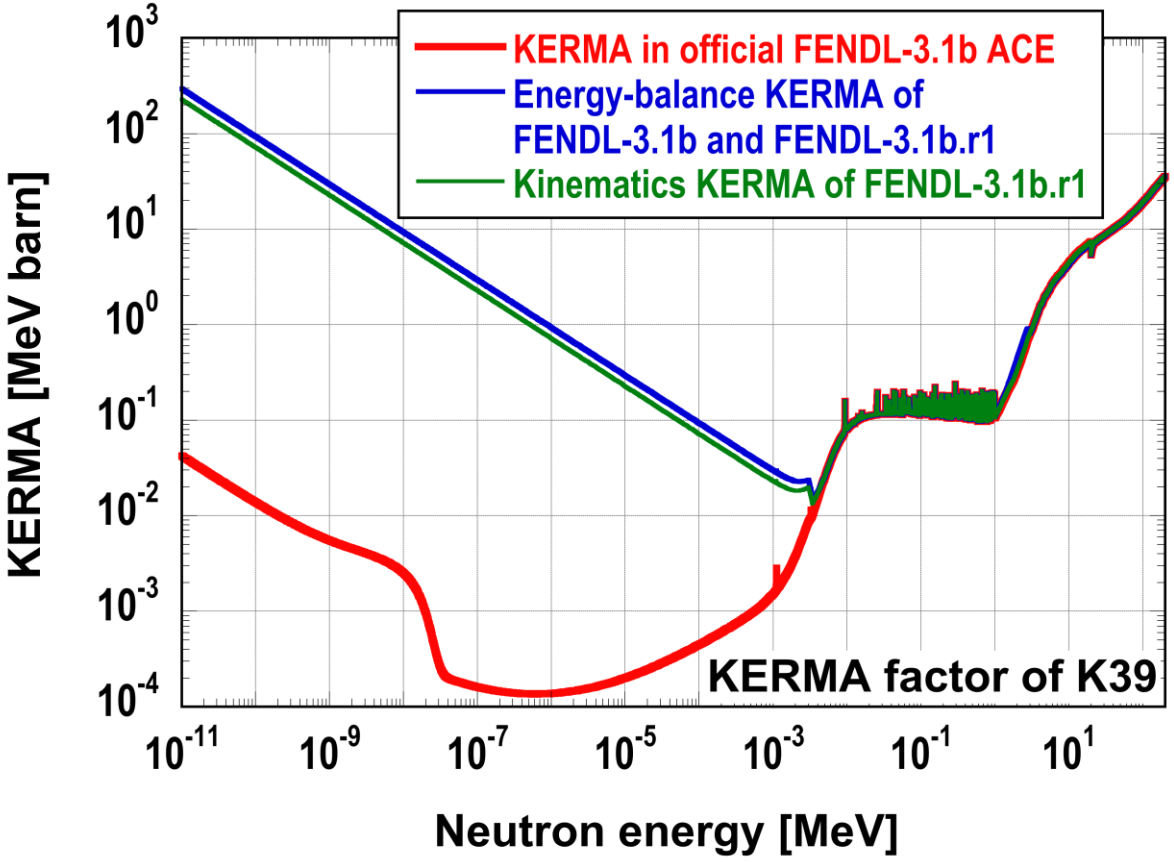


Probability density function (energy distribution) of residual nucleus in (n,α) reaction

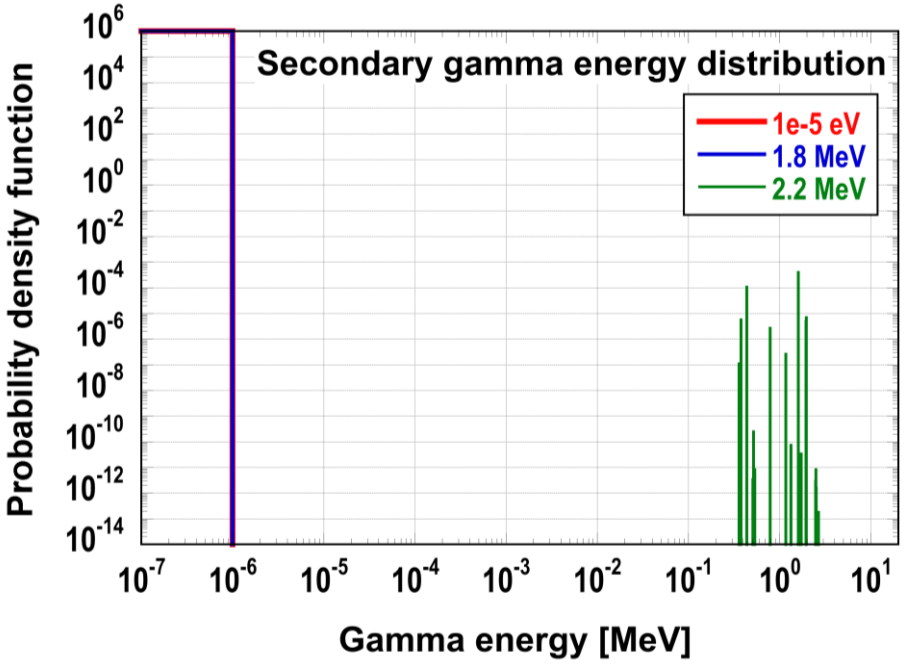
- Energy distribution data of secondary alpha and residual nucleus for neutrons of 10^{-5} eV in the (n,α) reaction should be replaced to those for neutrons of 20 keV.

Revision 1 of of ^{39}K in FENDL-3.1b

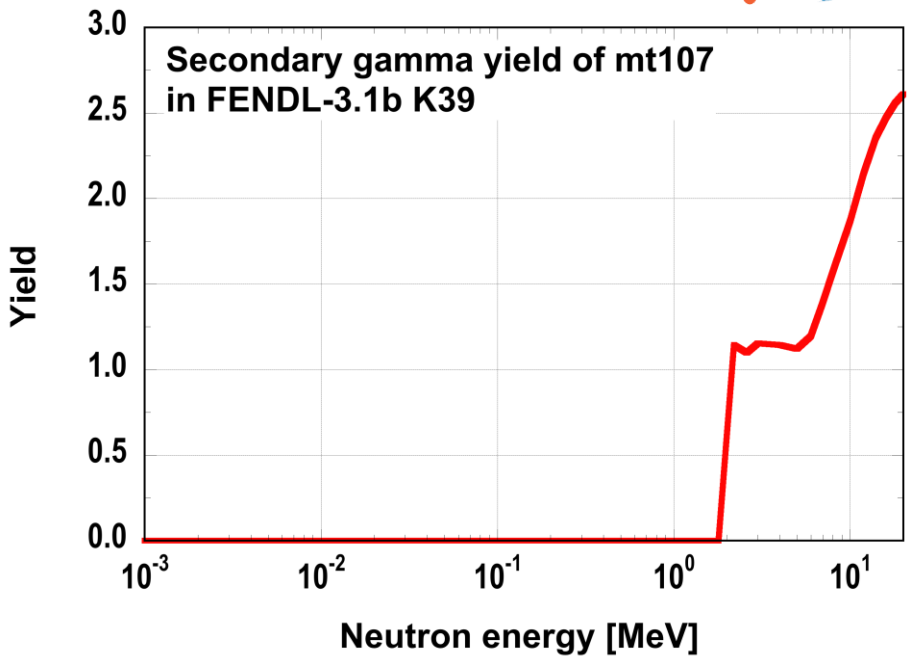
- Energy distribution data of secondary alpha and residual nucleus in the (n,α) reaction are modified (FENDL-3.1b.r1).
- Kinematics KERMA is close to energy-balance KERMA in FENDL-3.1b.r1, but is not equal.



Gamma data check of ^{39}K in FENDL-3.1b



Probability density function (energy distribution) of secondary gamma in (n,α) reaction

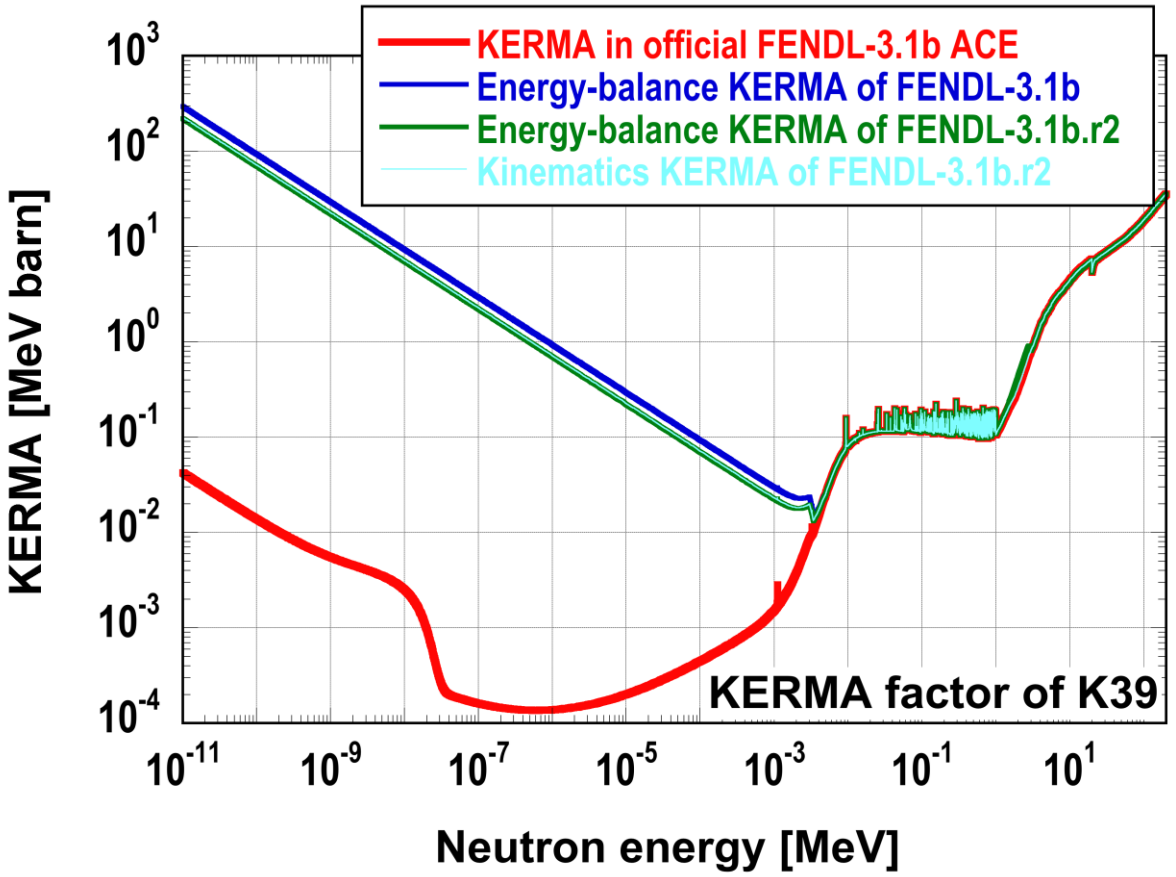


Yield of secondary gamma in (n,α) reaction

- **Energy distribution** data of secondary gamma for neutrons less than **2.2 MeV** in the (n,α) reaction should be replaced to those for neutrons of 2.2 MeV.
- **Yield** of secondary gamma for neutrons less than **2.2 MeV** in the (n,α) reaction should be modified to keep energy balance.

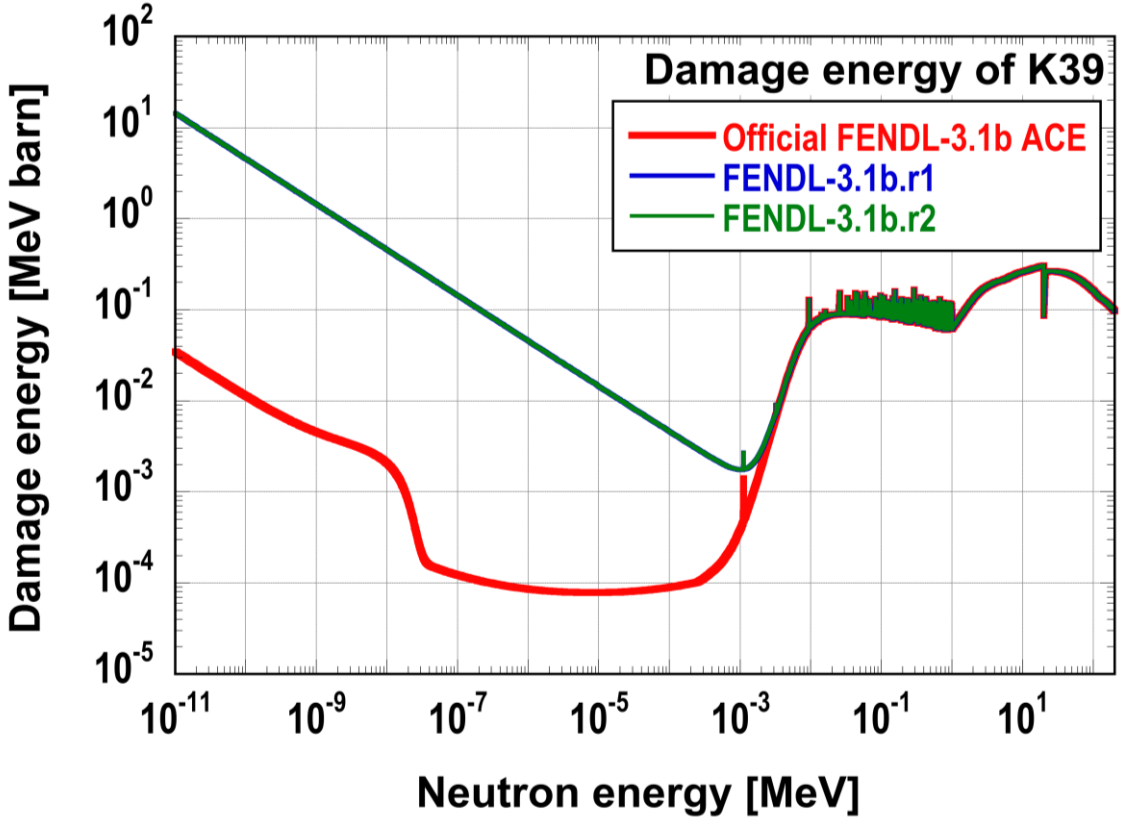
Revision 2 of ^{39}K in FENDL-3.1b

- Energy distribution and yield data of secondary gamma in (n,α) reaction are also modified (FENDL-3.1b.r2).
- Kinematics KERMA is almost the same as energy-balance KERMA in FENDL-3.1b.r2.
- Energy-balance KERMA of FENDL-3.1b is larger than that of FENDL-3.1b.r2, because it includes energy of secondary gamma in (n,α) reaction.



Damage energy of ^{39}K in FENDL-3.1b

- Damage energy includes contribution of alpha and residual nucleus in the (n,α) reaction in FENDL-3.1b.r2.
- Damage energies of FENDL-3.1b.r1 and FENDL-3.1b.r2 are the same because they are calculated by kinematics method.



Energy balance check ^{39}K in FENDL-3.1b.r2

ENERGY BALANCE SUMMARY: Q = 1.36126E+06

TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

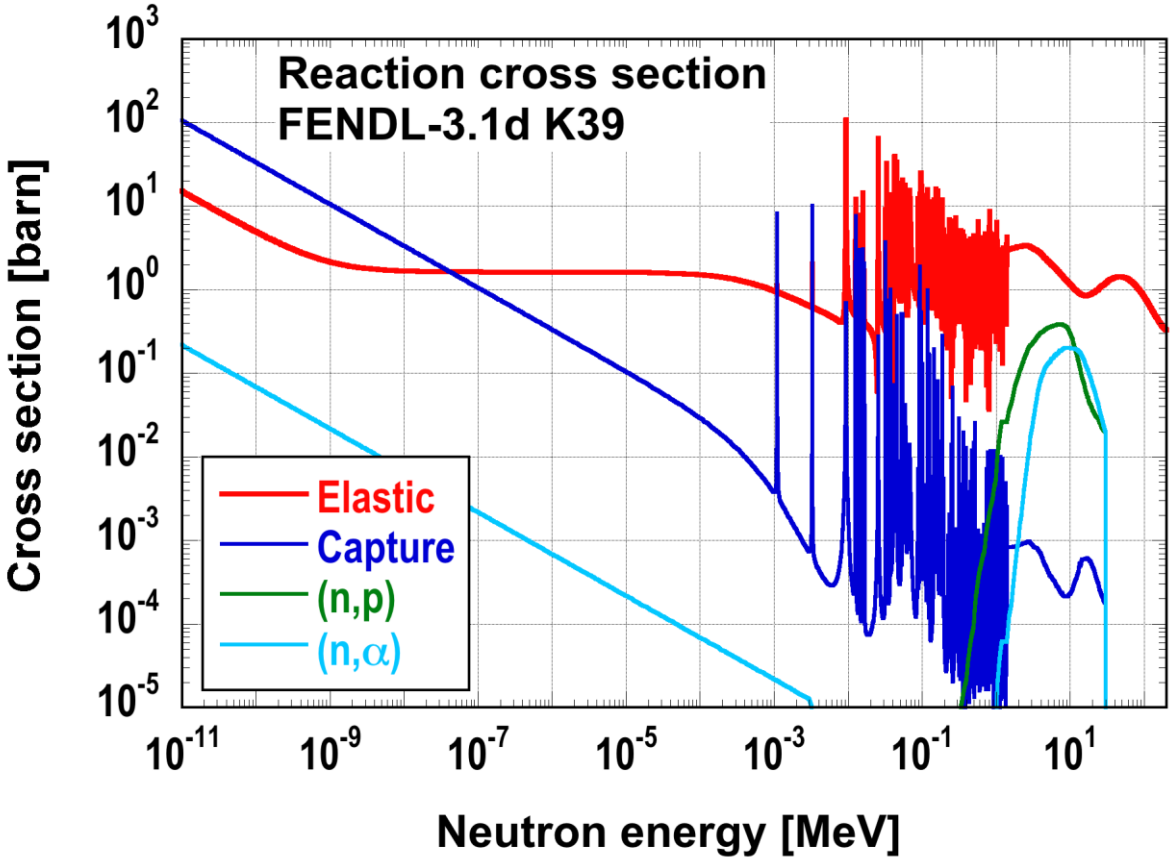
E	AVAIL	%DIFF	SUM	02004	17036	00000
1.00E-05	1.36E+06	1.23	1.38E+06	9.20E+05	1.17E+05	3.40E+05
2.00E+04	1.38E+06	0.28	1.38E+06	9.20E+05	1.17E+05	3.47E+05
5.00E+04	1.41E+06	1.67	1.43E+06	9.56E+05	1.21E+05	3.57E+05
1.00E+05	1.46E+06	-0.23	1.46E+06	9.56E+05	1.26E+05	3.73E+05
2.00E+05	1.56E+06	-1.81	1.53E+06	9.82E+05	1.40E+05	4.07E+05
4.00E+05	1.75E+06	3.21	1.81E+06	1.17E+06	1.64E+05	4.73E+05
6.00E+05	1.95E+06	-3.20	1.88E+06	1.16E+06	1.88E+05	5.40E+05
8.00E+05	2.14E+06	-6.45	2.00E+06	1.18E+06	2.11E+05	6.07E+05
1.00E+06	2.34E+06	-6.68	2.18E+06	1.27E+06	2.35E+05	6.73E+05
1.40E+06	2.73E+06	-3.87	2.62E+06	1.53E+06	2.83E+05	8.07E+05
1.80E+06	3.12E+06	0.23	3.12E+06	1.85E+06	3.29E+05	9.40E+05
2.20E+06	3.51E+06	0.00	3.51E+06	2.21E+06	3.76E+05	9.18E+05
2.60E+06	3.90E+06	0.00	3.90E+06	2.58E+06	4.22E+05	8.96E+05
3.00E+06	4.29E+06	0.00	4.29E+06	2.86E+06	4.68E+05	9.59E+05

PSYCHE output for (n,α) reaction of FENDL-3.1b.r2 (unit : eV)

- **FENDL-3.1b.r2 keeps energy balance.**

^{39}K in FENDL-3.1d (TENDL-2015)

Cross section check of ^{39}K in FENDL-3.1d



- Cross section of the (n,α) reaction is not so small in low energy neutrons. Thus partial KERMA and damage energy of the (n,α) reaction seem to be not so small.
- We examine the (n,α) reaction data in detail.

