Important comments on TENDL-2015

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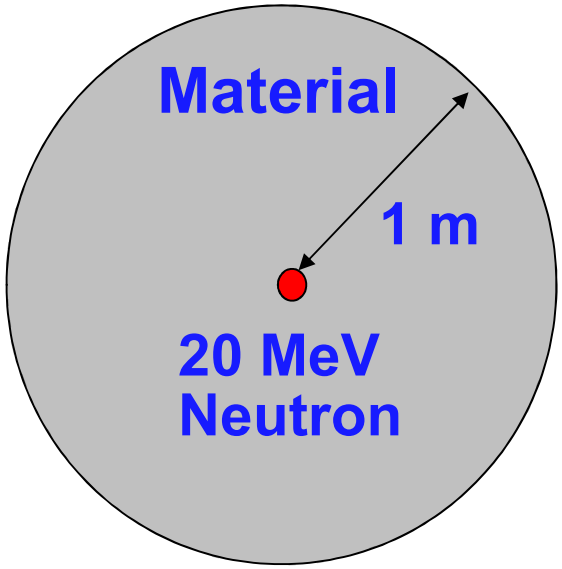
Contents

Introduction

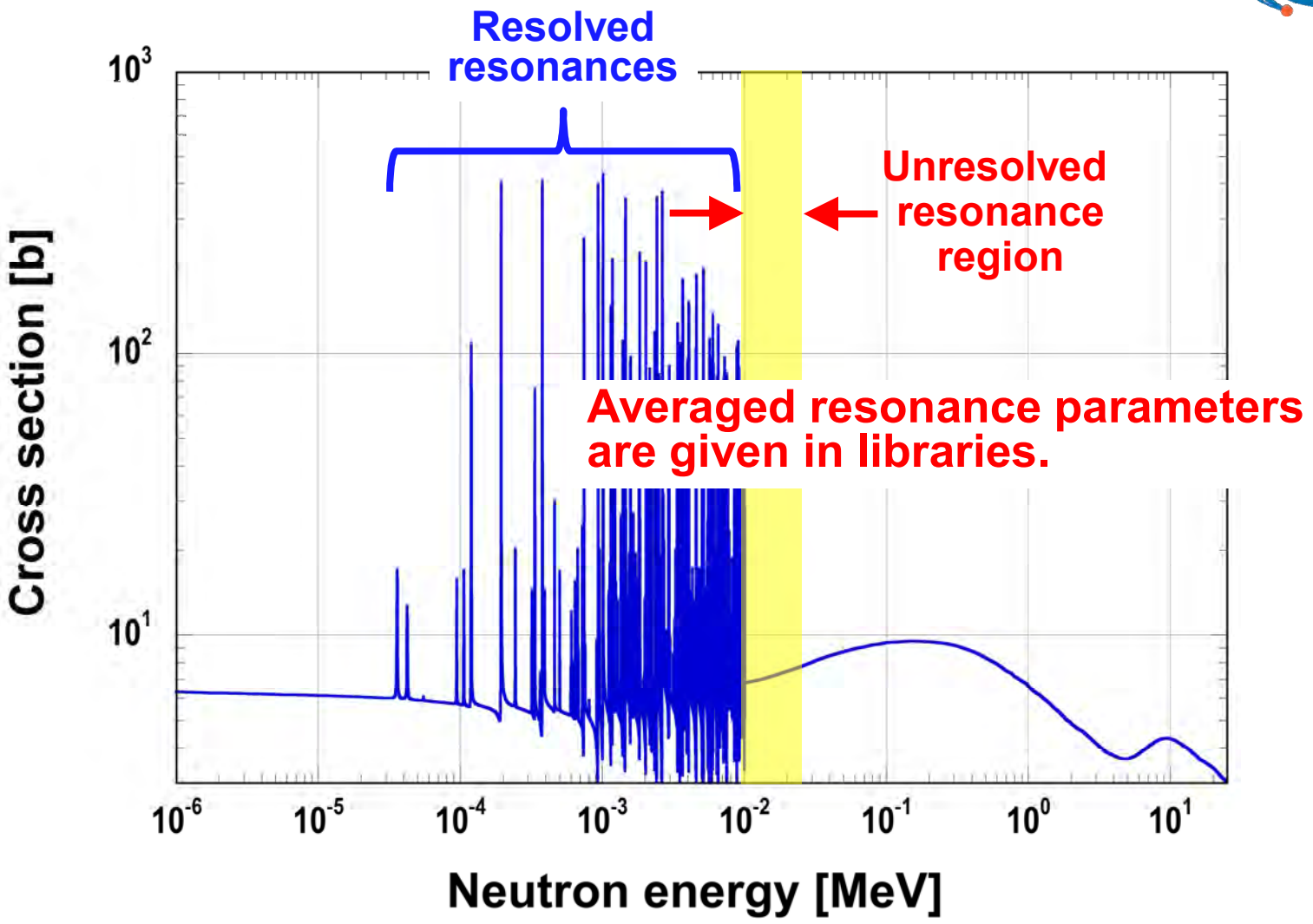
- TENDL-2015 up to 200 MeV has been used as one of the standard nuclear data libraries.
- Last year I started to use the TENDL-2015 neutron sub-library (called as "T15n") and its official ACE (A Compact ENDF) file and found the following issues.
  1. ACE file issues
     - No probability tables for unresolved resonance
     - No gamma production data
  2. T15n file issues
     - No high-energy gamma peaks in the capture reaction in low neutron energy
     - Inconsistent file 6 data of the (n,p) and (n,α) reactions in low neutron energy
- I explain these issues and their effects in detail.

Method

- T15n and its ACE file were checked.
- I produced ACE files (called as "JAEA ACE") of several nuclei in T15n with NJOY2012.50 adequately for comparison.
- Neutron and/or gamma spectra were calculated with MCNP by using the official and JAEA ACE files and compared each other. I adopted a very simple calculation model; a sphere of 1 m in radius.
  This sphere had an isotropic neutron source of 20 MeV at the center.
- KERMA and DPA data in the official and JAEA ACE files were extracted and compared.
- If necessary, the T15n files were modified temporarily.



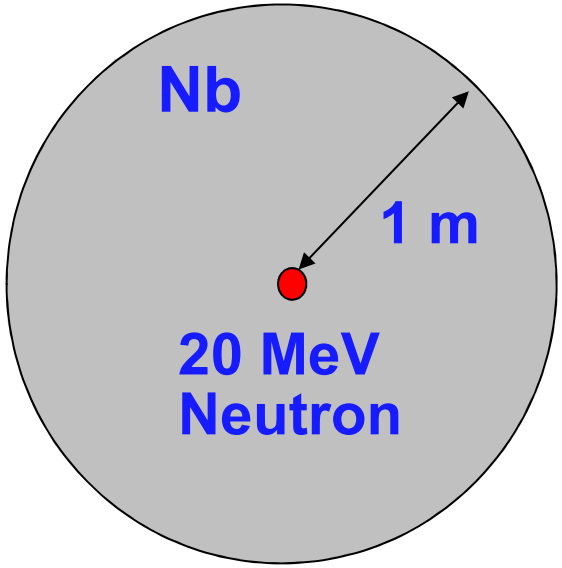
What is the unresolved resonance?



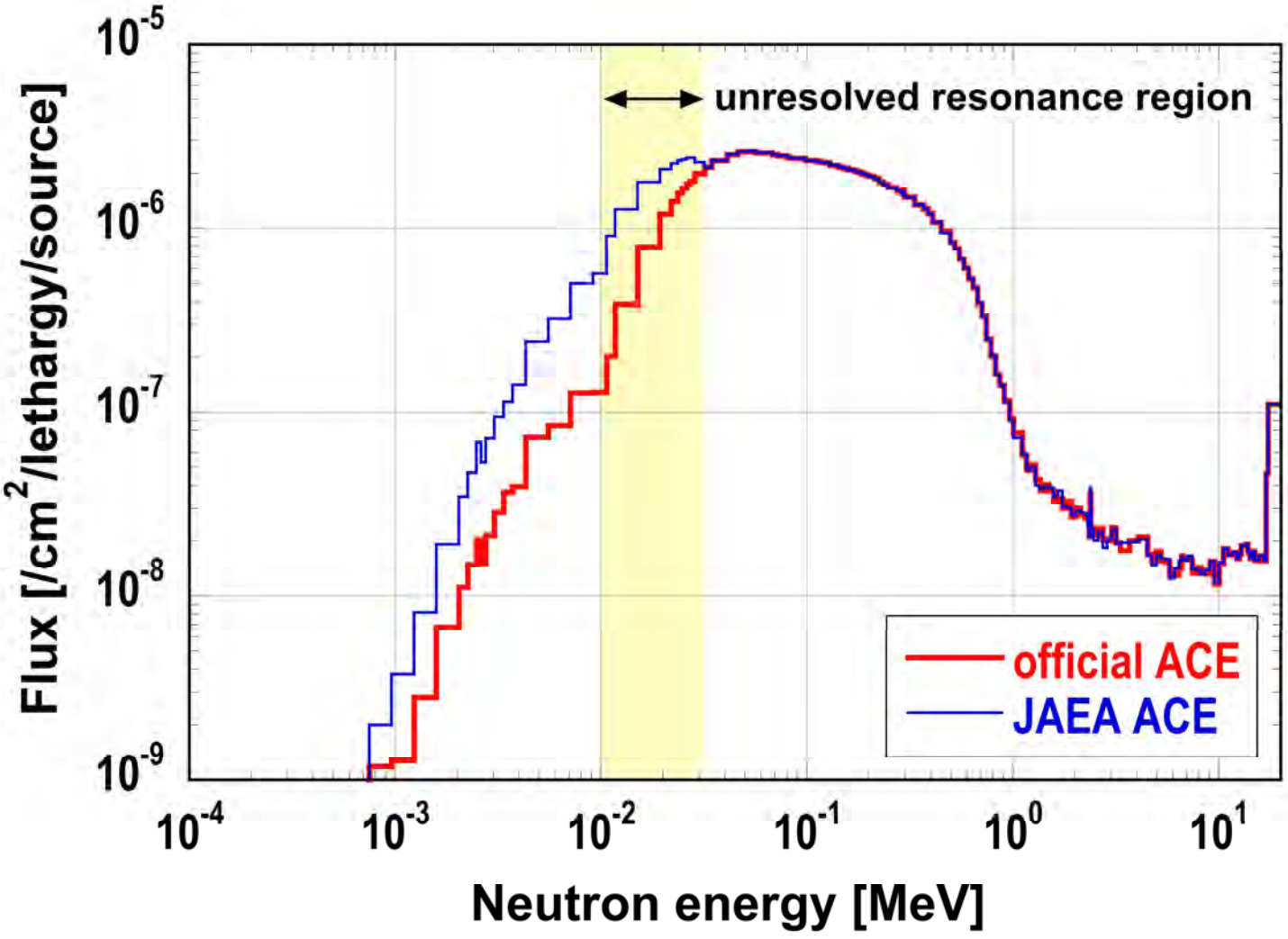
Total cross section of ^{93}Nb in T15n

Unresolved resonance data issue -(1)

- A lot of T15n 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.



Unresolved resonance data issue -(2)



Neutron spectra at 50 cm from niobium sphere center

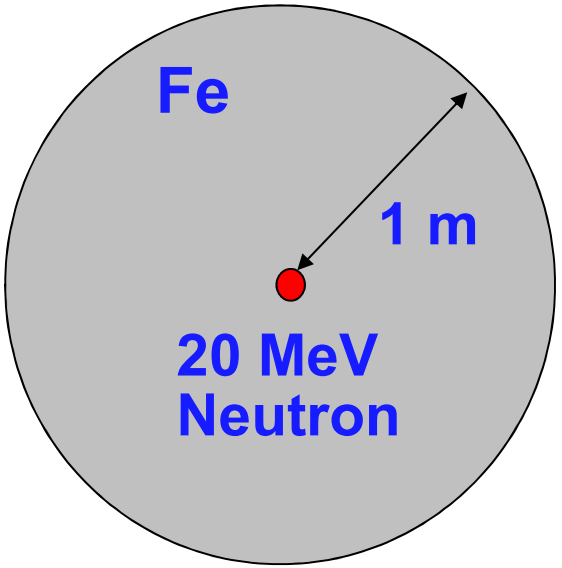
Unresolved resonance data issue -(3)

- The self-shielding correction is also important even in unresolved resonance region because the self-shielding effect is not so small.
- The solution of this issue is just to use the PURR module of the NJOY code in the processing, though it takes time.
- The official ACE files of T15n and/or the next TENDL should include probability table data for all nuclei with unresolved resonance data.
- If not, unresolved resonance data should be omitted in T15n and/or the next TENDL.