Energy balance check of ^{39}K in FENDL-3.1d

ENERGY BALANCE SUMMARY: Q = 1.34241E+06

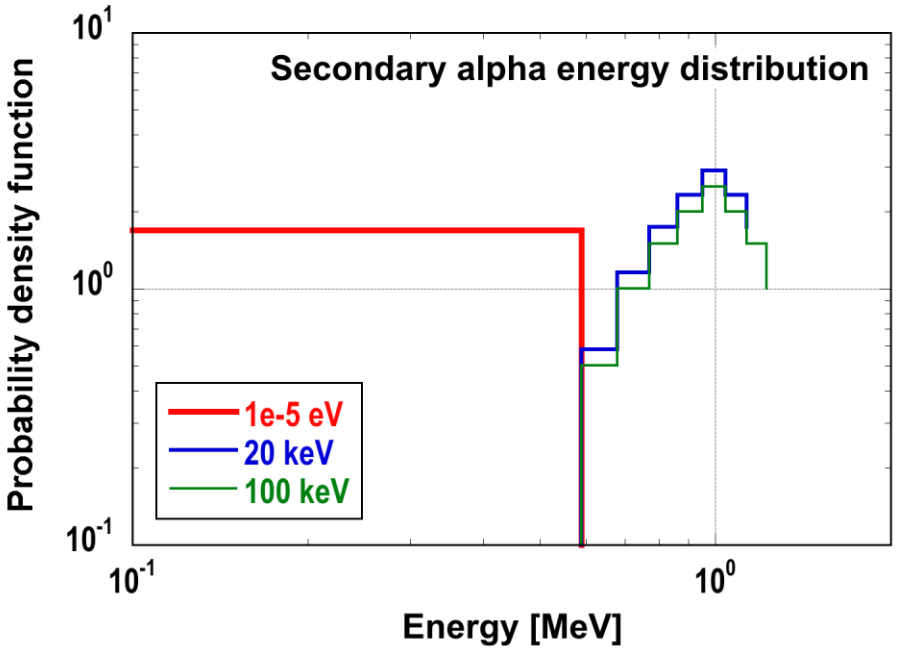
TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

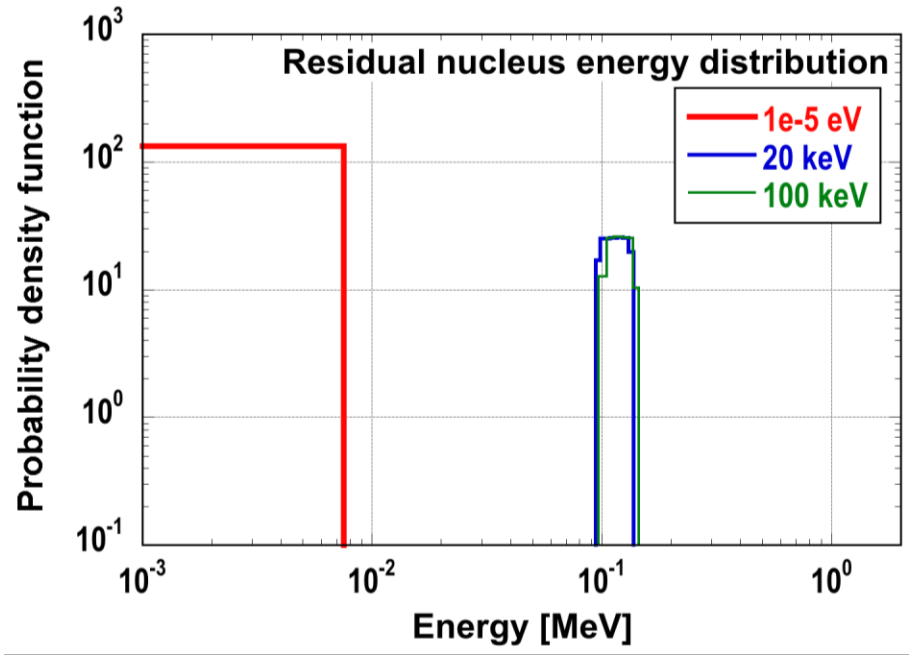
E	AVAIL	%DIFF	SUM	02004	17036	00000
1.00E-05	1.34E+06	-78.05	2.95E+05	2.95E+05	1.01E+02	9.97E-09
2.00E+04	1.36E+06	-32.18	9.24E+05	9.20E+05	3.15E+03	4.95E-06
6.00E+04	1.40E+06	-31.55	9.59E+05	9.56E+05	3.26E+03	1.48E-05
1.00E+05	1.44E+06	-33.40	9.59E+05	9.56E+05	3.37E+03	2.47E-05
2.00E+05	1.54E+06	-35.90	9.85E+05	9.82E+05	3.72E+03	4.95E-05
4.00E+05	1.73E+06	-35.93	1.11E+06	1.11E+06	4.37E+03	9.89E-05
6.00E+05	1.93E+06	-39.50	1.17E+06	1.16E+06	5.01E+03	1.48E-04
8.00E+05	2.12E+06	-43.96	1.19E+06	1.18E+06	5.66E+03	1.98E-04
1.00E+06	2.32E+06	-44.95	1.28E+06	1.27E+06	6.28E+03	2.47E-04
1.40E+06	2.71E+06	-43.27	1.54E+06	1.53E+06	7.57E+03	3.46E-04
1.80E+06	3.10E+06	-39.98	1.86E+06	1.85E+06	8.82E+03	4.45E-04
2.20E+06	3.49E+06	-36.42	2.22E+06	2.21E+06	1.01E+04	8.48E+02
2.60E+06	3.88E+06	-10.50	3.47E+06	2.57E+06	1.13E+04	8.88E+05
3.00E+06	4.27E+06	-10.58	3.82E+06	2.85E+06	1.25E+04	9.50E+05

PSYCHE output for (n,α) reaction (unit : eV)

- For neutrons of 10^{-5} eV, energies of secondary alpha, residual nucleus and secondary gamma are small.
- For neutrons up to 2.6 MeV, energies of secondary gamma are too small.

Charged particle data check of ^{39}K in FENDL-3.1d





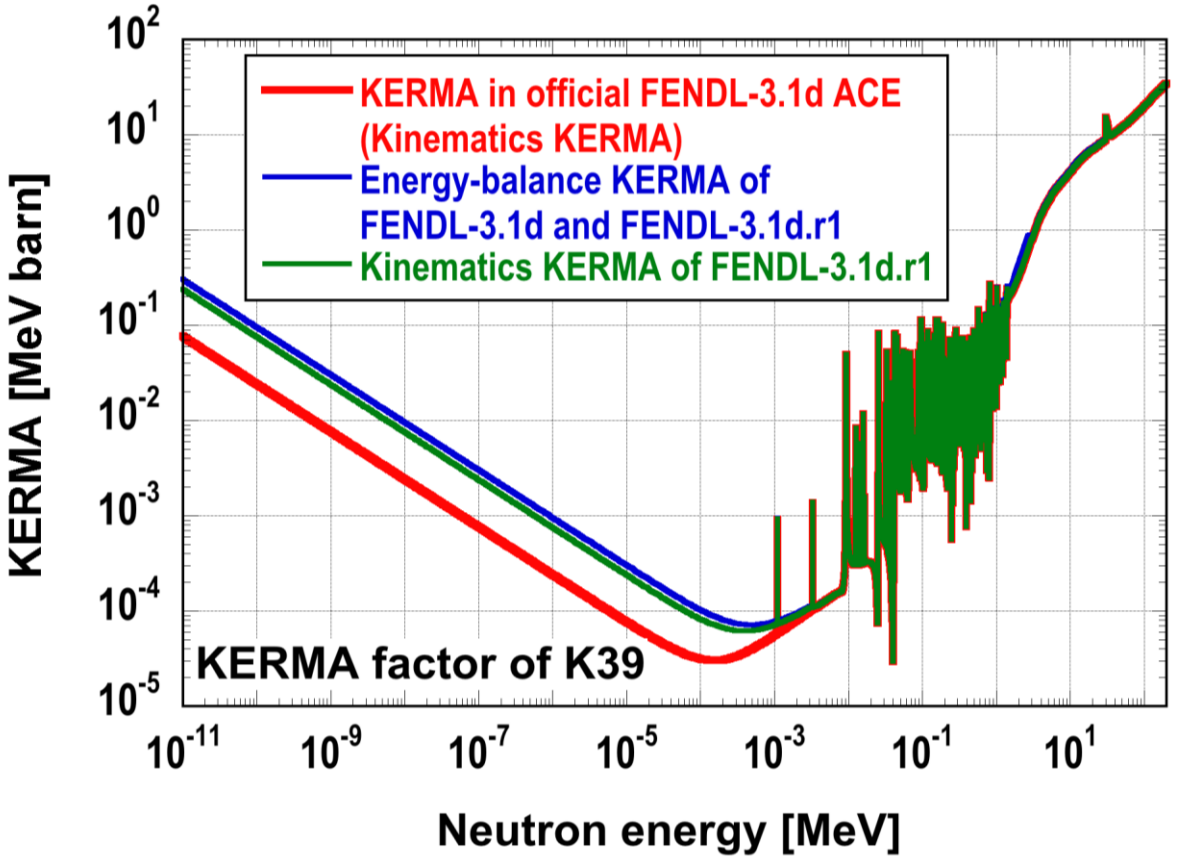
Probability density function (energy distribution) of secondary alpha in (n,α) reaction

Probability density function (energy distribution) of residual nucleus in (n,α) reaction

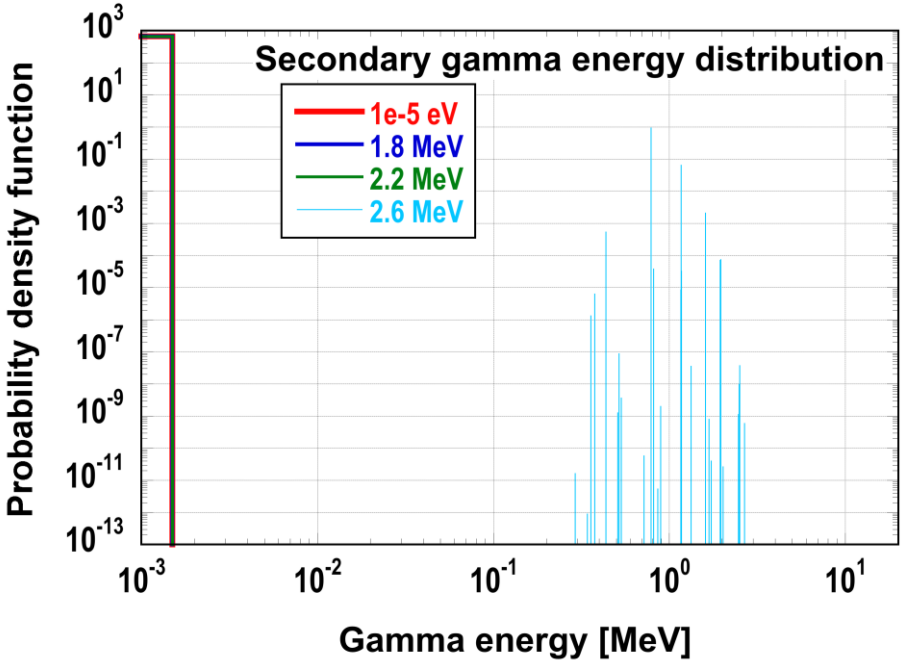
- Energy distribution data of secondary alpha and residual nucleus for neutrons of 10^{-5} eV in (n,α) reaction should be replaced to those for neutrons of 20 keV.

Revision 1 of ^{39}K in FENDL-3.1d

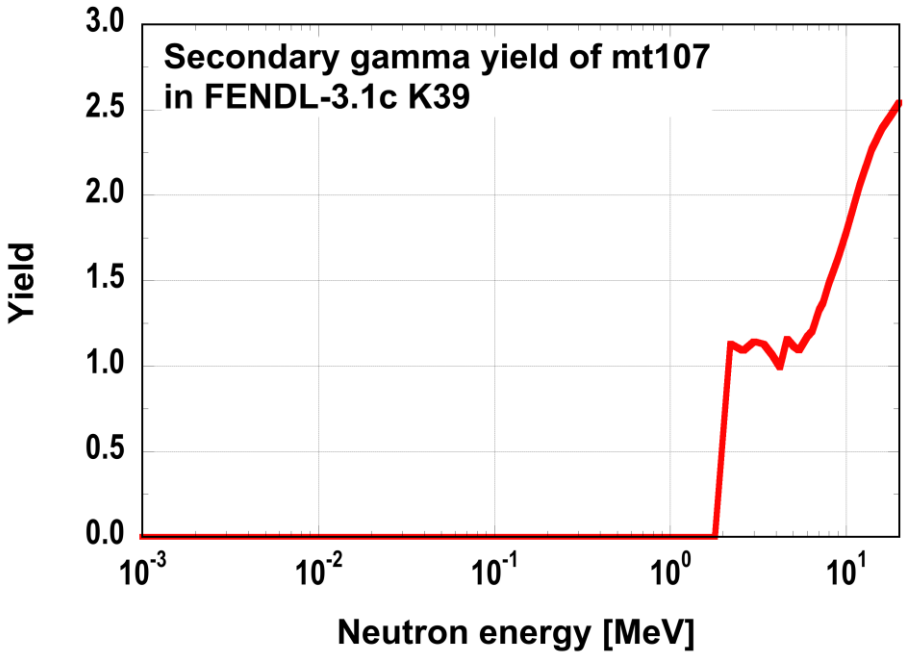
- Energy distribution data of secondary alpha and residual nucleus in (n,α) reaction are modified (FENDL-3.1d.r1).
- Kinematics KERMA is close to energy-balance KERMA in FENDL-3.1d.r1, but is not equal.



Gamma data check of ^{39}K in FENDL-3.1d



Probability density function (energy distribution) of secondary gamma in (n,α) reaction

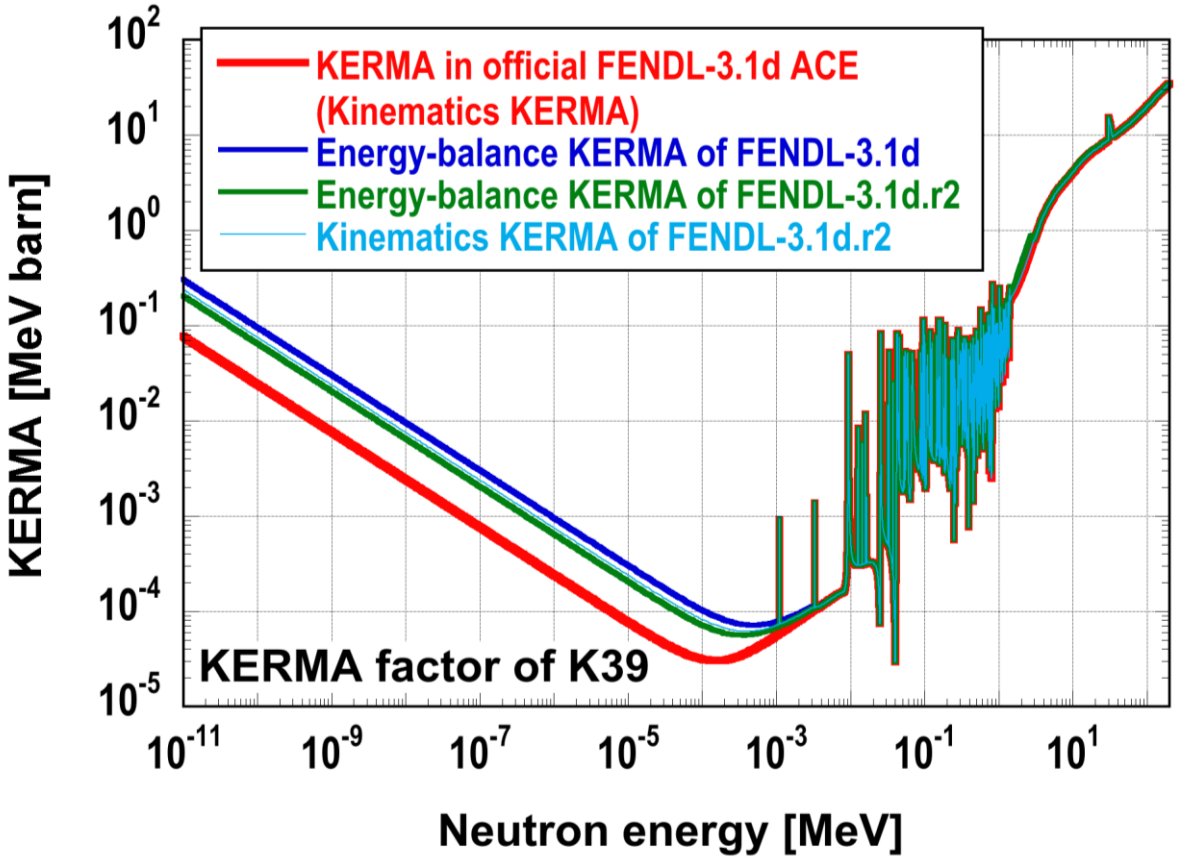


Yield of secondary gamma in (n,α) reaction

- **Energy distribution** data of secondary gamma for neutrons less than **2.6 MeV** in the (n,α) reaction should be replaced to those for neutrons of 2.6 MeV.
- **Yield** of secondary gamma for neutrons less than **2.6 MeV** in the (n,α) reaction should be modified to keep energy balance.

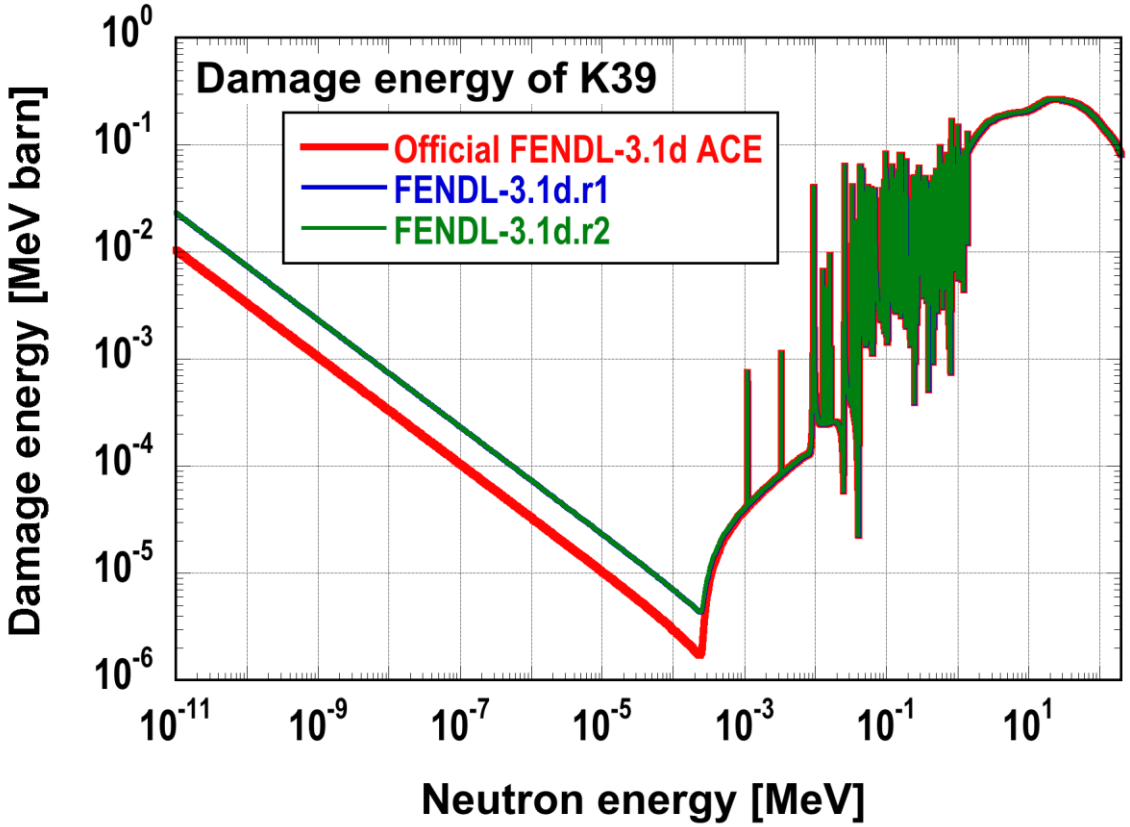
Revision 2 of ^{39}K in FENDL-3.1d

- Energy distribution and yield data of secondary gamma in the (n,α) reaction are also modified (FENDL-3.1d.r2).
- Kinematics KERMA is almost the same as energy-balance KERMA in FENDL-3.1d.r2.
- Energy-balance KERMA of FENDL-3.1d is larger than that of FENDL-3.1d.r2, because it includes energy of secondary gamma in the (n,α) reaction.



Damage energy of ^{39}K in FENDL-3.1d

- Damage energy includes contribution of alpha and residual nucleus in the (n,α) reaction in FENDL-3.1d.r2.
- Damage energies of FENDL-3.1d.r1 and FENDL-3.1d.r2 are the same because they are calculated by kinematics method.