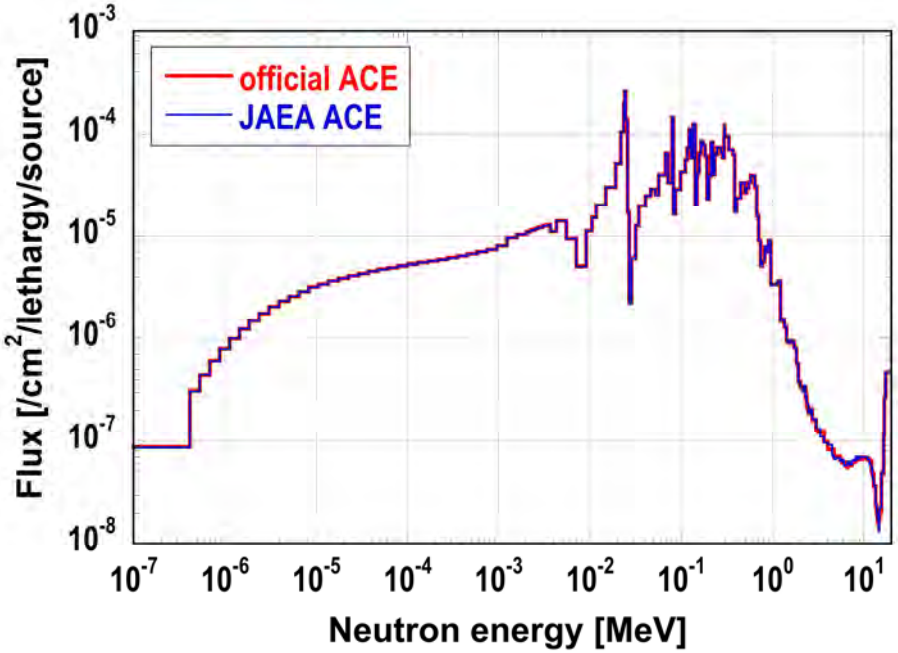
1. Introduction
2. TENDL-2015 ACE file issues
   - 2.1 Unresolved resonance data issue
   - 2.2 Gamma production data issue
3. TENDL-2015 issues
   - 3.1 High-energy gamma data issue
   - 3.2 File 6 data issue
4. Summary

Gamma production data issue

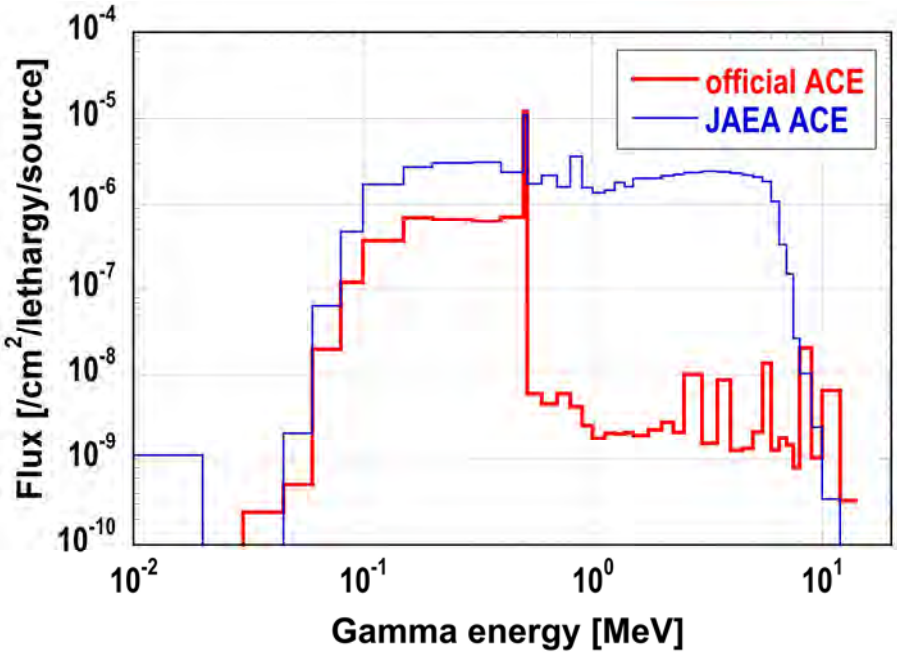
- The secondary gamma data are required in neutron-gamma coupling calculations.
- However there are no gamma production data in the official T15n ACE files except for 13 nuclei (^{1}H, ^{2}H, ^{6}Li, ^{7}Li, ^{9}Be, ^{10}B, ^{11}B, ^{12}C, ^{14}N, ^{15}N, ^{16}O, ^{19}F and ^{239}Pu).
- Thus secondary 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.