Energy balance check ^{39}K in FENDL-3.1d.r2 #24

ENERGY BALANCE SUMMARY: Q = 1.34241E+06

TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

E	AVAIL	%DIFF	SUM	02004	17036	00000
1.00E-05	1.34E+06	2.48	1.38E+06	9.20E+05	3.15E+03	4.52E+05
2.00E+04	1.36E+06	1.70	1.39E+06	9.20E+05	3.15E+03	4.61E+05
6.00E+04	1.40E+06	2.70	1.44E+06	9.56E+05	3.26E+03	4.80E+05
1.00E+05	1.44E+06	1.22	1.46E+06	9.56E+05	3.37E+03	4.98E+05
2.00E+05	1.54E+06	-0.47	1.53E+06	9.82E+05	3.72E+03	5.45E+05
4.00E+05	1.73E+06	0.87	1.75E+06	1.11E+06	4.37E+03	6.37E+05
6.00E+05	1.93E+06	-1.62	1.90E+06	1.16E+06	5.01E+03	7.30E+05
8.00E+05	2.12E+06	-5.20	2.01E+06	1.18E+06	5.66E+03	8.23E+05
1.00E+06	2.32E+06	-5.45	2.19E+06	1.27E+06	6.28E+03	9.15E+05
1.40E+06	2.71E+06	-2.62	2.64E+06	1.53E+06	7.57E+03	1.10E+06
1.80E+06	3.10E+06	1.53	3.14E+06	1.85E+06	8.82E+03	1.29E+06
2.20E+06	3.49E+06	1.32	3.53E+06	2.21E+06	1.01E+04	1.32E+06
2.60E+06	3.88E+06	-10.50	3.47E+06	2.57E+06	1.13E+04	8.88E+05
3.00E+06	4.27E+06	-10.58	3.82E+06	2.85E+06	1.25E+04	9.50E+05

PSYCHE output for (n,α) reaction of FENDL-3.1d.r2 (unit : eV)

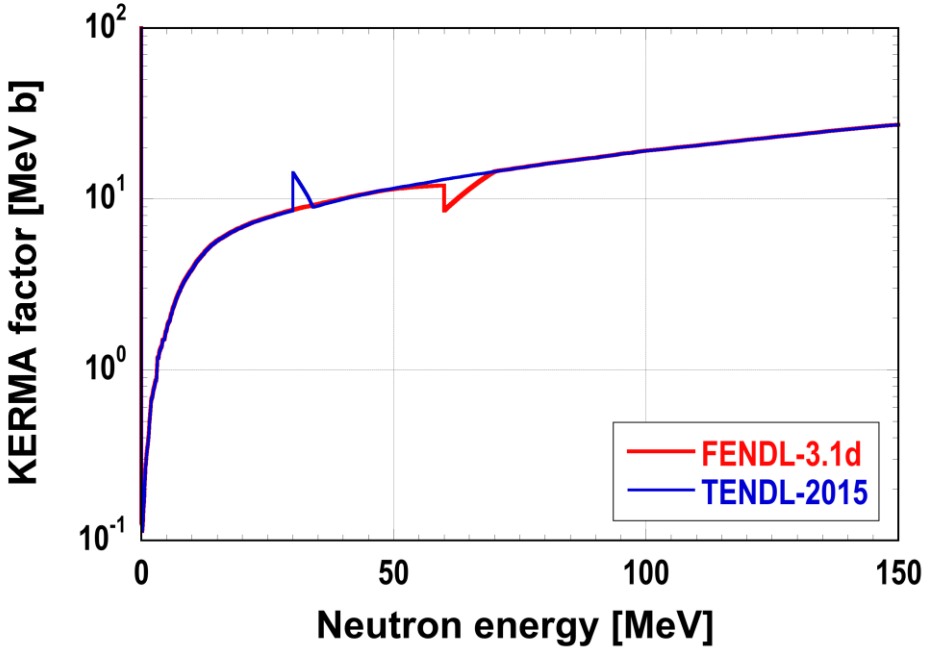
- **FENDL-3.1d.r2 keeps energy balance.**

Concluding Remarks

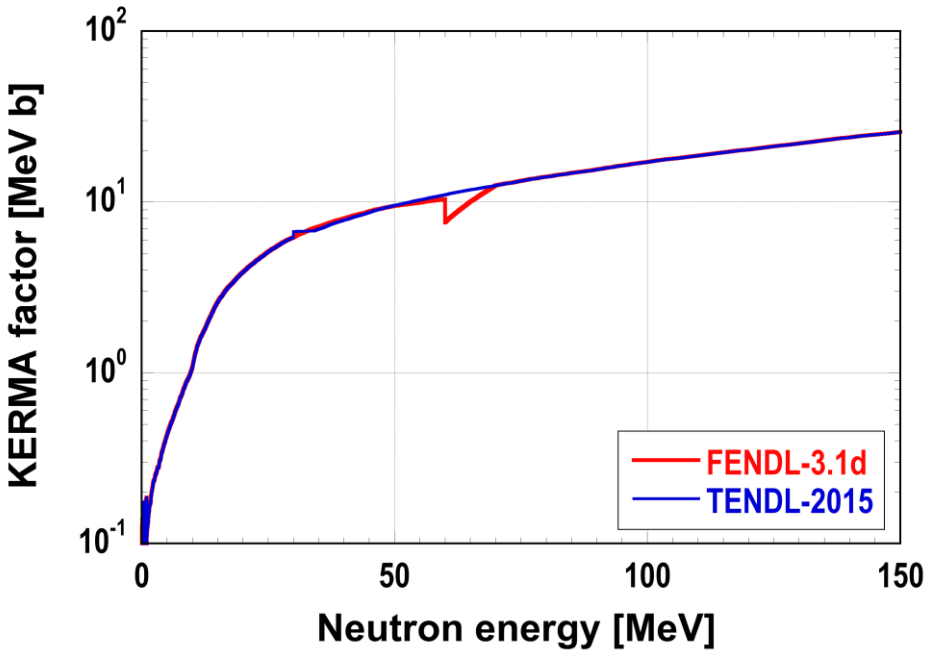
- We re-investigated reasons of difference between kinematics and energy-balance KERMA factors of ^{39}K in FENDL-3.1b (TENDL-2012) and -3.1d (TENDL-2015) in detail.
- We found out the followings.
  - This issue is not due to NJOY, but due to the ^{39}K data themselves of FENDL-3.1b and -3.1d.
  - Secondary gamma yield and energy distribution data of secondary alpha, residual nucleus and secondary gamma of the (n,α) reaction in ^{39}K of FENDL-3.1b and -3.1d seem to be incorrect, which causes this issue and wrong damage energy.
- ^{40}K in FENDL-3.1b (TENDL-2012) and -3.1d (TENDL-2015) also has the same problem.
- Note that the same issue also occurs in ^{39}K and ^{40}K in TENDL-2017.

Appendix

- ^{40}K and ^{41}K data in FENDL-3.1d are not identical to those in the TENDL-2015 official site.
  - FENDL-3.1d : mt=5 is above 60 MeV.
  - TENDL-2015 : mt=5 is above 30 MeV.
- We are afraid that users are confused.



^{40}K KERMA factor



^{41}K KERMA factor

Problem on p-table in ACE file of FENDL-3.1d

Japan Atomic Energy Agency
Chikara Konno

Contributor : Saerom Kwon (QST)

Consultants' Meeting on the FENDL Library for fusion neutronics calculations
15-18 October 2018
IAEA Headquarters, Vienna, Austria

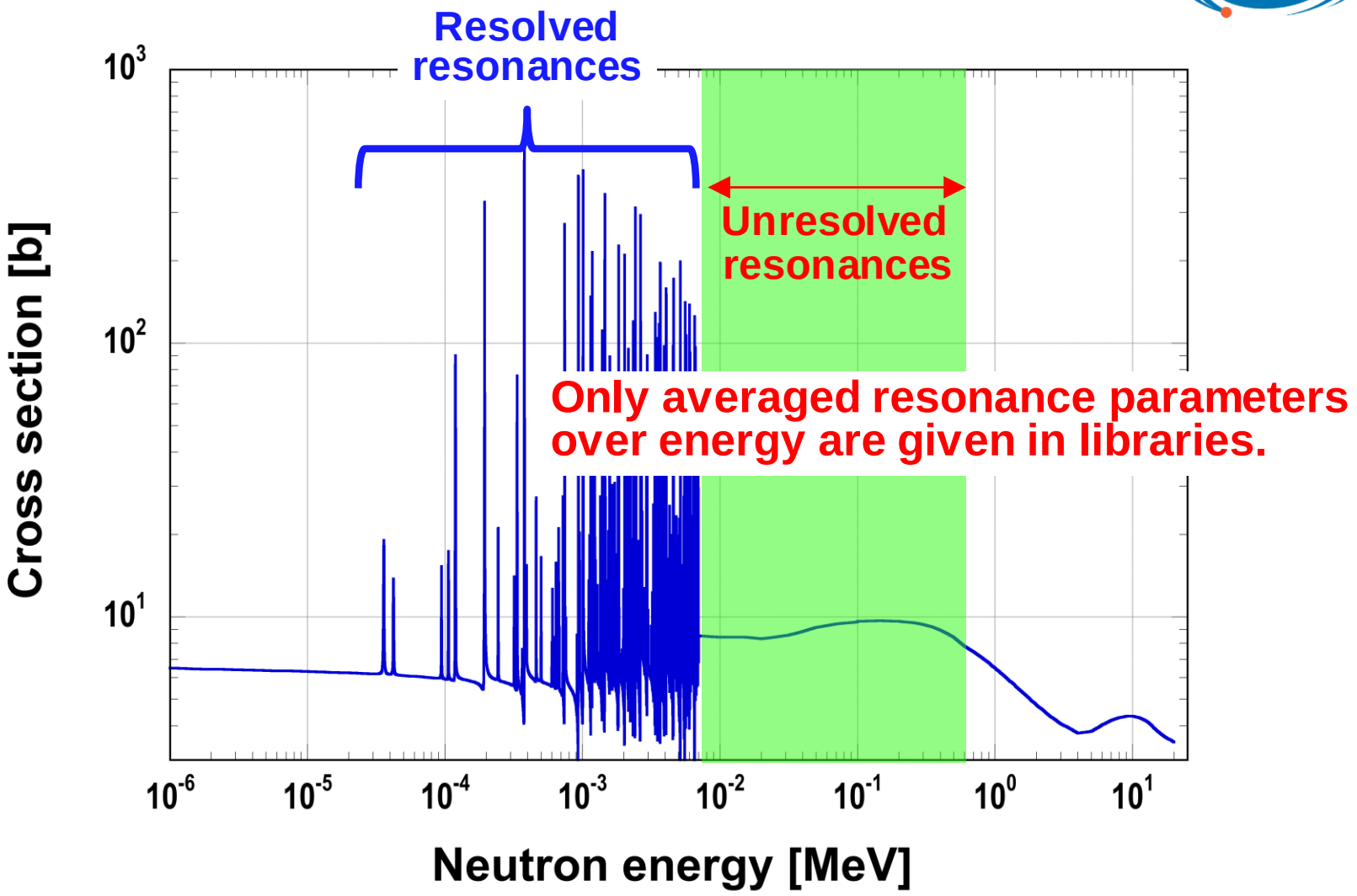
Introduction -(1)

- IAEA decided to adopt kinematics upper limit KERMA as KERMA in all the official ACE and MATXS files of FENDL-3.1d except for ^{40}K and ^{41}K in order to avoid energy-balance problem.
- Thus the heating numbers [KERMA/(total cross section)] in the official ACE file of FENDL-3.1d are always positive.
- However, we found out that several p-tables (probability tables) of the heating number in the ACE files of the following 33 nuclei were negative.

  Ga69, Ga71, Br79, Br81, Mo92, Mo94, Mo95, Mo96, Mo97, Mo98, Mo100, Rh103, Cd108, Cd110, Cd112, Cd113, Cd114, Cd116, Sb121, Sb123, Ba130, Ba132, Ba134, Ba135, Ba136, Ba137, Ce142, Hf174, Hf176, Hf177, Hf178, Hf179, Hf180

- We examine why several heating numbers of the p-tables in the ACE files of the above nuclei are negative.

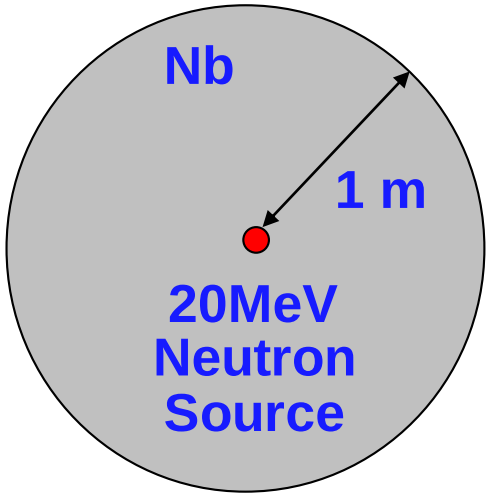
What are unresolved resonance data?



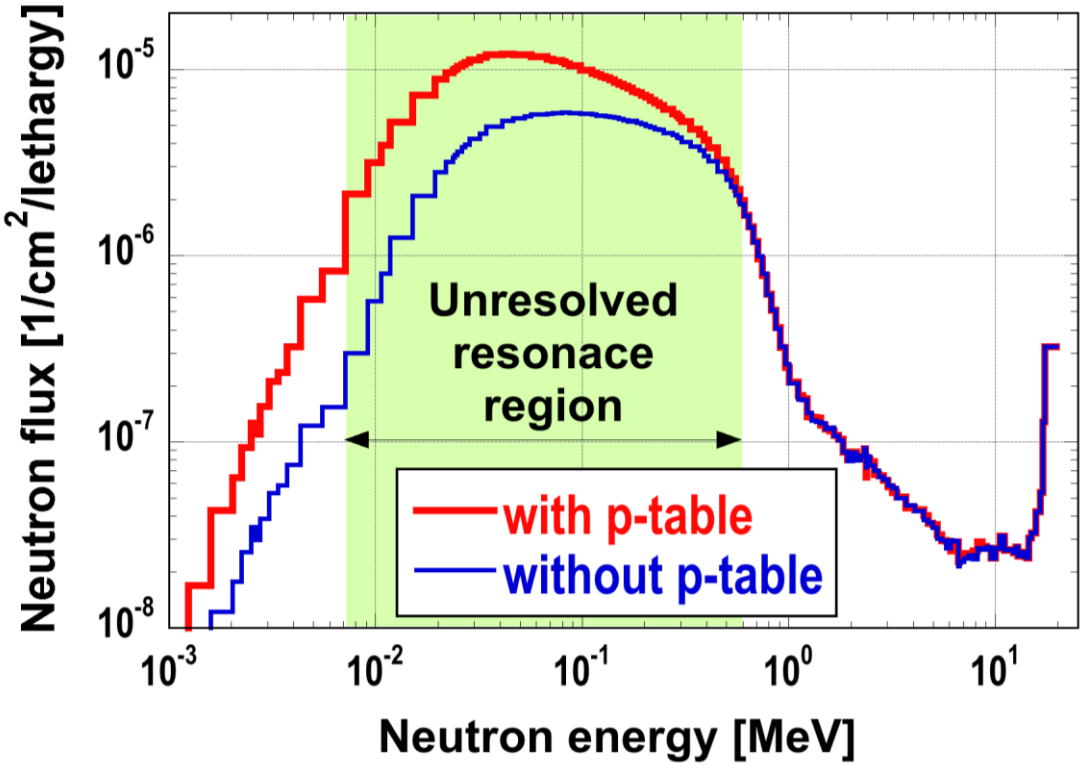
Total cross section of ^{93}Nb in FENDL-3.1d

Effect of unresolved resonances

- The unresolved resonance also cause the cross section **self-shielding**, which affects neutron spectra in the deep penetration problem though it is a very rare case.



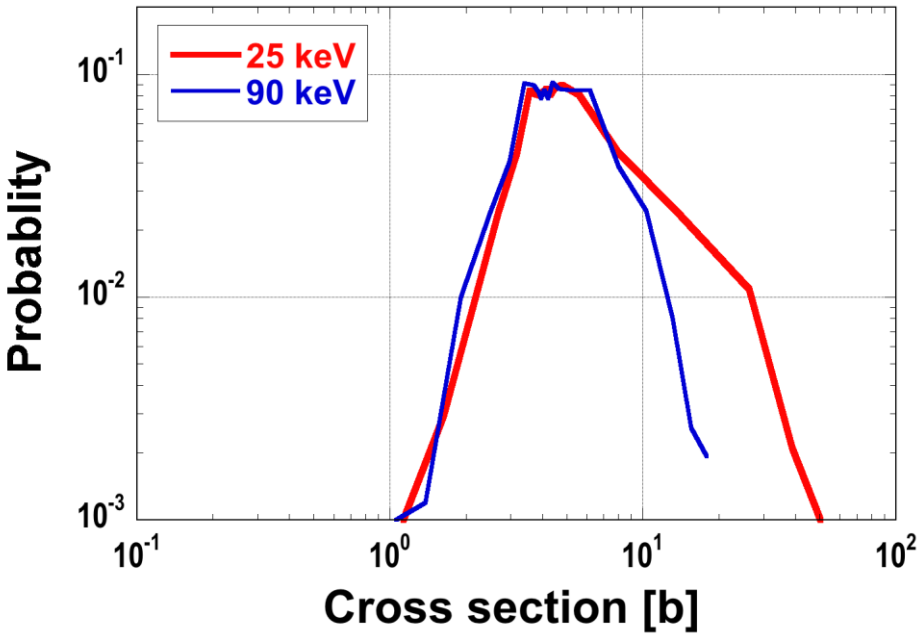
Calculation model



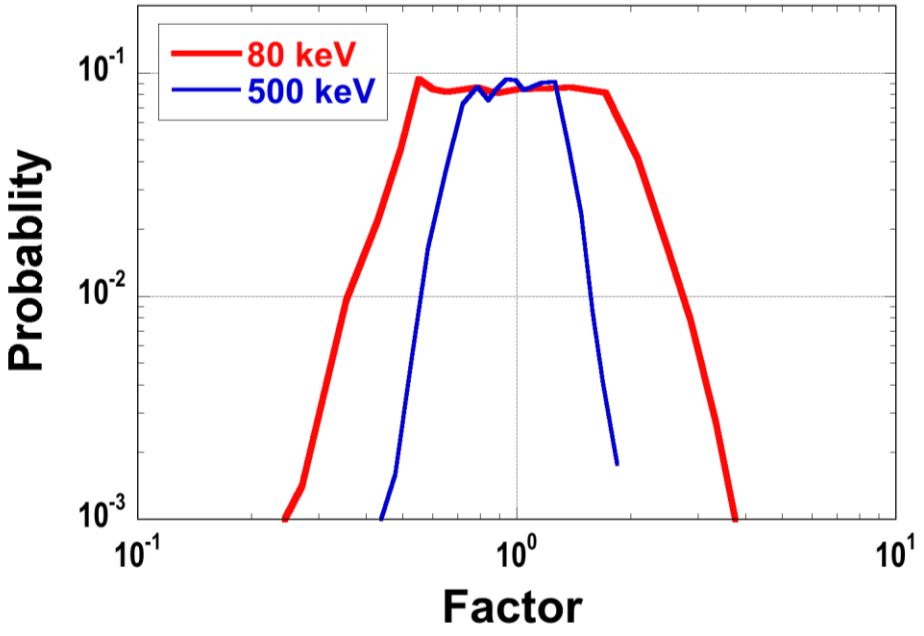
Neutron spectra at 60cm from Nb sphere center calculated with MCNP

Cross sections of unresolved resonances

- The unresolved resonance data are given as averaged resonance parameters over energy.
- The p-table in ACE files expresses relation between a cross section (heating number) or a factor for the average cross section and probability.

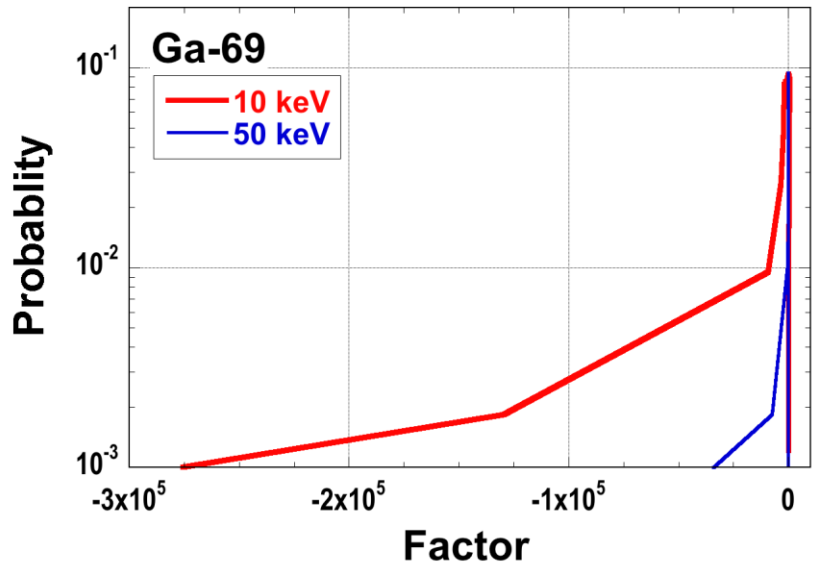


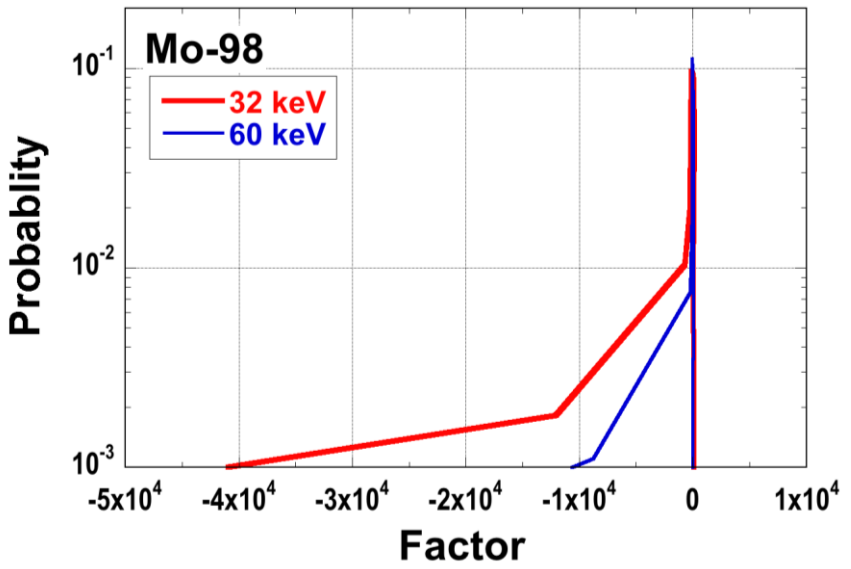
p-table for total x-sec. in ^{137}Ba of FENDL-3.1d

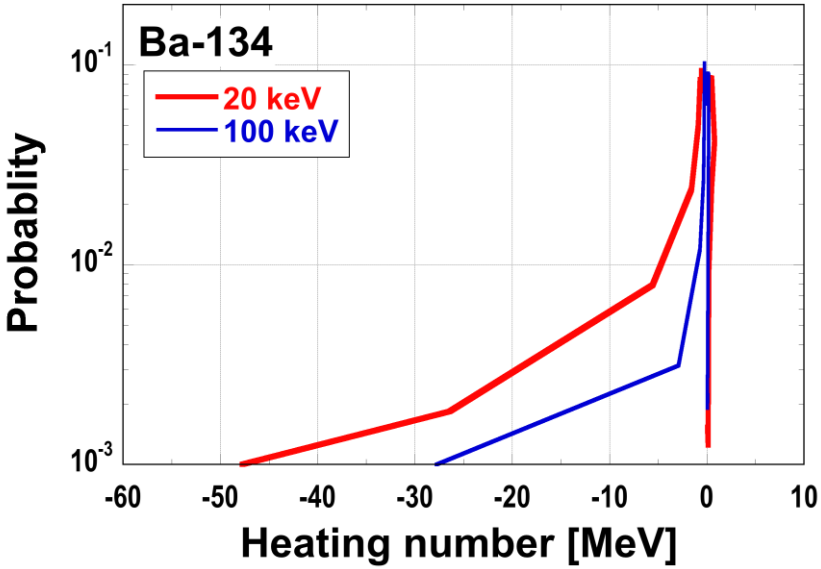


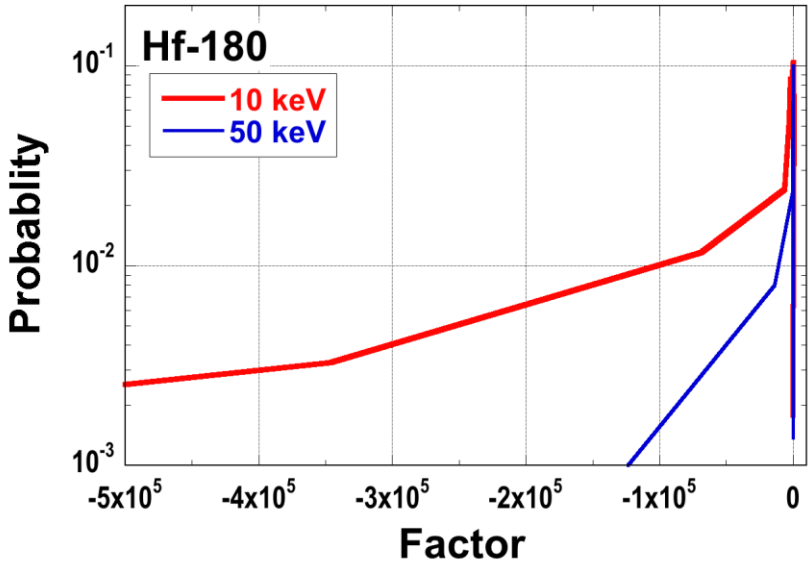
p-table for total x-sec. in ^{93}Nb of FENDL-3.1d

Negative p-tables of heating number









Why are p-tables of heating number negative? -(1)

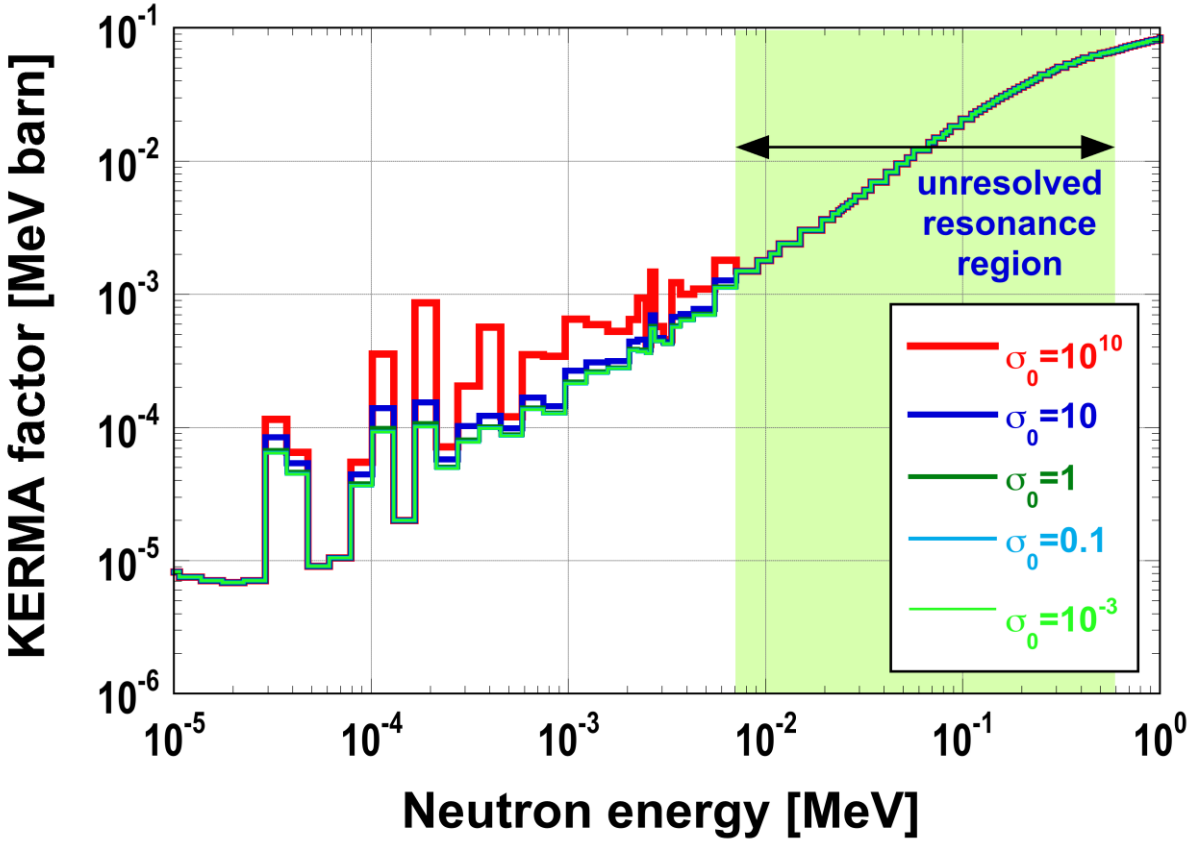
- The p-table of heating number is produced in the PURR module of NJOY with KERMA calculated in the HEATR module of NJOY.
- We examined NJOY and FENDL-3.1d in detail. Then we found out that partial KERMA of the capture reaction were too large. We also specified its reason.
  - The problematic nuclei have no secondary gamma data of the capture reaction or secondary gamma data of the capture reaction in the nuclei are stored in file12-15 mt=3, not mt=102.
  - The partial KERMA of the capture reaction includes secondary gamma energy because it is calculated with the energy-balance method.
  - Thus the partial KERMA of the capture reaction becomes too large.

Why are p-tables of heating number negative? -(2)

- In the PURR module, the total KERMA is subtracted by partial KERMAs of the elastic scattering, fission and capture reactions.
- In FENDL-3.1d, the total KERMA is calculated with the kinematics method, not the energy-balance method. Thus the total KERMA does not include secondary gamma energy.
- The subtracted total KERMA becomes negative if the partial KERMA factor of the capture reaction includes secondary gamma energy.
- Finally the p-table of KERMA also becomes negative.

Solution of the problem -(1)

- How is the self-shielding effect of KERMA in the unresolved resonance region? → *Negligibly small !*



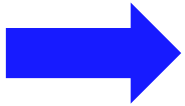
KERMA of ^{93}Nb in FENDL-3.1d generated from GENDF file

(p-table is positive.)

Solution of the problem -(2)

- The self-shielding effect for KERMA in the unresolved resonance region is very small. It is considered that the p-table of heating number is not necessary.
- The NJOY2016 manual describes that the PURR module sets the p-table of heating number to "1.0" or an average heating number in the case that the partial KERMAs of the elastic scattering, fission and capture reactions are not calculated in the HEATR module.
- We modified the HEATR input.

```
heatr
-21 -23 -24 34/
4243 7 0 0 0 2 0 1/
302 304 318 402 404 443 444/
```



```
heatr
-21 -23 -24 34/
4243 4 0 0 0 2 0 1/
304 404 443 444/
```

Input change in the HEATR module(^{98}Mo)

- The problem is solved.

Concluding Remarks

- We found out that several p-tables (probability tables) of the heating number in the ACE files of 33 nuclei were negative.
- We examined why several heating numbers of the p-tables in the ACE files of the above nuclei were negative.
- We specified that the reason of the negative p-table is because the problematic nuclei have no secondary gamma data of the capture reaction or secondary gamma data of the capture reaction in the nuclei are stored in file12-15 mt=3, not mt=102.
- The self-shielding effect for KERMA in the unresolved resonance region is very small. Thus we adopted a method to set the p-table of heating number to "1.0" or an average heating number with no calculation of the partial KERMAs of the elastic scattering, fission and capture reactions in the HEATR module.

Problem on MATXS file of FENDL-3.1d due to NJOY unresolved resonance processing

Japan Atomic Energy Agency
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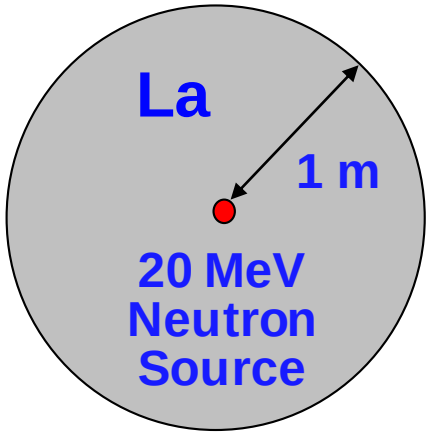
Contributor : Saerom Kwon (QST)

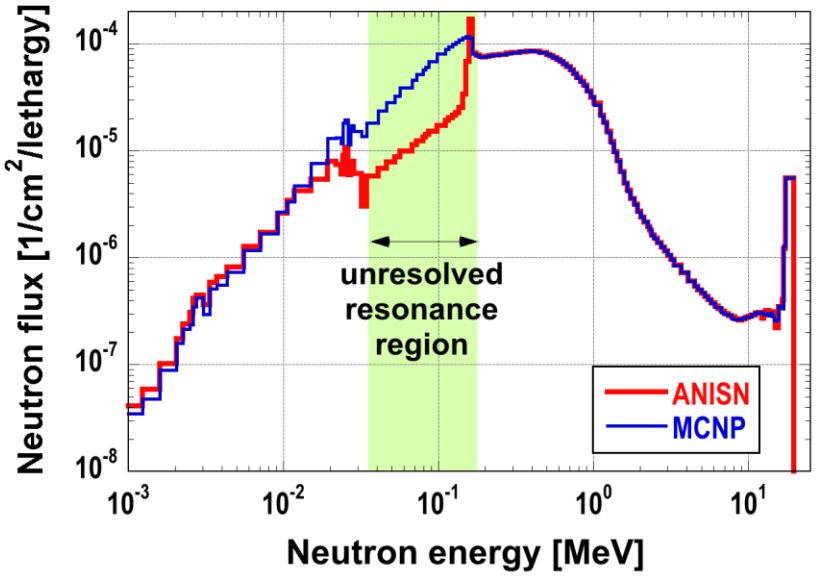
Consultants' Meeting on the FENDL Library for fusion neutronics calculations
15-18 October 2018
IAEA Headquarters, Vienna, Austria

Introduction

- We encountered a problem that neutron spectra calculated with ANISN and MCNP (Library : FENDL-3.1d) were drastically different for a La sphere of 1 m in radius with an isotropic neutron source of 20 MeV at the center.
- The La isotope data in FENDL-3.1d have unresolved resonance (URR) data, which seem to cause the problem.
- We examine reasons of the difference.

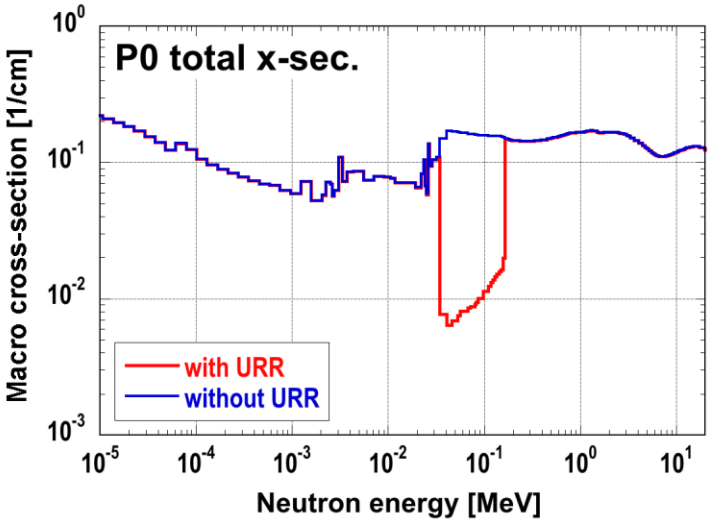


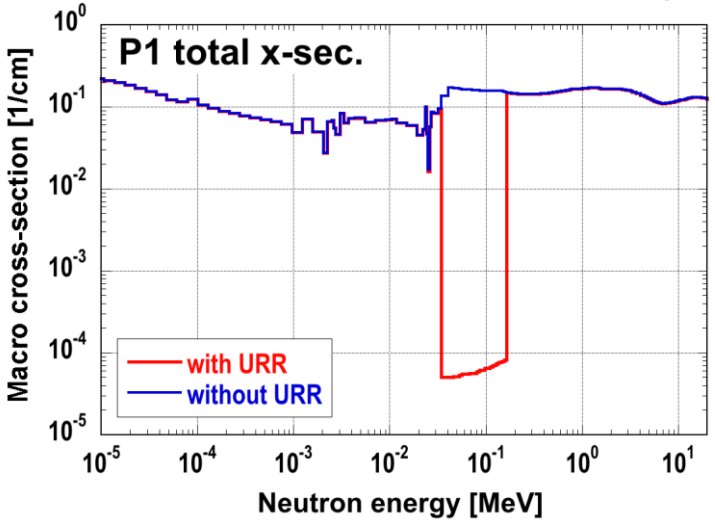
Calculation model

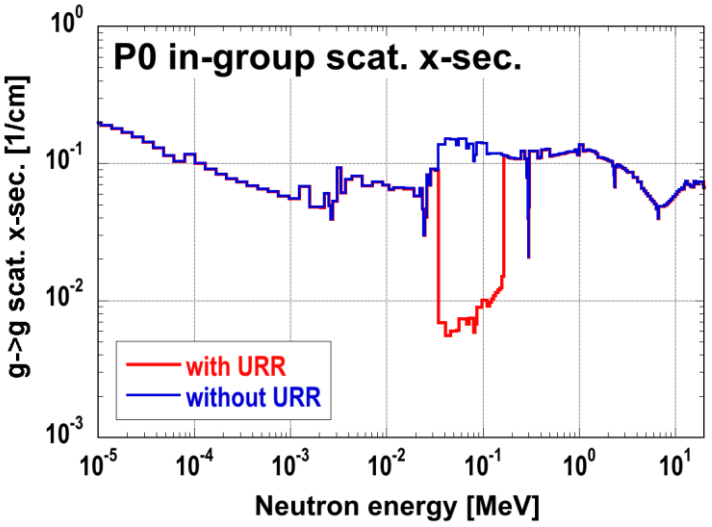


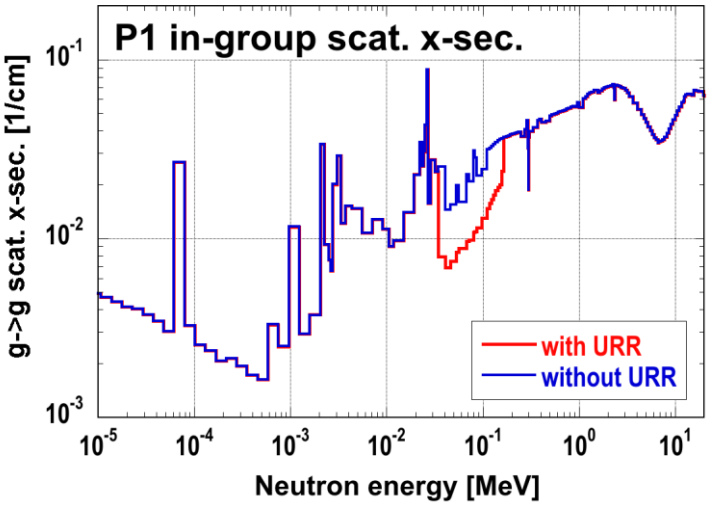
Neutron spectra at 60 cm from La sphere center

Macroscopic multigroup library of La





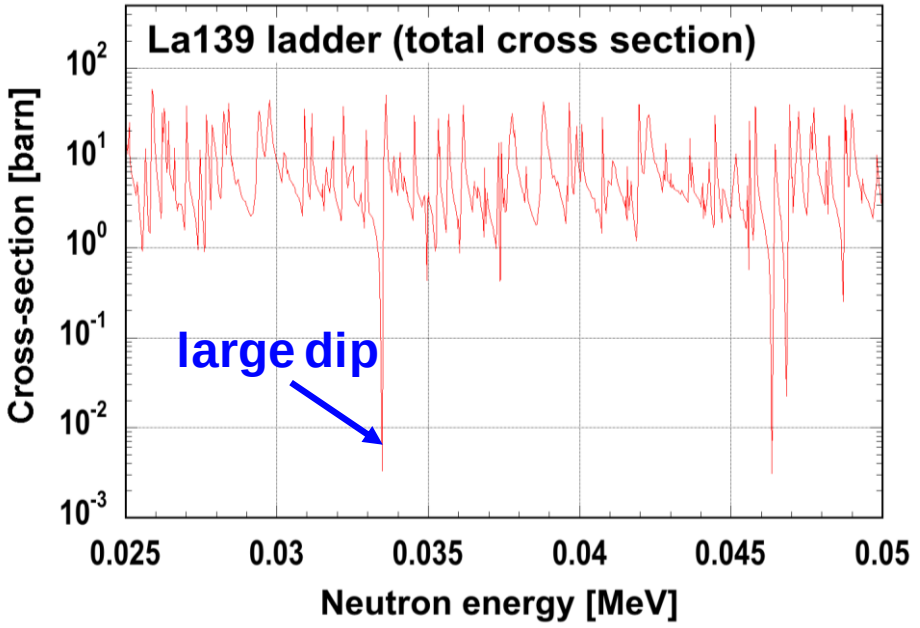




The self-shielding correction in URR is large!