Neutron and gamma spectra



Neutron spectra at 50 cm
from iron sphere center



Gamma spectra at 50 cm
from iron sphere center

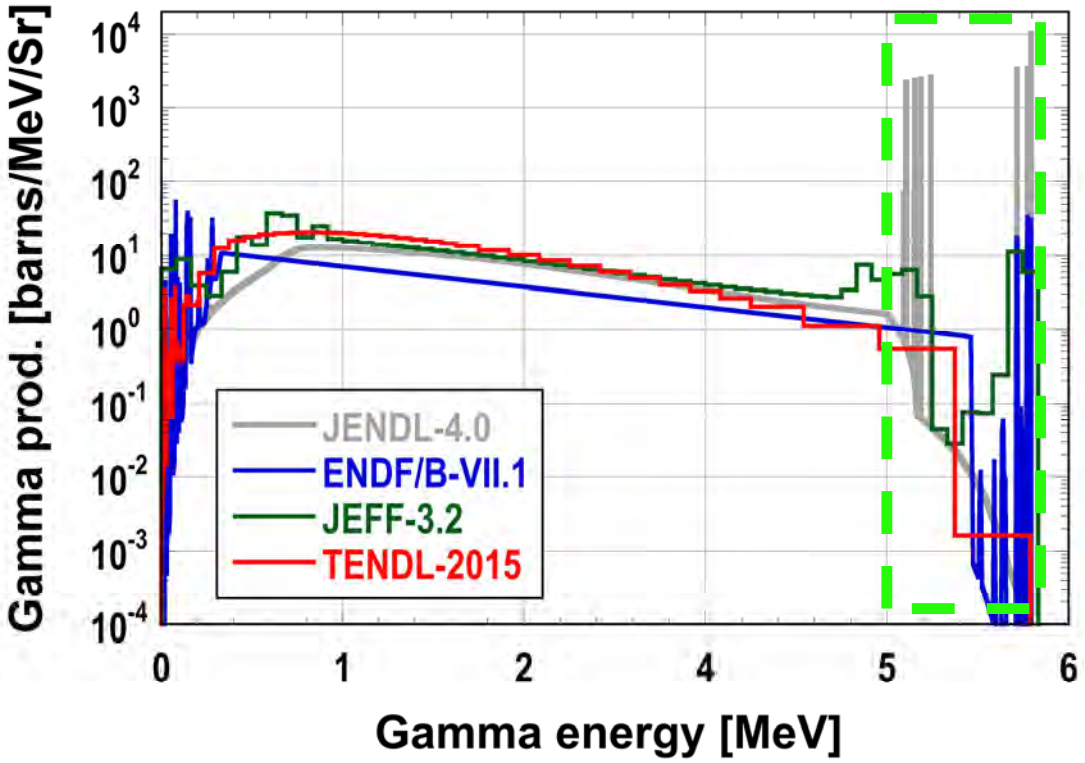
- The official ACE files have no gamma production data, but the MCNP calculation with the official ACE file produced gamma.
- I specified the reason; MCNP misidentifies and misuses particle production data (mt=5 data in T15n) in the official ACE file as gamma production data.

Reason of no gamma production data

- I 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 T15n.
- This issue also occurs in the official ACE files of TENDL-2015 proton, deuteron, triton, He-3, and alpha sub-libraries.
- Thus if T15n is re-processed by using NJOY with iopp=1, this issue is resolved. I hope that the next TENDL will be processed with iopp=1.

High-energy gamma data issue

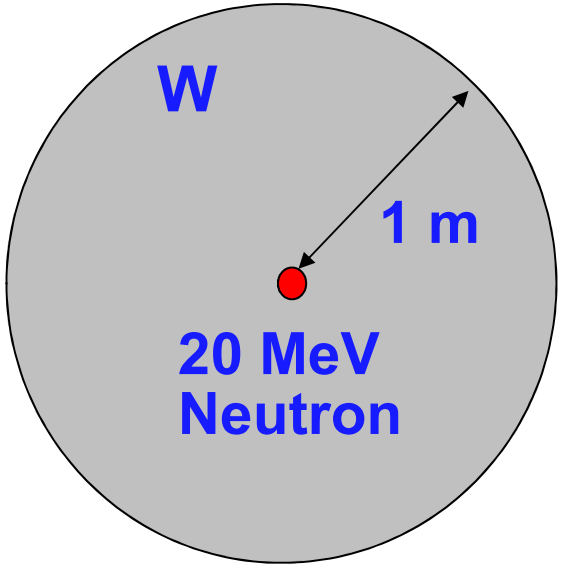
- The secondary gamma spectra from the capture reaction of a lot of nuclei in T15n have fewer high-energy gamma peaks than those in other nuclear data libraries. (e.g. gamma peaks above 5 MeV in the below figure)



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

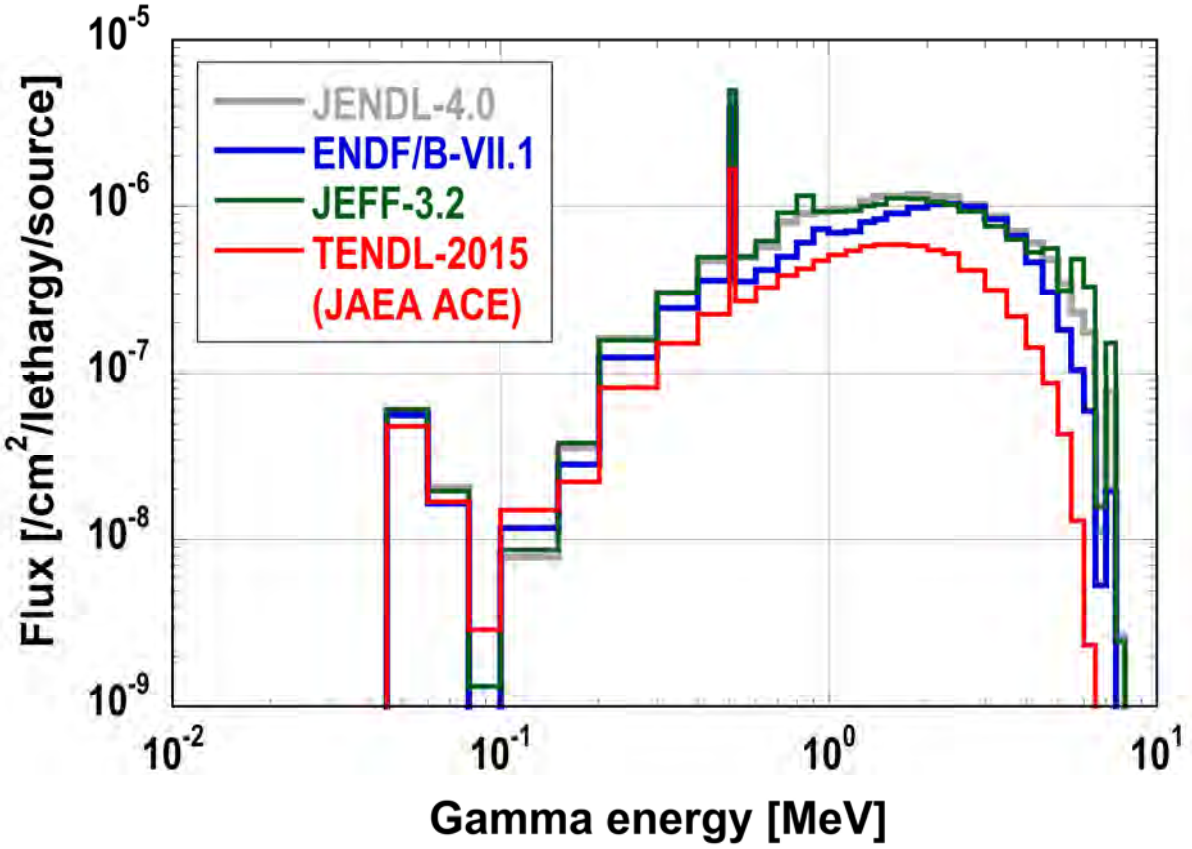
Gamma spectra -(1)

- 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 the JAEA ACE (with gamma production data) files and ACE files of other nuclear data libraries.