Why is the self-shielding effect of URR large? -(1)

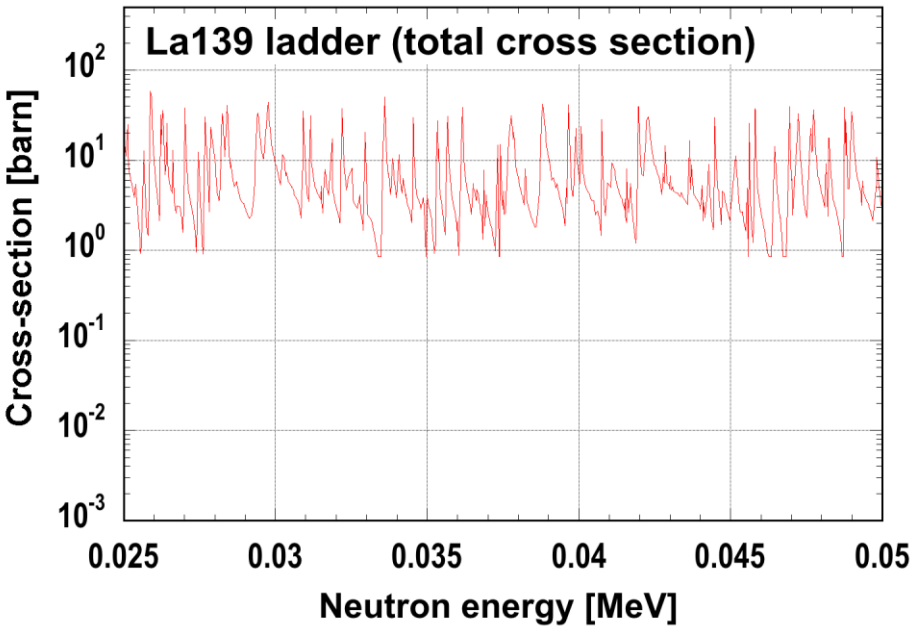
- **PURR module of NJOY**
  - ① A lot of plausible sets [ladder] of elastic scat., fission and capture reaction cross sections with pseudo resolved resonances are generated from unresolved resonance data with random number.
  - ② The range between the smallest and largest total cross sections are divided to several bins. The p-table is calculated from frequency how the total cross section hits each bin.



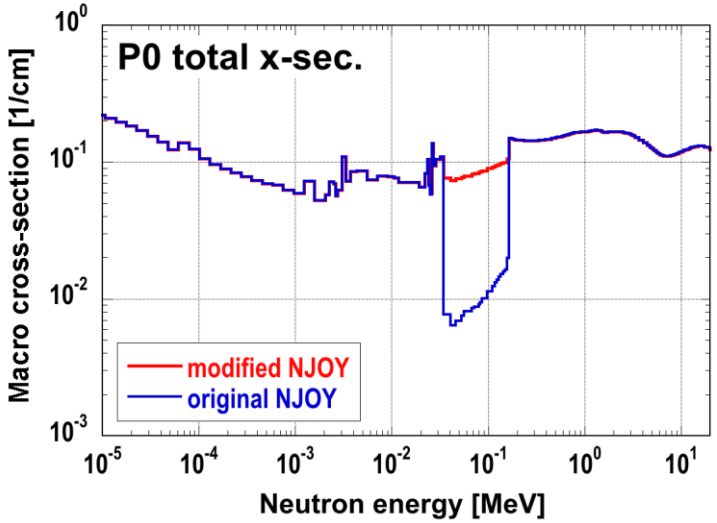
- **Large dips among resonances appear in ladders.**

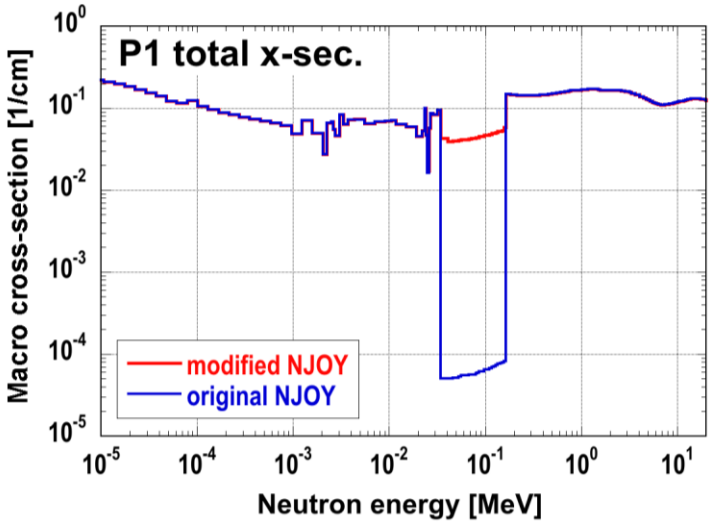
Why is the self-shielding effect of URR large? -(2)

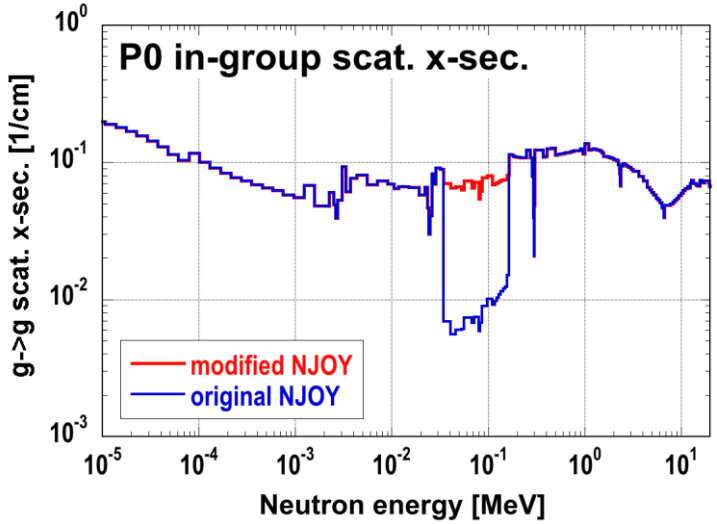
- In the case of a small background x-sec. such as 10^{-3} b, the contribution of smaller total x-sec. increases more in URR because the weighting function is invers or invers square of the total x-sec. Then the self-shielding correction in URR becomes large.
- The NJOY manual describes "the unrealistic cross sections in the dips between resonances will eventually make even the PURR results suspect at low values."
- We modified NJOY2016 where the total x-sec. below 1/10 of infinite diluted total x-sec. is set to 1/10 of infinite diluted total x-sec. [just trial]

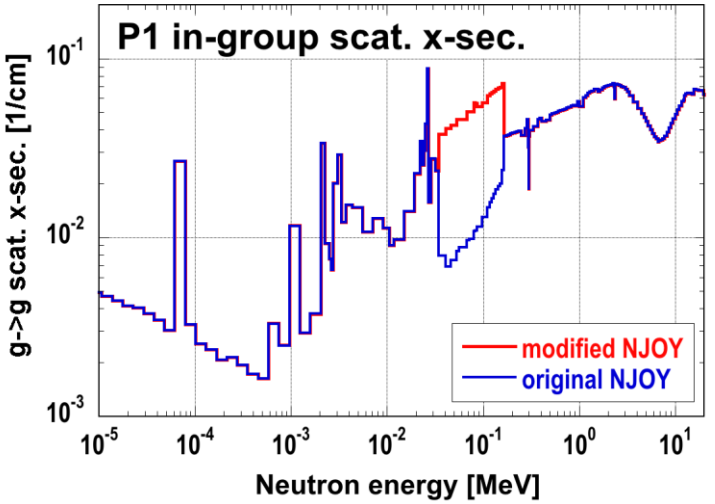


Modified macroscopic multigroup library of La





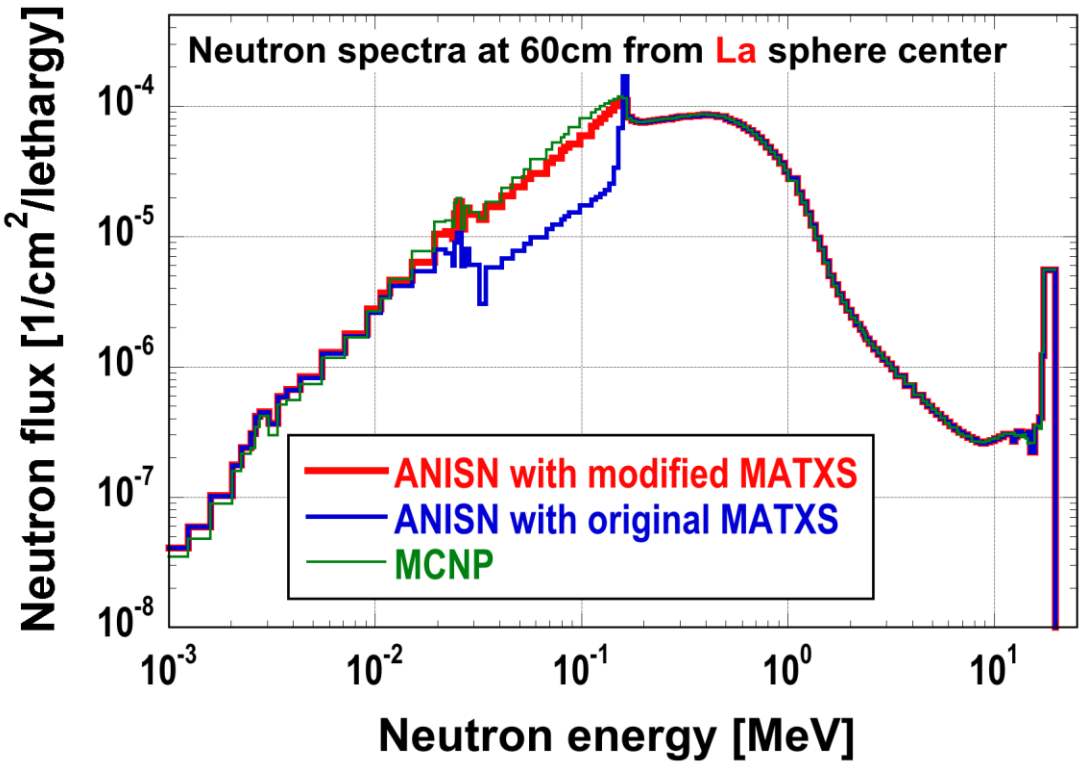




The self-shielding correction of URR becomes smaller!

Calculation with modified MATXS file

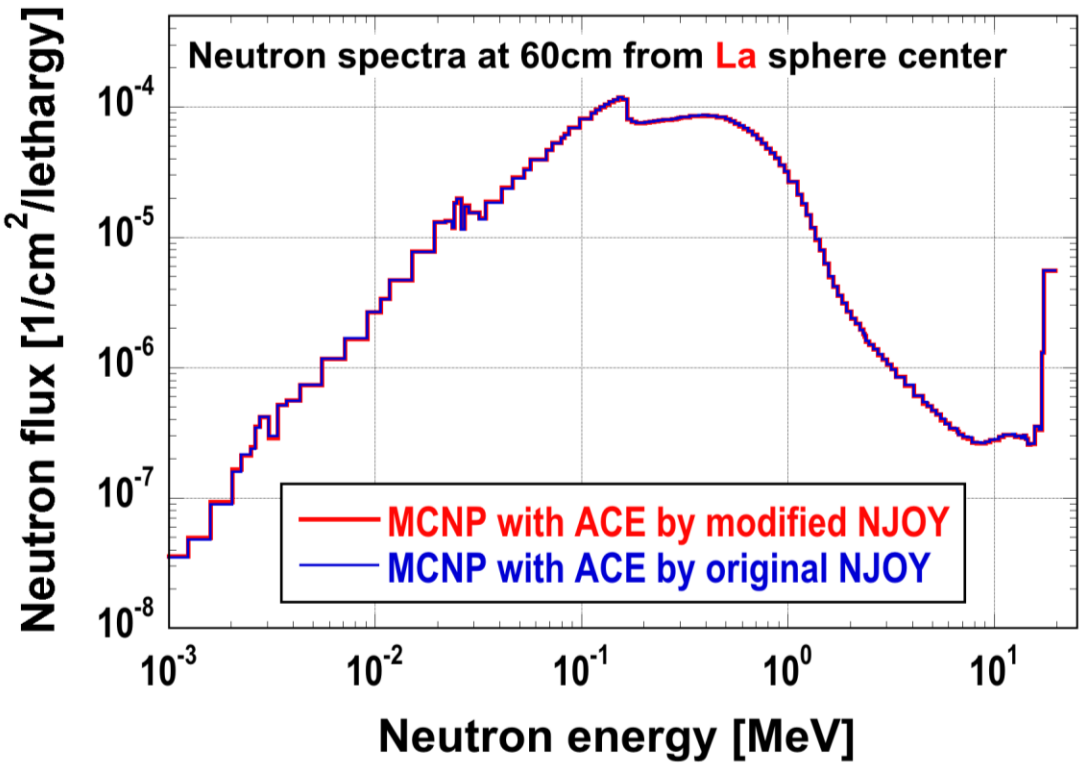
- We performed the same ANISN calculation as the first one with the new MATXS file.



The ANISN calculation with modified MATXS is close to one with MCNP!

Calculation with modified ACE file

- We also produced a new ACE file of FENDL-3.1d with the modified NJOY2016 and performed the same MCNP calculation as the first one with the new ACE file.



ACE files with the modified NJOY do not affect MCNP calculation results.

Concluding remarks

- We encountered a problem in a simple calculation for a La sphere with ANISN and the MATXS file of FENDL-3.1d. We examined reasons of the problem.
- We found out that the self-shielding effect in the unresolved resonance region was large.
- We specified that unrealistic cross sections in the dips between resonances caused the above issue.
- We modified NJOY2016 so as to improve the unrealistic cross sections in the dips between resonances.
- We confirmed that MATXS files with the modified NJOY2016 gave better results.
- ACE files with the modified NJOY did not affect MCNP calculation results.

IAEA patch effects for TRANSX

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Consultants' Meeting on the FENDL Library
for fusion neutronics calculations
15-18 October 2018
IAEA Headquarters, Vienna, Austria

Introduction -(1)

- The TRANSX2.15 code has been used worldwide since 1994 in order to generate macroscopic multigroup libraries with self-shielding correction from MATXS files produced with the NJOY code for shielding analyses.
- IAEA released two unofficial patches generated by Dr. Kazuaki Kosako for TRANSX2.15 for the MATXS file (FENDL/MG-2.0) of Fusion Evaluated Nuclear Data Library (FENDL) version 2.0 in 1998.
- The first patch is for all MATXS files and its effect has not been demonstrated.
- The second patch is only for MATXS files with mixed data types such as FENDL/MG-2.0, which are very rare. TRANSX2.15 cannot process them without the second patch. Thus, the effect of the second patch is trivial.
- Here we focus only on the first patch.

Introduction -(2)

IAEA Patches

Patch 1. to increase the insufficient array size (2 lines)

```
*d up14.4 [maxds=5+5*(nl+1)]
      maxds=5+12*(nl+1)
```

Patch 2. to allow for simultaneous processing of MG files for different materials out of which some contain thermal scattering data and others do not (30 lines)

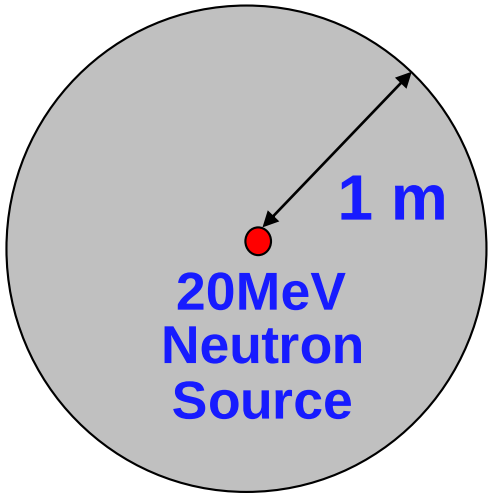
```
*/ 1998/08/10
*/ modify for processing the matxs files
with different ntypes
*i transx.674
      ntypes=0
*d transx.707,708
      if (ntypes.eq.0) then
        ntypes=ntype
        do 235 i=1,ntype
 235 htypnm(i)=ha(l1h1+npart+i)
      elseif (ntype.ne.ntypes) then
        do 236 i=1,min(ntype,ntypes)
  236   if (htypnm(i).ne.ha(l1h1
     &   +npart+i)) call error(
     &   'inconsistent hollerith
     &   identification for data type')
        if (ntype.gt.ntypes) then
          do 237 i=ntypes+1,ntype
  237     htypnm(i)=ha(l1h1+npart+i)
          ntypes=ntype
        endif
      endif
      nwds=(npart+20+nmat)*mult+npart+2
     & *20+2*nmat
*i up10.91
      nwds=6
      irec=2
      call reed(nin,irec,a(l1),nwds,0)
      ntype=ia(l1+1)
*i up10.122
      nwds=6
      irec=2
      call reed(nin,irec,a(l1),nwds,0)
        ntype=ia(l1+1)
```

Introduction -(3)

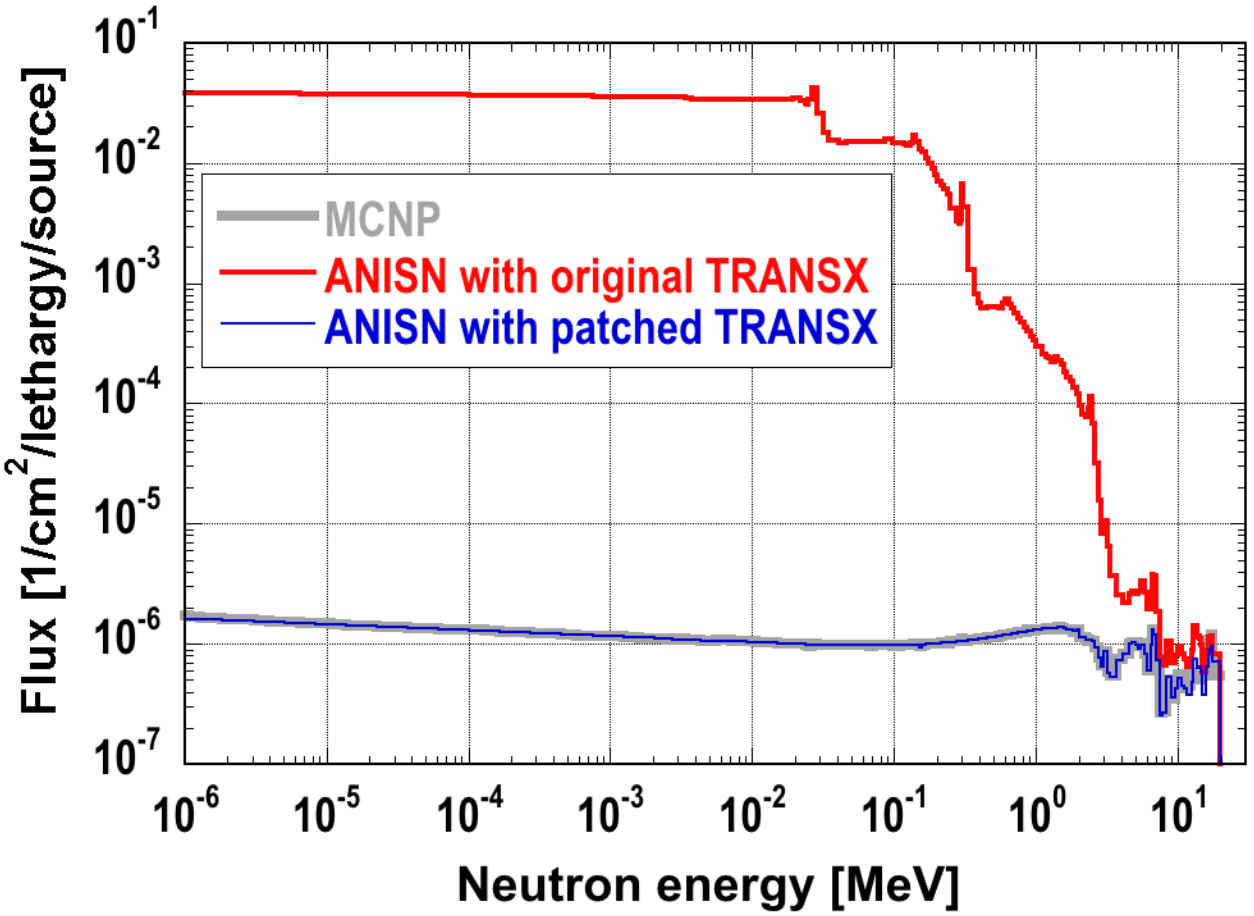
- Dr. Hideo Kitagawa announced a similar issue as the first patch to Japanese nuclear data community in 2004.
- The ENEA Bologna group also released a similar patch with MATJEFF31.BOLIB in 2009.
- However, no one including us has demonstrated effects of this patch.
- Recently we found out that self-shielding corrected multigroup libraries produced with the original TRANSX2.15 caused extremely large neutron fluxes and the first patch solved this problem.
- Unfortunately, the first patch has not been known well because it is not included in the official TRANSX2.15 release. Thus, we present this issue in order to alert TRANSX2.15 users widely that the first patch is essential.

Calculation Method

- In order to examine effects of the first patch, we calculated neutron spectra inside a sphere of 1 m in radius with an isotropic neutron source of 20 MeV at the center with the ANISN code, changing a material of the sphere.
- The macroscopic multigroup libraries with self-shielding correction of FENDL-3.1d were produced from the FENDL-3.1d MATXS file (neutron 211 group) by using TRANSX2.15 with and without the first patch.
- For comparison, the neutron spectra were calculated with the MCNP6.1 code and the FENDL-3.1d ACE file.
- The three calculated neutron spectra are compared to demonstrate effects of the patch.



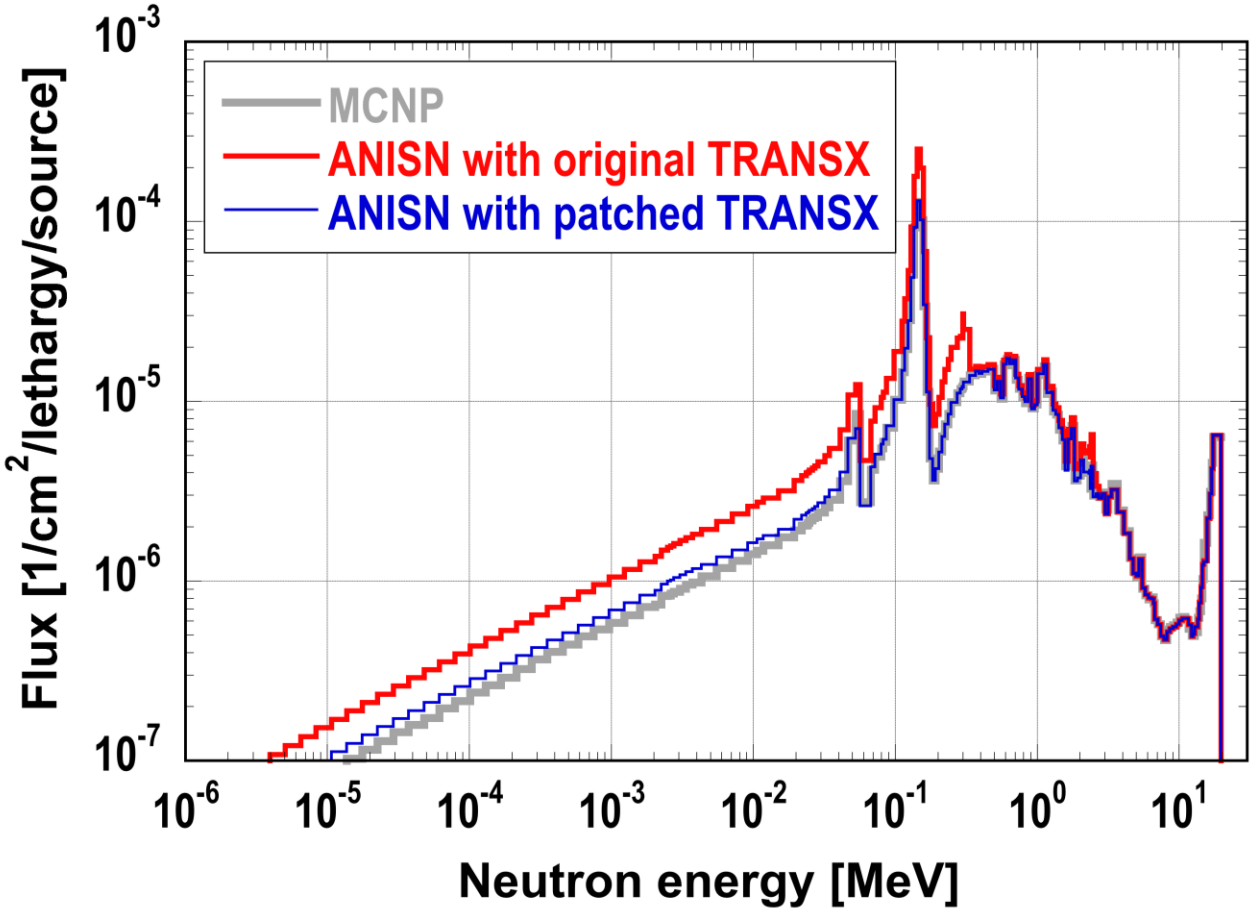
Calculated Neutron Spectra -(1)



Calculated neutron spectra at 60 cm from graphite sphere center

The neutron spectrum with ANISN and original TRANSX2.15 is much larger than that with MCNP6.1.

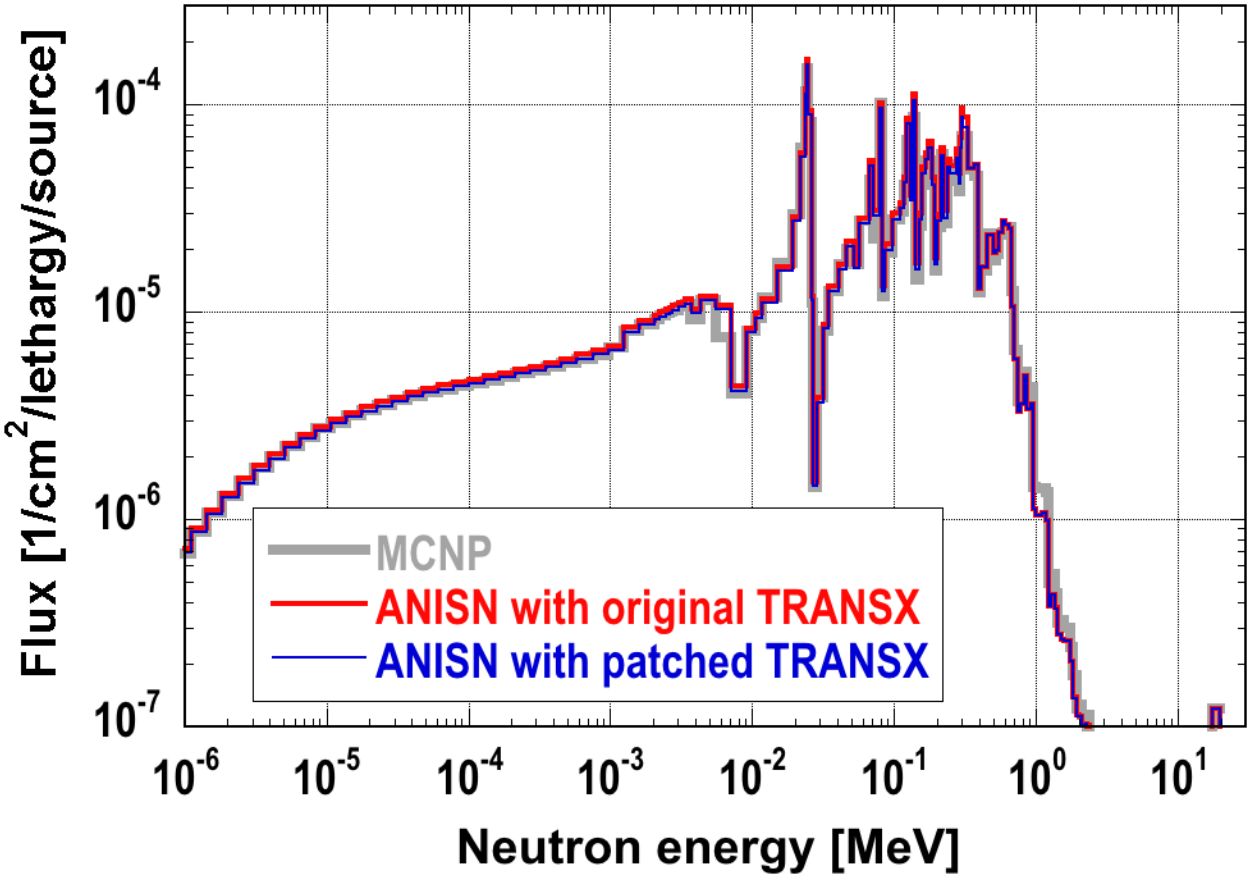
Calculated Neutron Spectra -(2)



Calculated neutron spectra at 60 cm from silicon sphere center

The neutron spectrum with ANISN and original TRANSX2.15 is larger than that with MCNP6.1.

Calculated Neutron Spectra -(3)

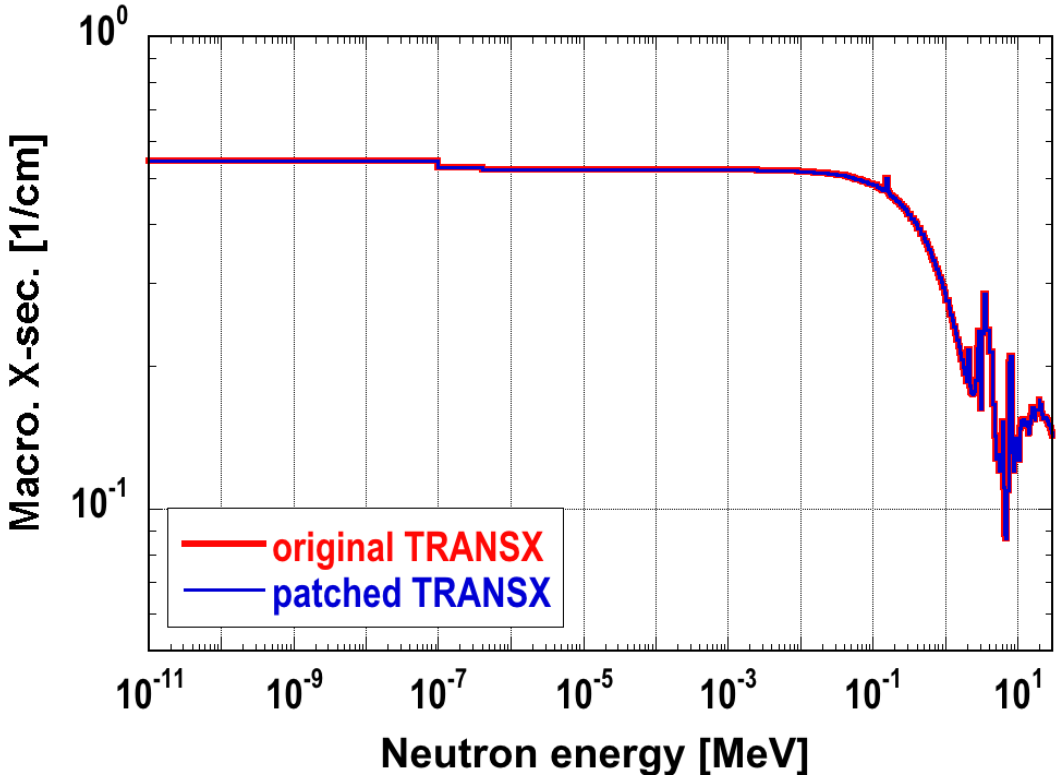


Calculated neutron spectra at 60 cm from iron sphere center

The neutron spectrum with ANISN and original TRANSX2.15 is almost the same as that with MCNP6.1.

Comparison of macro cross sections -(1)

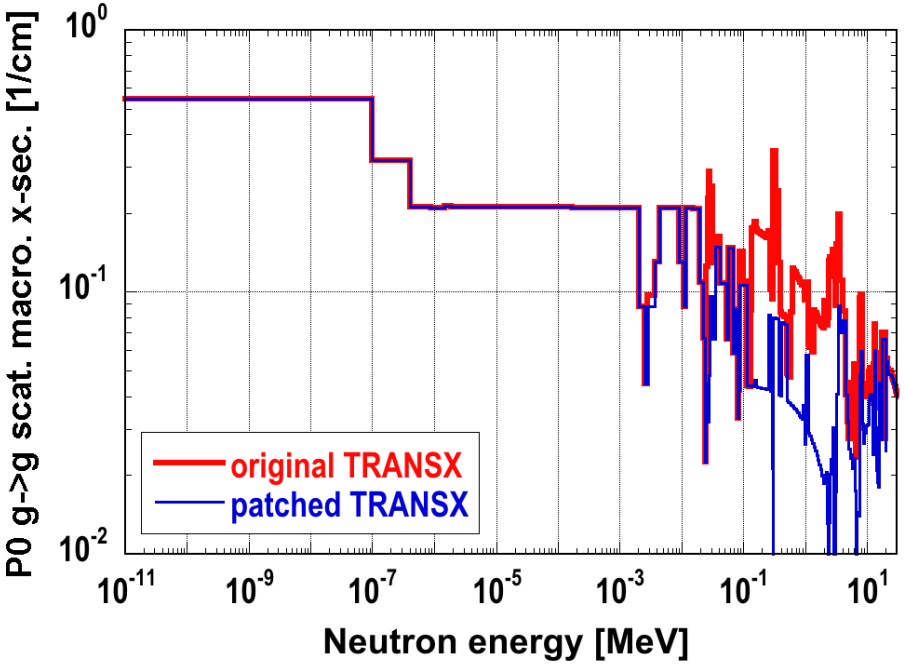
- The effect of the patch is very large in the graphite sphere.
- We compare macroscopic cross sections for graphite sphere produced with original and patched TRANSXs.

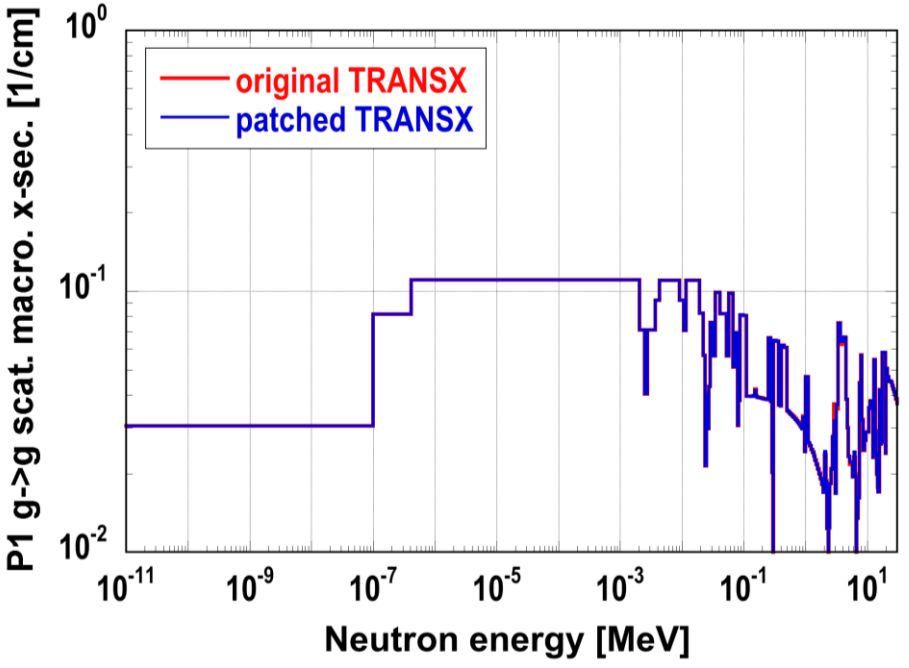


Macroscopic total cross sections for graphite sphere

Same!

Comparison of macro cross sections -(2)





(a) P0 **(b) P1**

Macroscopic in-group scattering cross sections for graphite sphere

Different! *Almost same!*

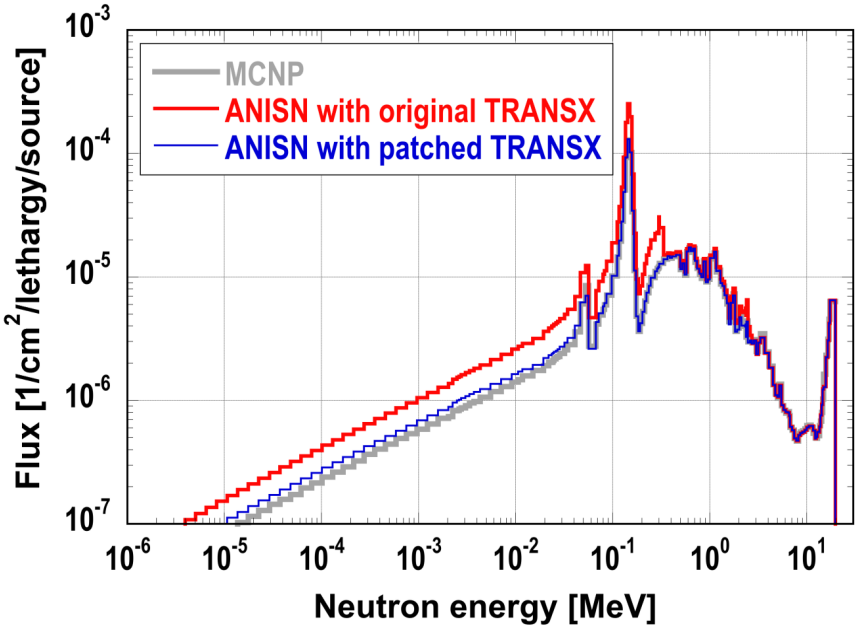
It is considered that the different P0 in-group scattering cross section data lead to the different neutron spectra.

TRANSX code check -(1)

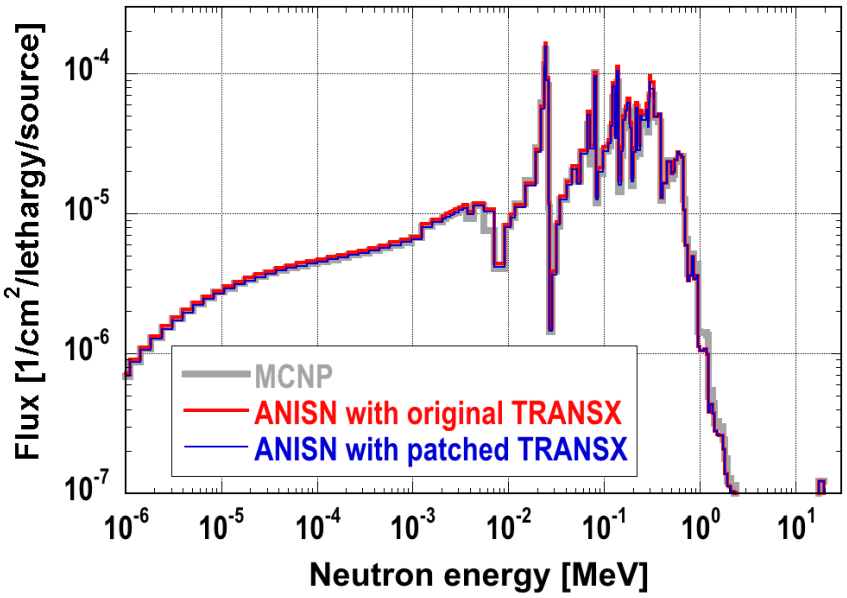
- Why are the macroscopic P0 in-group scattering cross section data different?
- We examined the source program of TRANSX in detail.
- The first patch replaces "maxds=5+5*(nl+1)" to "maxds=5+12*(nl+1)".
- "maxds=5+5*(nl+1)" is introduced in the official TRANSX up14 patch in order to generalize the down-scatter limit due to elastic scattering for self-shielding, which is described as a comment in the official TRANSX up14 patch.
- "maxds=5+5*(nl+1)" means that the down-scatter group number is 5, but 11 down-scatter groups at maximum are required for the MATXS file of FENDL-3.1d ^{12}C.
- The first patch extends the down-scatter group number from 5 to 12.

TRANSX code check -(2)

- The first patch is more effective for lighter nuclei, because the larger down-scatter group number is necessary for lighter nuclei.
- Thus, the effect of the first patch is not so large in the silicon sphere and is very small in the iron sphere.