- The official T15n ACE file was not used because it has no secondary gamma data.

Gamma spectra -(2)

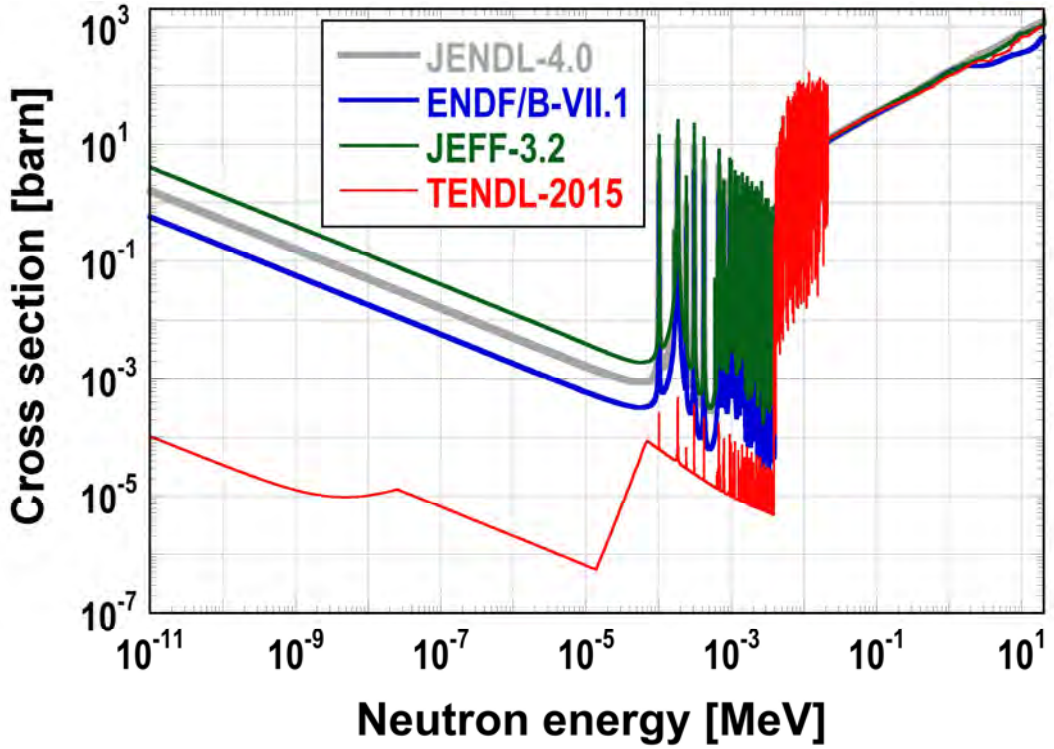


Gamma spectra at 50 cm from tungsten sphere center

- The calculated gamma spectrum with **JAEA ACE** is **smaller** than those with the other libraries and is shifted to lower gamma energy.

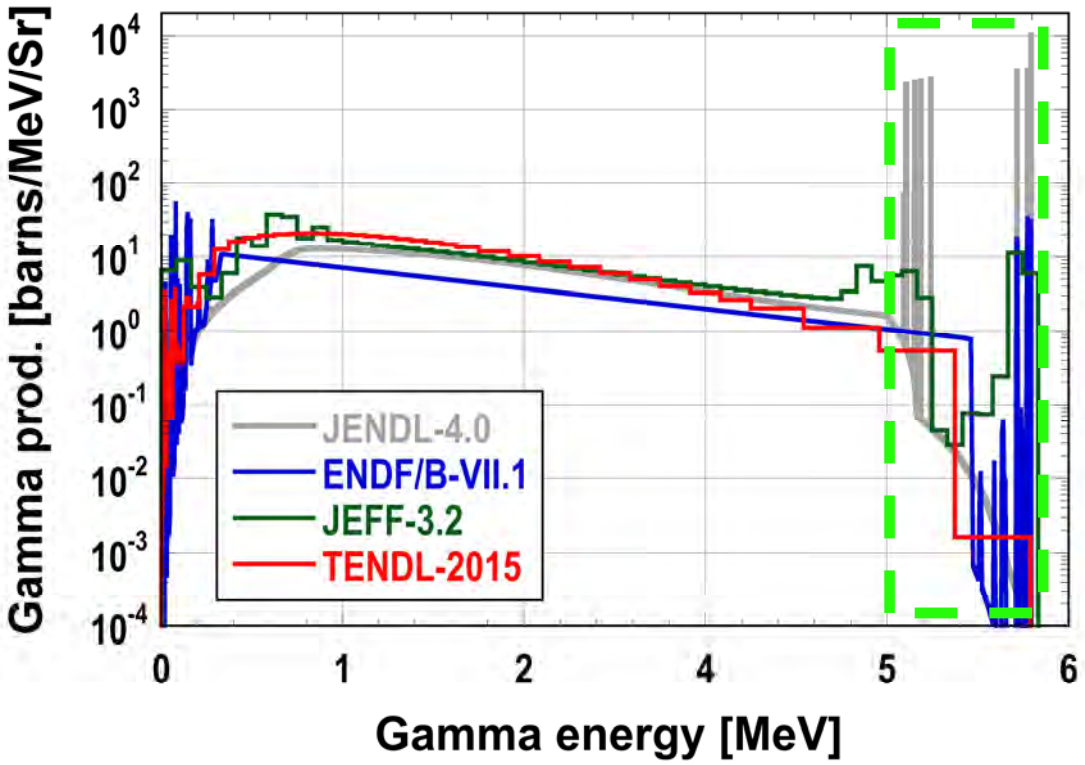
DPA and KERMA data -(1)

- This issue also causes much smaller DPA cross-section data, particularly for nuclei with a larger displacement energy such as ^{184}W (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 larger displacement energy.