(a) Silicon

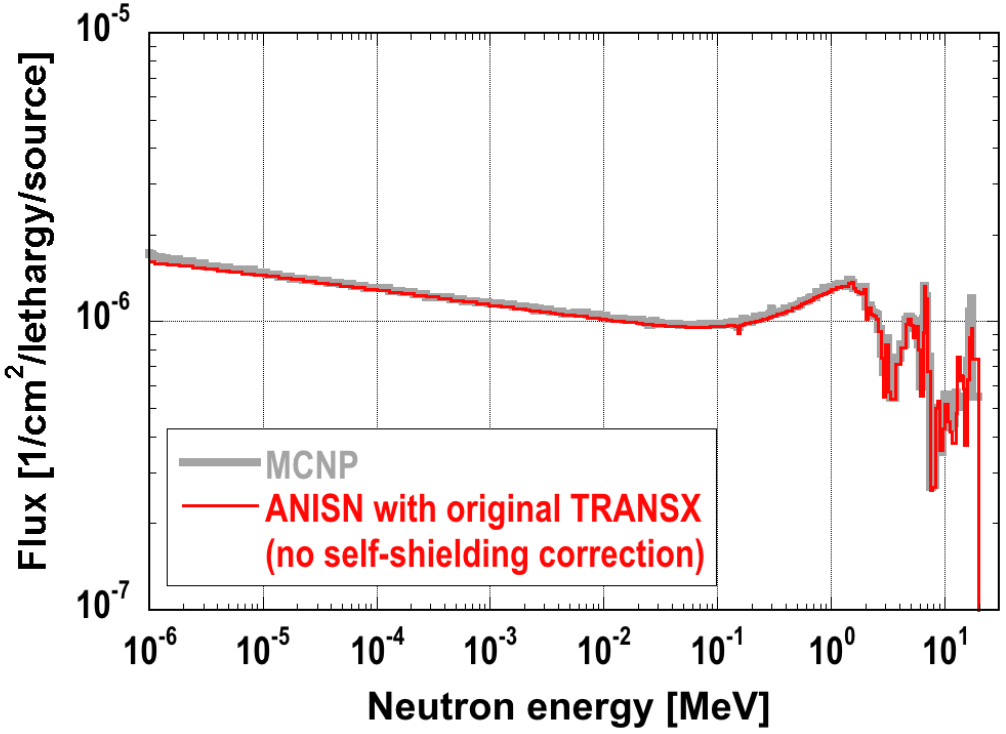


(b) Iron

Calculated neutron spectra at 60 cm from sphere center

TRANSX code check -(3)

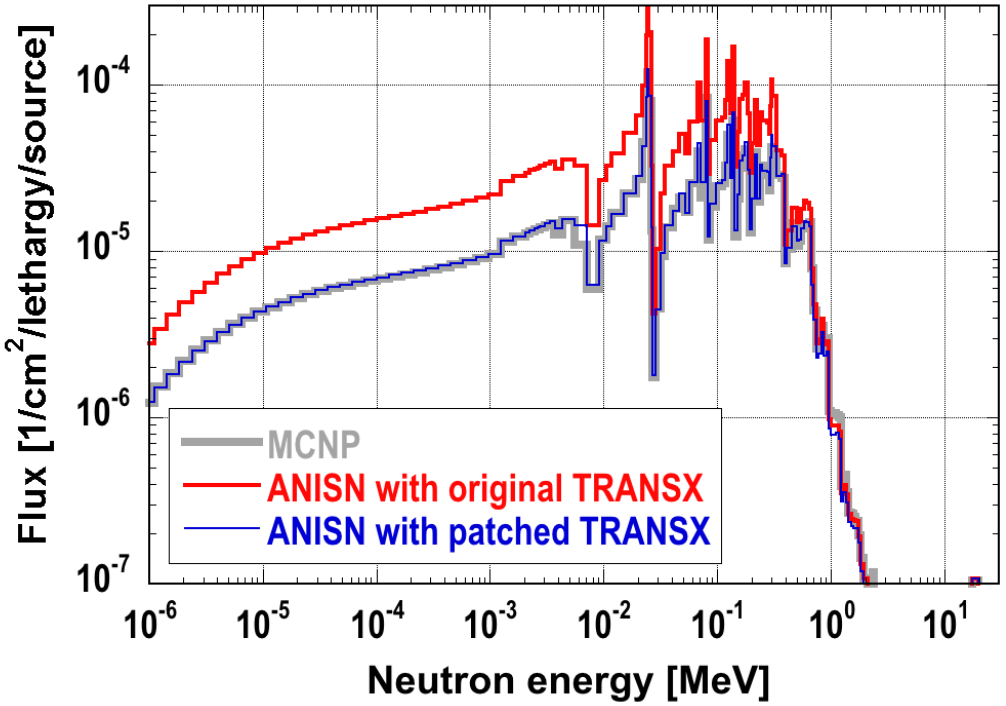
- The TRANSX check indicates the first patch is necessary only in the case of self-shielding correction, while it is not in case of no self-shielding correction.
- For example, the first patch is not necessary for the graphite sphere because the self-shielding effect is very small.



Calculated neutron spectra at 60 cm from graphite sphere center

TRANSX code check -(4)

- However the self-shielding correction is necessary, for example, in the carbon steel (carbon : 1 wt %) sphere.

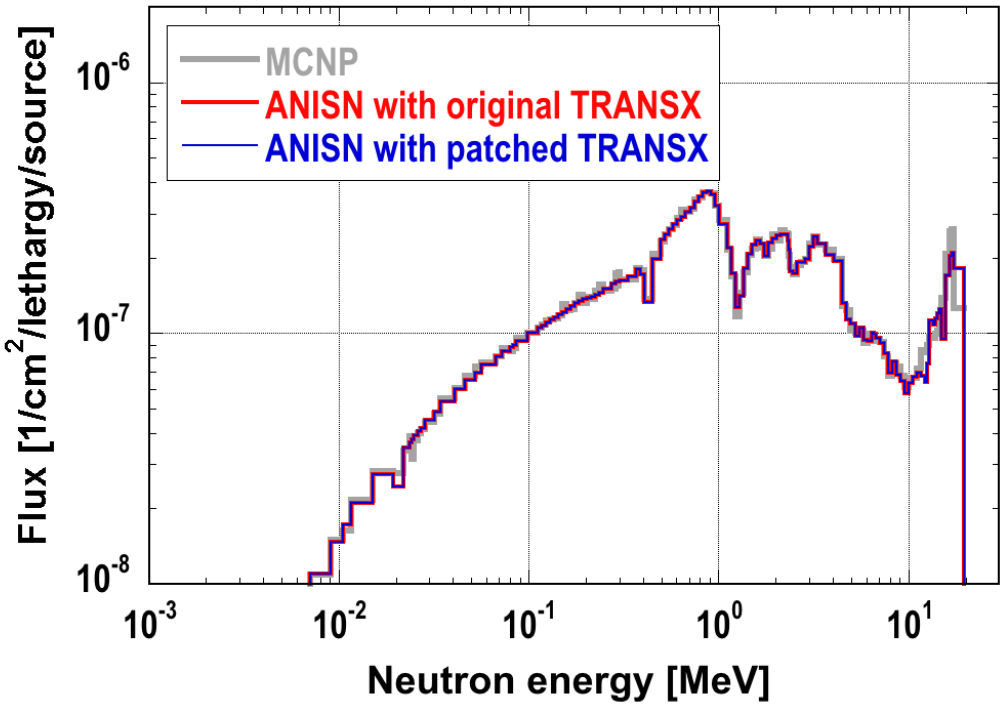


Calculated neutron spectra at 60 cm from carbon steel (carbon : 1 wt%) sphere center

- The first patch is also essential for carbon in the carbon steel.

TRANSX code check -(5)

- **TRANSX2.15 does not apply the self-shielding correction to nuclei with atomic mass number of smaller than 11.5. Thus, the first patch does not matter for nuclei with atomic mass number of smaller than 11.5.**

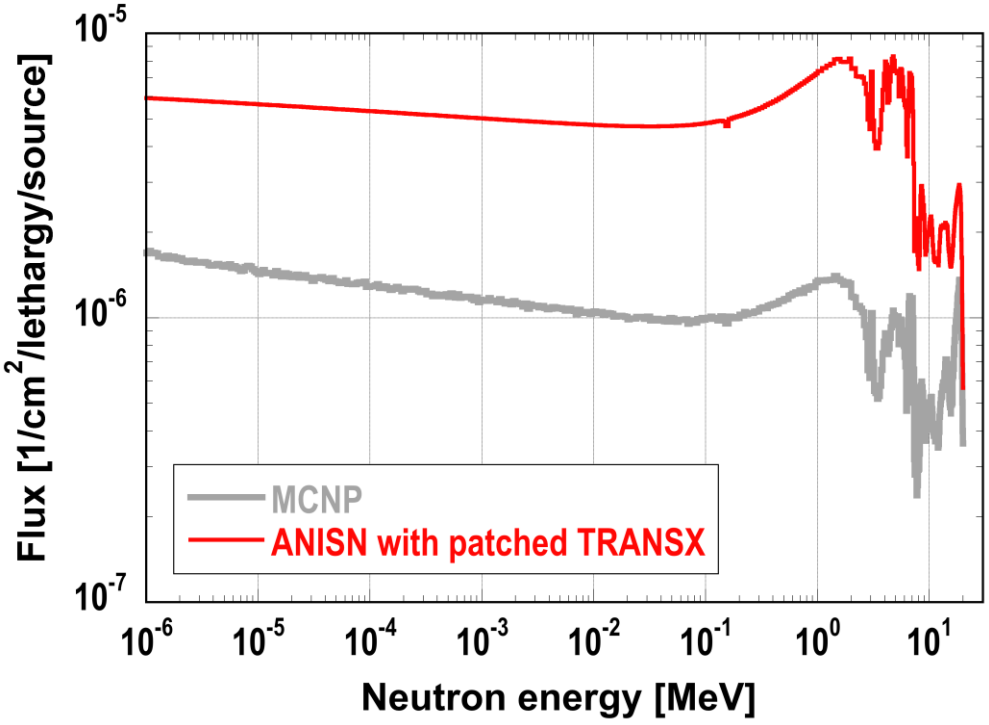


Calculated neutron spectra at 60 cm from boron (atomic mass number < 11.5) sphere center

MATXS files with larger neutron group number -(1)

- The first patch is enough for the MATXS file of FENDL-3.1d, where the neutron group number is 211.
- However, it is not enough for MATXS files with a larger neutron group number.
- We produced a MATXS file of FENDL-3.1d with the SAND-IIA group structure (neutron group number : 640) by using NJOY2016 and calculated neutron spectra inside the graphite sphere of 1 m in radius with an isotropic neutron source of 20 MeV at the center by using ANISN and MCNP6.1.

MATXS files with larger neutron group number -(2)

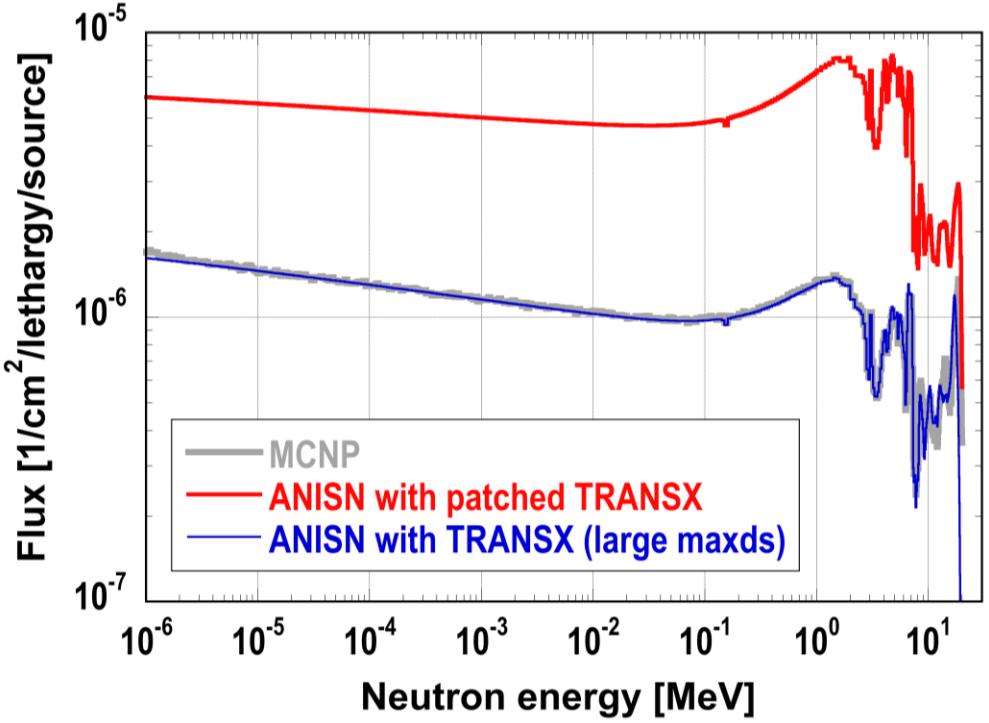


Calculated neutron spectra at 60 cm from graphite sphere center

Even the ANISN result with the patched TRANSX2.15 code is different from the MCNP one.

MATXS files with larger neutron group number -(3)

- Thus, we also carried out a new ANISN calculation with a multigroup library produced by TRANSX2.15, where "maxds" is enough large, i.e., maxds=5+64*(nl+1).



Calculated neutron spectra at 60 cm from graphite sphere center

If users adopt larger neutron group number for MATXS files, they should modify "maxds" adequately.

Concluding remarks

- We examined effects of the first one of IAEA unofficial patches for the TRANSX2.15 code with a simple calculation model and the MATXS file of FENDL-3.1d.
- The followings were found out.
  1) Large neutron fluxes appear in calculation results with self-shielding corrected multigroup libraries produced by the original TRANSX2.15 code. This effect is larger for lighter nuclei.
  2) The first IAEA patch solves this problem. It should be modified for MATXS files with a larger neutron group number.
- The first IAEA patch or modified one should be included in the official TRANSX2.15 release, for users to obtain correct results.

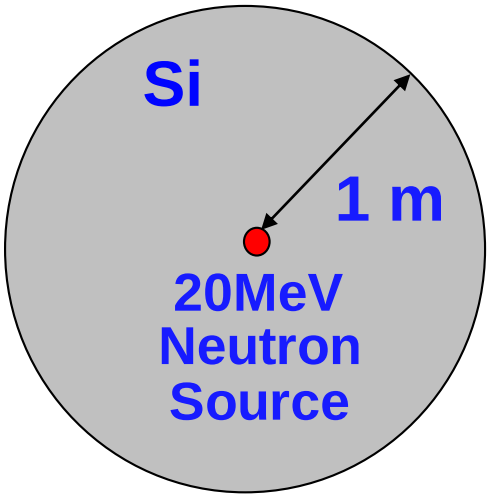
Appendix 1

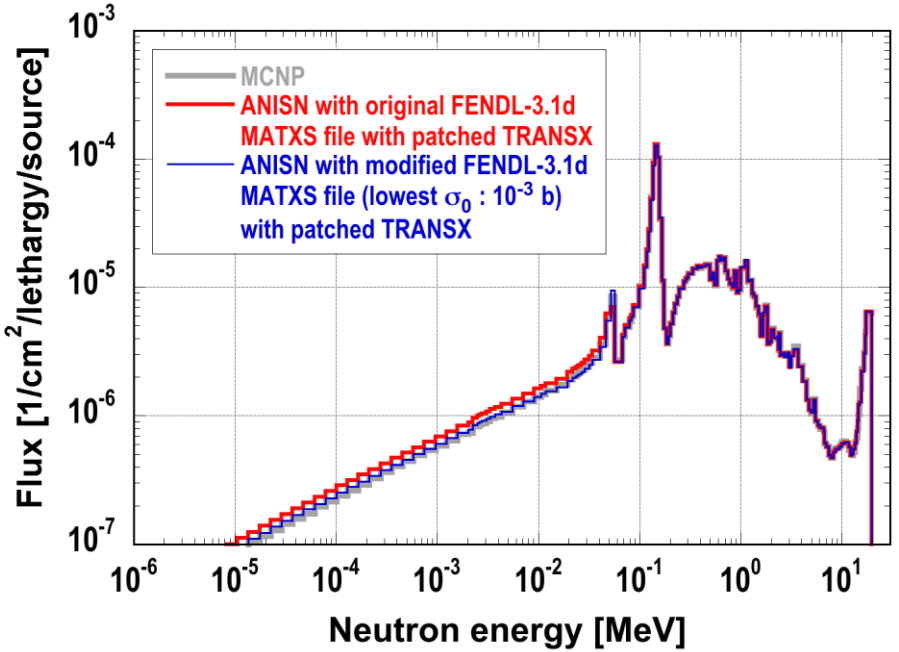
- The MATXS file of FENDL-3.1d ^{56}Fe caused an error in being read by the original TRANSX2.15 code.
- We specified the reason. Data in MATXS files are stored in unit of 5000 ("maxw") data. The data size is checked in TRANSX2.15, but this check is not correct when the data size is just equal to 5000 such as the MATXS file of FENDL-3.1d ^{56}Fe, which is a rare case.
- The patch for this issue is as follows.

```
*d transx.1364 [if (nwds+nk.gt.maxw) go to 230]
      if (nwds+nk.ge.maxw) go to 230
*d transx.2298 [if (nwds+nk.gt.maxw) go to 215]
      if (nwds+nk.ge.maxw) go to 215
```

Appendix 2

- The background cross sections in the MATXS file of FENDL-3.1d are not always adequate; for example,
  - ^{23}Na, $^{24-26}$Mg, ^{27}Al : only infinite dilution
  - $^{28-30}$Si : the lowest background cross section is 1 b
- Thus the self-shielding correction for these nuclei is not sufficient.





Calculated neutron spectra at 60 cm from silicon sphere center

Comments on TENDL-2017

Japan Atomic Energy Agency
Chikara Konno

Contributor : Saerom Kwon (QST)

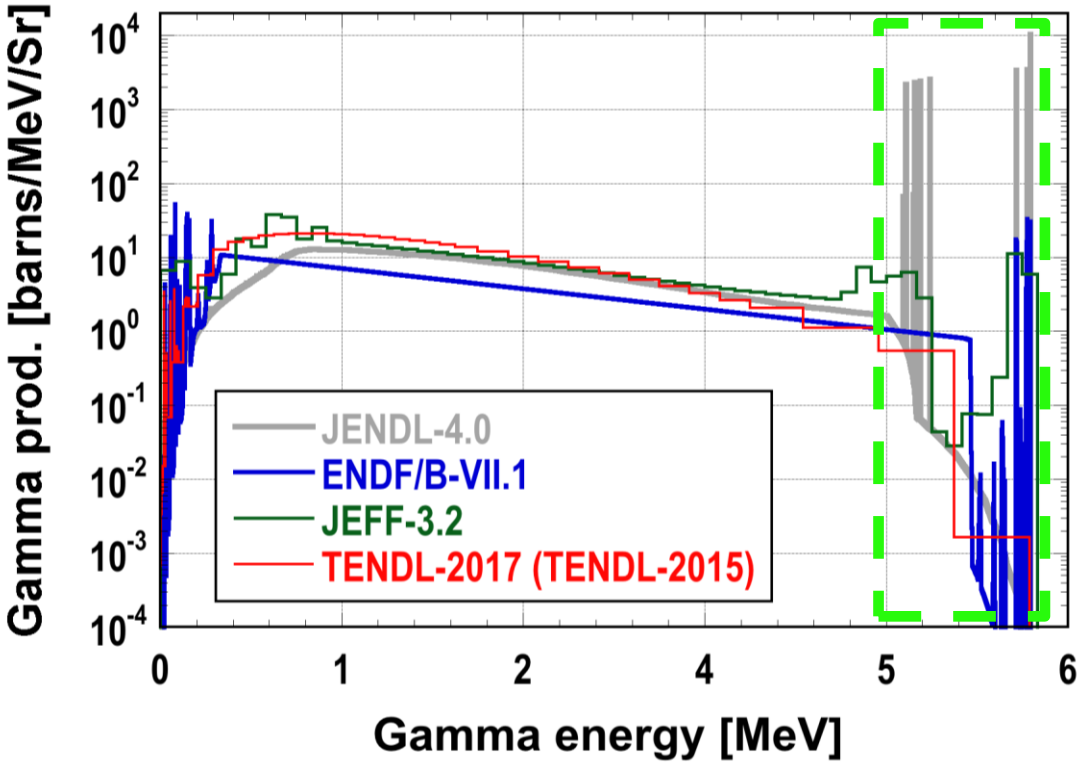
Consultants' Meeting on the FENDL Library
for fusion neutronics calculations
15-18 October 2018
IAEA Headquarters, Vienna, Austria

Introduction

- FENDL-3.1d adopted a lot of data from TENDLs. It is expected that the next FENDL will also adopt a lot of data from the latest TENDL.
- Thus we examined the latest TENDL, TENDL-2017. We found out two problems in TENDL-2017.
  - Secondary neutron spectra for mt=5 at 30 MeV (the next presentation by Dr. Kwon)
  - High-energy gamma data in secondary gamma spectra of the capture reaction
- Here we present the second issue.