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

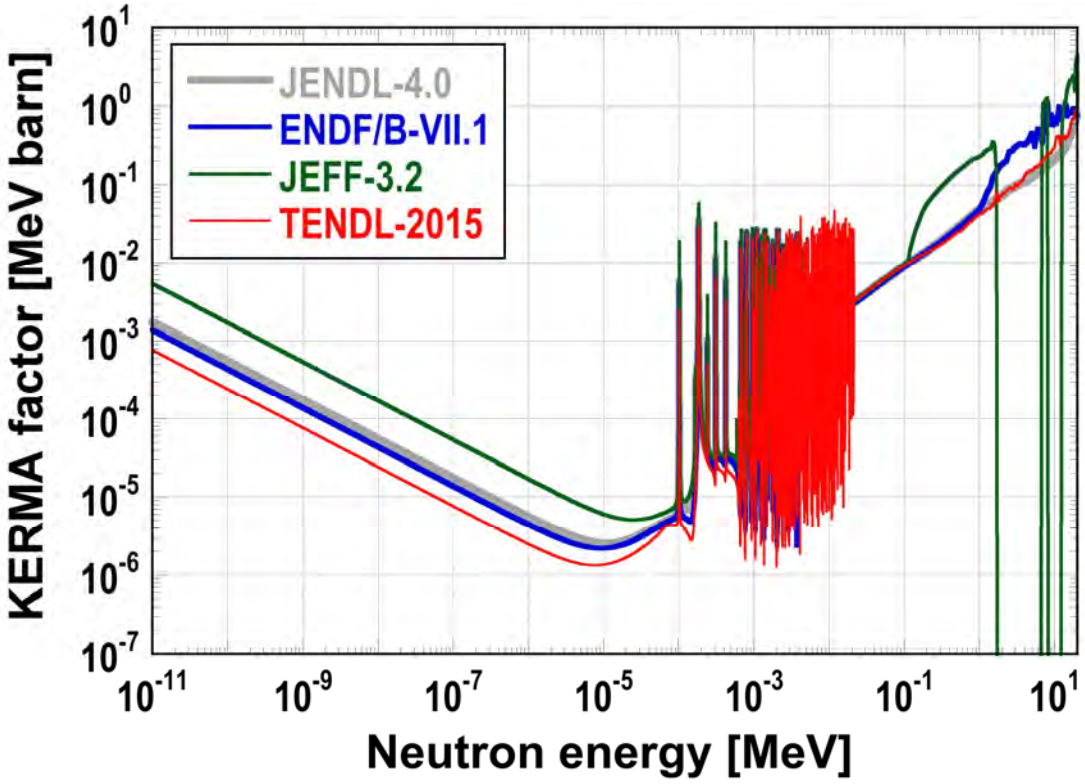
Secondary gamma spectra



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

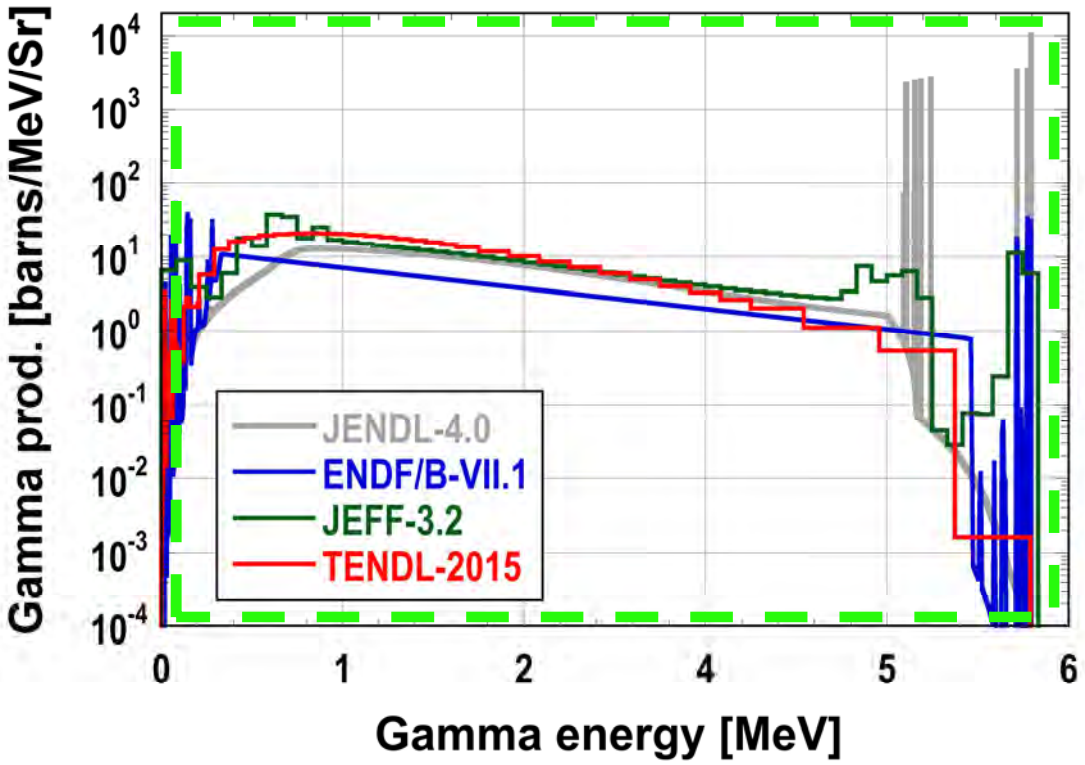
DPA and KERMA data -(2)

- On the contrary, this issue does not affect the KERMA factor so much.
- This is because KERMA factors consider total gamma energies, which are not so different among the nuclear data libraries.