High-energy gamma data issue

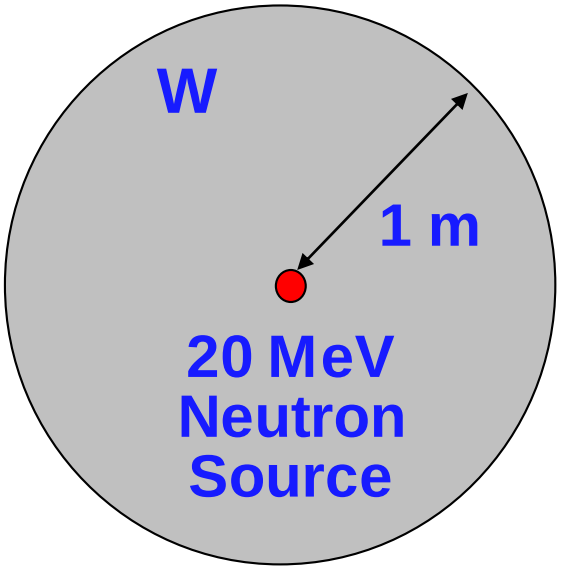
- The secondary gamma spectra from the capture reaction of a lot of nuclei in TENDL-2017 have fewer high-energy gamma peaks than those in other nuclear data libraries. (e.g. gamma peaks above 5 MeV in the below figure)



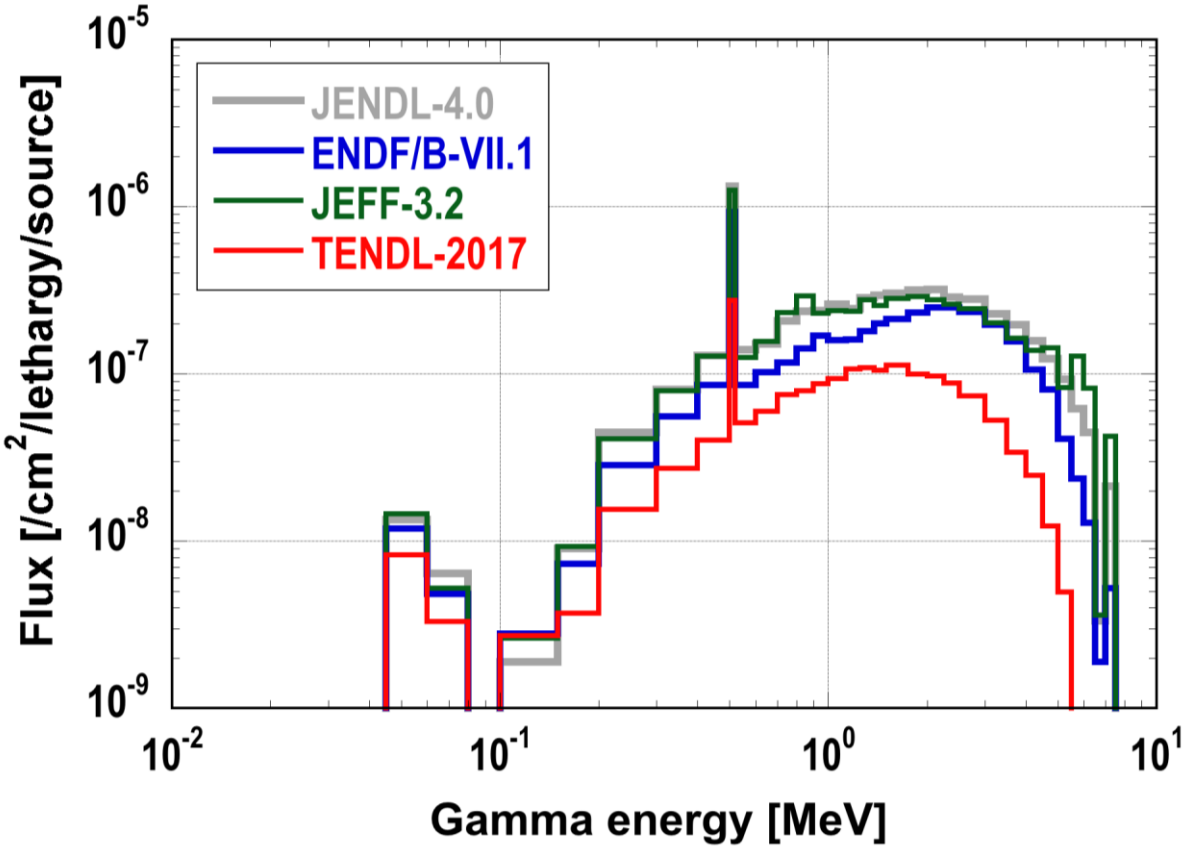
Secondary gamma spectra from capture reaction of ^{184}W in neutron energy of 10^{-5} eV

Gamma spectra -(1)

- This issue causes smaller gamma fluxes in neutron-gamma coupling calculations than those with other nuclear data libraries.
- In order to demonstrate this effect, gamma spectra inside a tungsten sphere of 1 m in radius with an isotropic neutron source of 20 MeV at the center were calculated with MCNP by using JENDL-4.0, ENDF/B-VII.1, JEFF-3.2 and TENDL-2018.



Gamma spectra -(2)

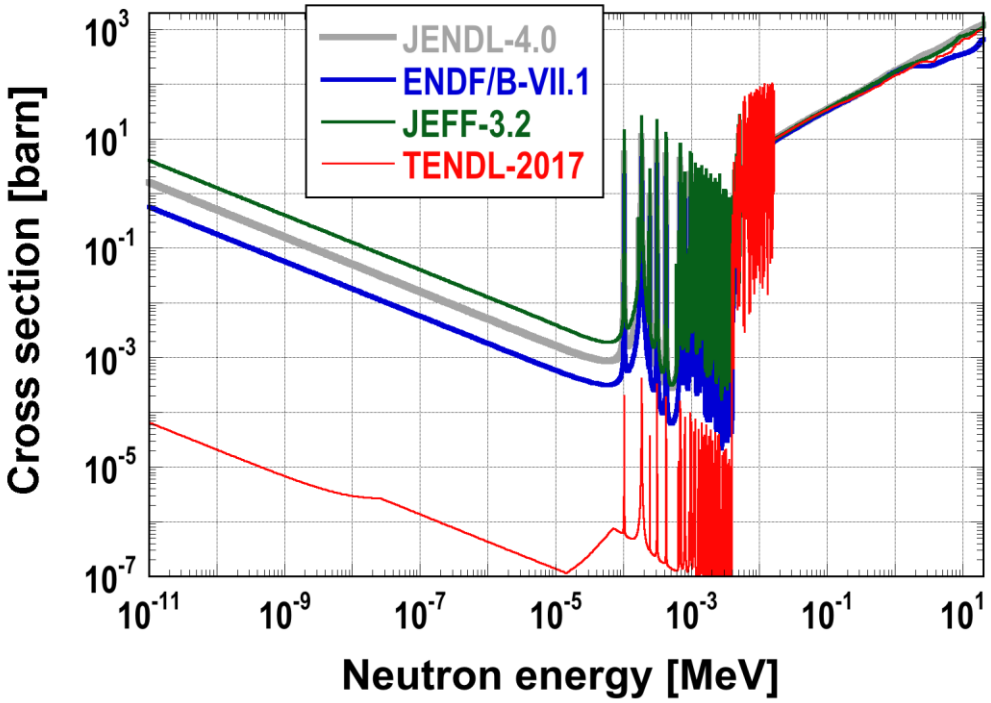


Gamma spectra at 60 cm from tungsten sphere center

- The calculated gamma spectrum with TENDL-2017 is smaller than those with the other libraries and is shifted to lower gamma energy.

DPA cross section

- This issue also causes much smaller DPA cross-section data, particularly for nuclei with a larger displacement energy such as tungsten (displacement energy : 90 eV) below ~ 1 keV than those of other nuclear data libraries.
- This is because only higher energy gammas contribute to DPA cross-section data due to the larger displacement energy.



DPA cross-section of ^{184}W in ACE files

Concluding remarks

- We examined TENDL-2017.
- We found out that secondary gamma spectra from the capture reaction of a lot of nuclei in TENDL-2017 had fewer high-energy gamma peaks than those in other nuclear data libraries.
- This problem causes smaller gamma fluxes in neutron-gamma coupling calculations than those with other nuclear data libraries.
- This problem also causes much smaller DPA cross-section data, particularly for nuclei with a larger displacement energy such as tungsten (displacement energy : 90 eV) below ~ 1 keV than those of other nuclear data libraries.

Appendix 1

- **Two ACE files of TENDL-2017 released from the TENDL official site are different.**
  - **tar file of 556 nuclei (good)**
  - **single file of each nucleus (no p-table, no secondary gamma)**
- **No information for differences between the two ACE files in the TENDL home page.**

tar & ACE files

Last update: 26 April 2018

The TENDL-2017 library can be retrieved with tar (*.tgz) files for each sub-library. To untar the files, use the command: tar -zxvf.

Mirror pages: here (cloud servers).

1. Neutron

   2813 ENDF files (3.1 Gb),
   2807 EAF files (175 Mb), and 2807 EAF covariance files (10 Mb).
   List of MAT numbers: iso-mat.tendl-n.txt.

   List of 556 ZAID numbers for ACE: Ace-Readme.tendl17c.txt.
   556 ACE files files (2.1 Gb),

TENDL-2017 Nucl

Neutron sub-library for

Tabulated data (fast neutron range)

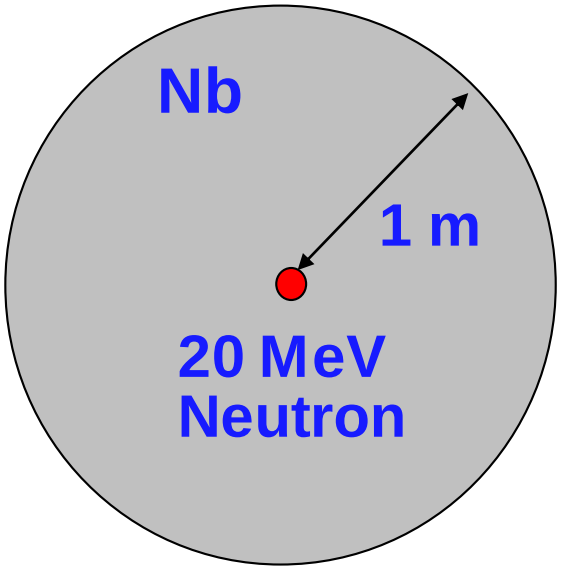
1. Tabular elastic angular distributions (En - angle - cross section)
2. Tabular (n,inl_1) angular distributions (En - angle - cross section)
3. Tabular gamma-ray intensities (En - Eg - cross section)
4. Tabular residual cross sections (En - Residual product - cross section)
5. Tabular spectra (En - Eout - particle - cross section)
6. Tabular total and partial cross sections (En - cross section)

Evaluated formatted data (i.e. ENDF)

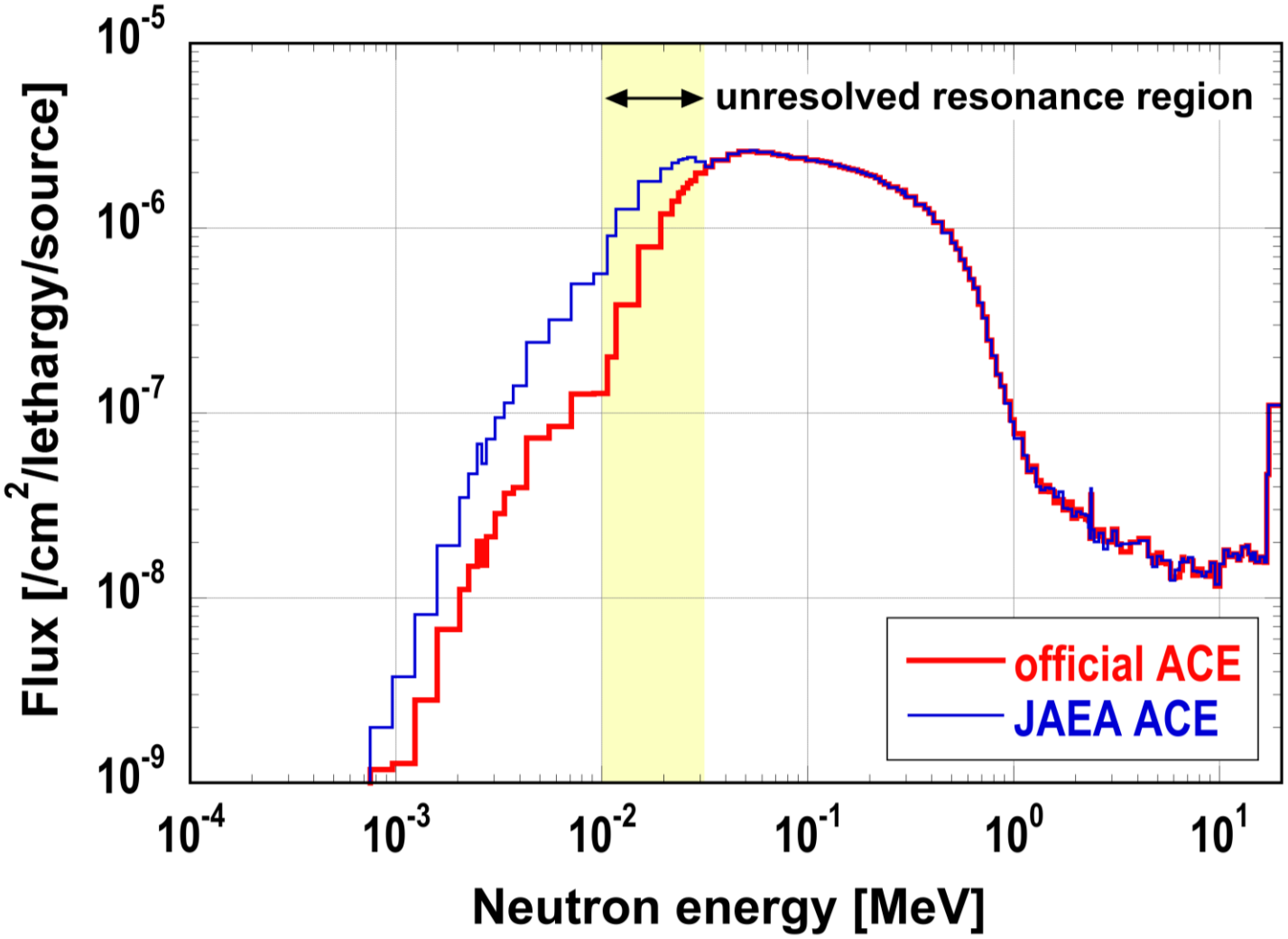
1. The TENDL file
2. Pointwise cross sections at 293 K (pendf)
3. ACE file at 293 K (ace.gz and xsdir)
4. Special ENDF file with MF32c and MF12/MT102 (so-called s20 file)
5. EAF file (European Activation File) and associated covariances
6. ACF file (Activation File)

Appendix 2 -(1)

- A lot of TENDL-2015 files (2513 nuclei) have unresolved resonance data.
- However there are no probability table (p-table) data of unresolved resonances in the official T15n ACE files except for three nuclei (^{235}U, ^{235m}U and ^{238}U).
- Thus self-shielding correction in the unresolved resonance region is incomplete if most of the official ACE files are used.
- In order to demonstrate this effect, neutron spectra were calculated with MCNP by using the official (without p-table data) and JAEA ACE (with p-table data) files. The calculation model was a niobium sphere of 1 m in radius. The sphere had an isotropic neutron source of 20 MeV at the center.



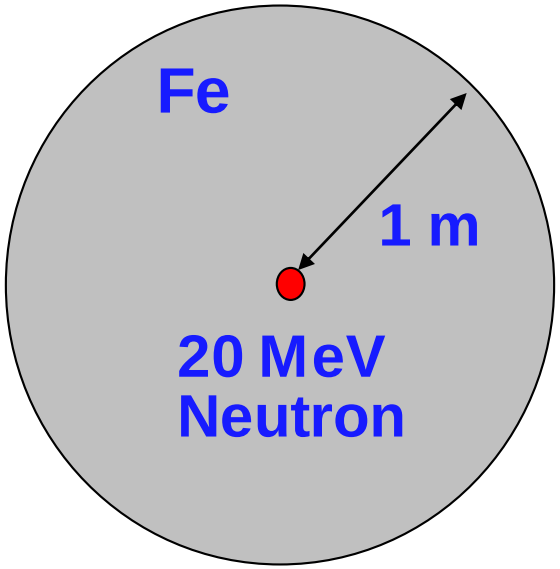
Appendix 2 -(2)



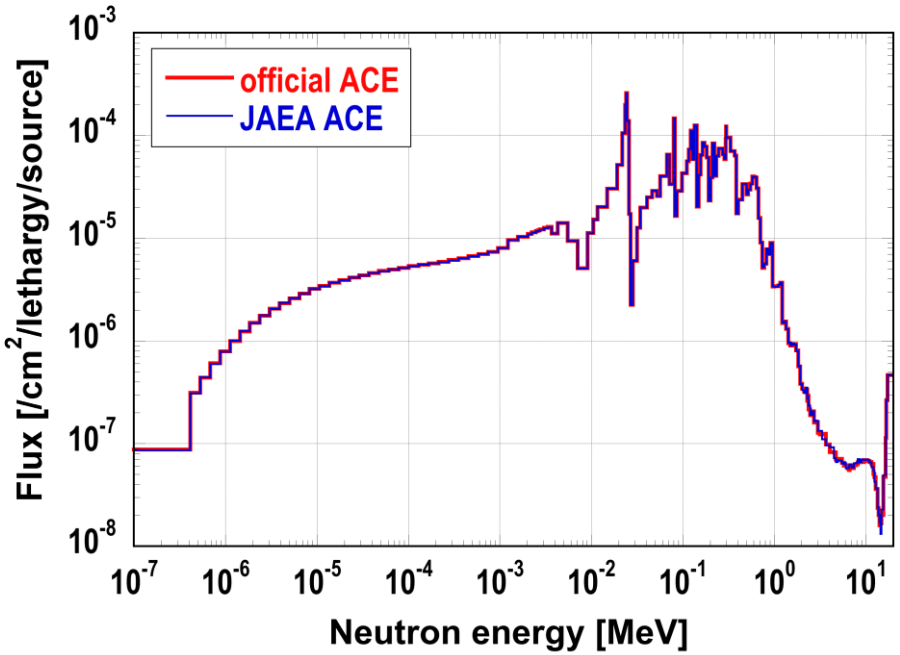
Neutron spectra at 50 cm from niobium sphere center

Appendix 3 -(1)

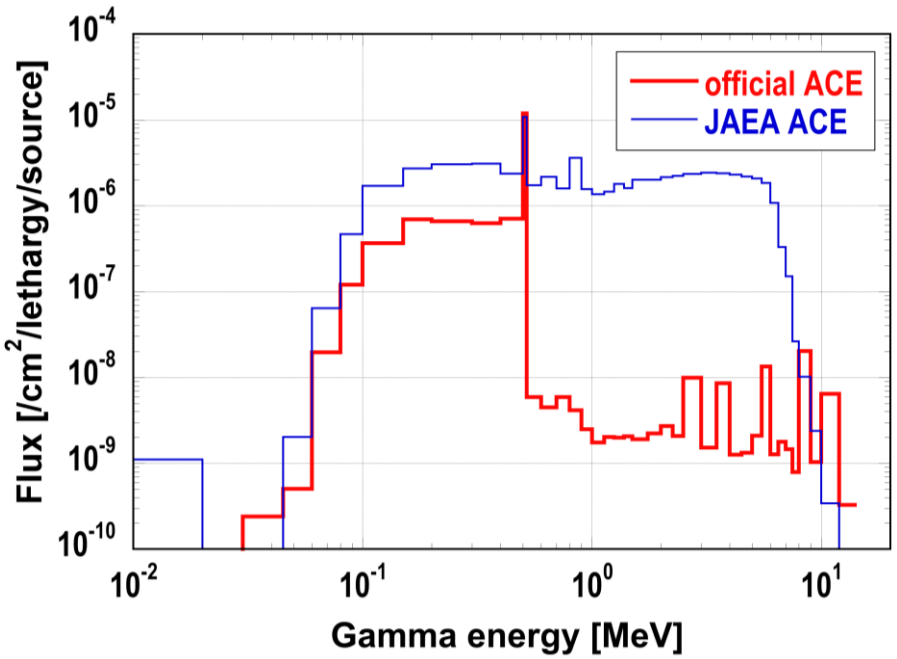
- The secondary gamma data are required in neutron-gamma coupling calculations.
- However there are no gamma production data in the official TENDL-2015 ACE files except for 13 nuclei (^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{12}C, ^{14}N, ^{15}N, ^{16}O, ^{19}F and ^{239}Pu).
- Thus secondary gammas are not produced in neutron-gamma coupling MCNP calculations with the official ACE files.
- In order to demonstrate this effect, neutron and gamma spectra inside an iron sphere of 1 m in radius with an isotropic neutron source of 20 MeV at the center were calculated with MCNP by using the official (without gamma production data) and JAEA ACE (with gamma production data) files.



Appendix 3 -(2)



Neutron spectra at 50 cm from iron sphere center



Gamma spectra at 50 cm from iron sphere center

- The official ACE files have no gamma production data, but the MCNP calculation with the official ACE file produced gamma.
- We specified the reason; MCNP misidentifies and misuses particle production data (mt=5 data in TENDL-2015) in the official ACE file as gamma production data.

Appendix 3 -(3)

- We guessed the reason of no gamma production data in the official ACE files.
  - "iopp" (input parameter for "detailed photons", 0=no, 1=yes) in ACER input of NJOY2012 was set to 0, which requires obsolete 20x30 photon matrix data. However the obsolete 20x30 photon matrix data were not supplied in the NJOY processing. Thus only gamma production cross section data were included in the official ACE files, but outgoing photon energy data were not included.
  - It is not known why iopp=0 was used in processing of TENDL-2015.
- This issue also occurs in the official ACE files of TENDL-2015 proton, deuteron, triton, He-3, and alpha sub-libraries.

Thank you for your attention!