KERMA factor of ^{184}W in ACE files

Secondary gamma spectra

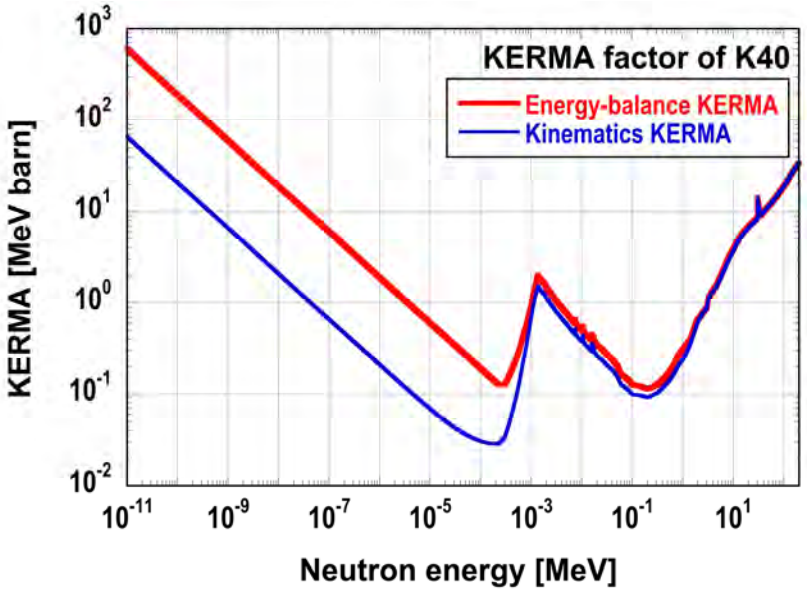


Secondary gamma spectra from capture reaction of ^{184}W in neutron energy of 10^{-5} eV

1. Introduction
2. TENDL-2015 ACE file issues
   - 2.1 Unresolved resonance data issue
   - 2.2 Gamma production data issue
3. **TENDL-2015 issues**
   - 3.1 High-energy gamma data issue
   - **3.2 File 6 data issue**
4. Summary

Introduction

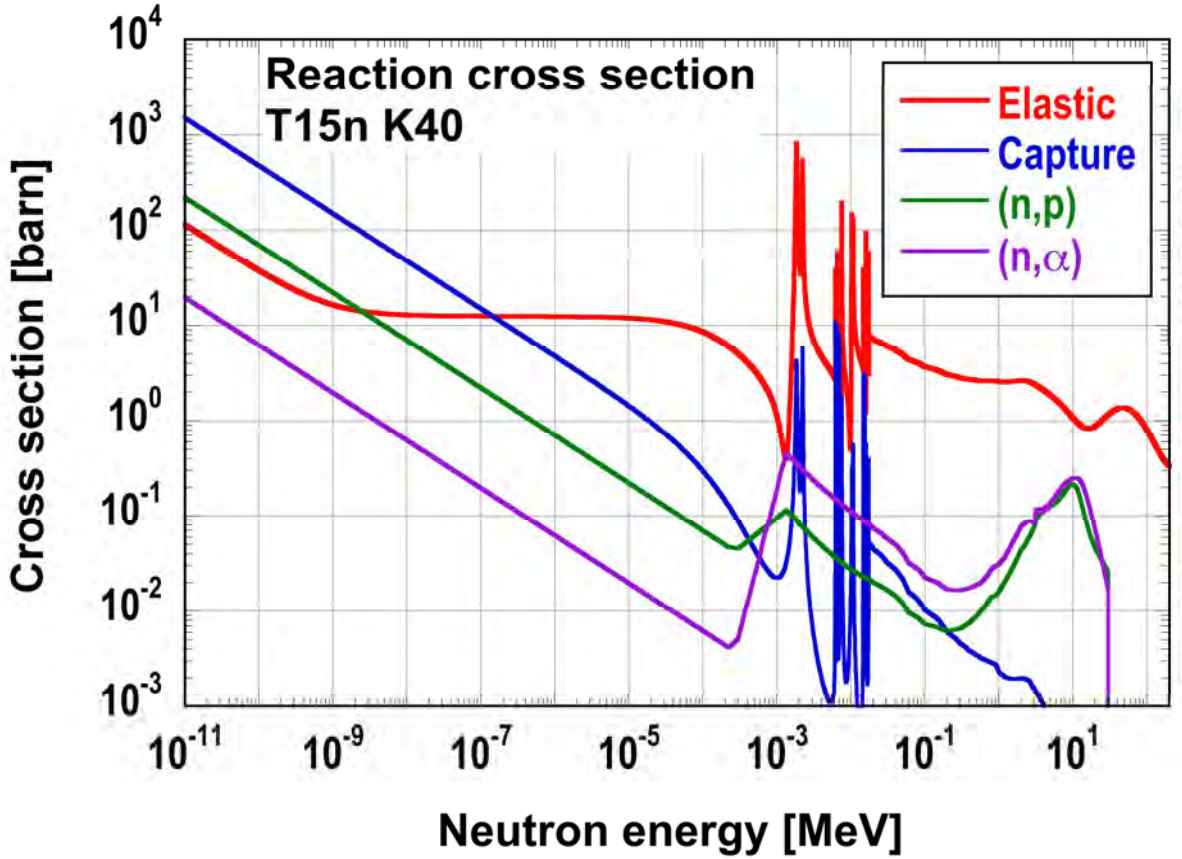
- Recently I calculated and compared energy-balance and kinematics (upper limit) KERMA factors of several nuclei in T15n.
- It is written in the NJOY manual that the kinematics KERMA factor should be larger than the energy-balance KERMA factor. However the kinematics KERMA factor is much smaller than the energy-balance KERMA factor in lower neutron energy for some nuclei such as ^{39}K and ^{40}K in T15n.
- Thus I investigated this issue in more detail by using T15n ^{40}K.



Method

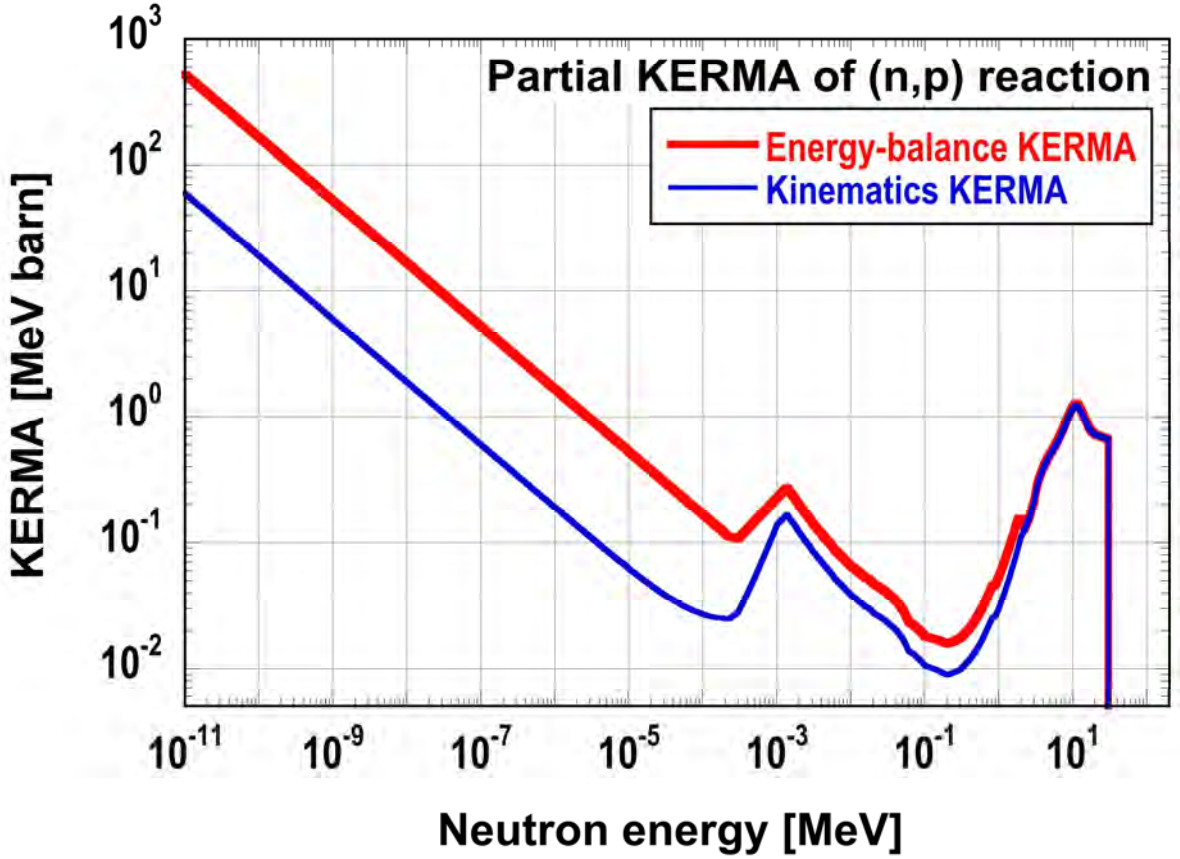
- The T15n ^{40}K data are checked.
  - Reaction cross section data and energy-balance
  - Kinematics (upper limit) and energy-balance KERMAs
  - data of proton, residual nucleus and gamma in the (n,p) reaction [File 6 data]
  - data of alpha, residual nucleus and gamma in the (n,α) reaction [File 6 data]
  - DPA cross-section data
- Code
  - PSYCHE code for energy-balance check
  - NJOY2016.3, which is modified to output partial kinematics KERMAs, are used for calculation of KERMA factor, DPA cross section, etc.
- The T15n ^{40}K data are modified temporarily.

Cross section check



- The cross sections of the (n,p) and (n,α) reactions are not so small in low neutron energy. Thus the (n,p) and (n,α) reactions probably contribute to KERMA and DPA data in low neutron energy.
- I examine the (n,p) and (n,α) reaction data in detail.

Partial KERMA of (n,p) reaction



- Partial **kinematics** KERMA factor of the **(n,p)** reaction is **smaller** than partial **energy-balance** KERMA factor below a few MeV, like the total KERMA.

Energy-balance check of (n,p) reaction

ENERGY BALANCE SUMMARY: Q = 2.37533E+06

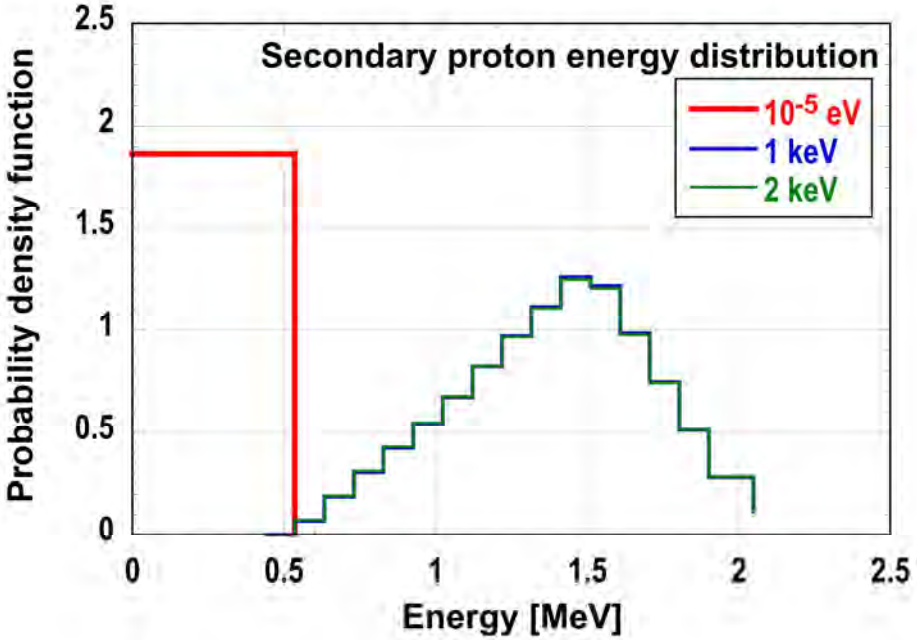
TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

E	AVAIL	%DIFF	SUM	01001	18040	00000
1.00E-05	2.38E+06	-88.71	2.68E+05	2.68E+05	3.05E+01	2.08E-02
1.00E+03	2.38E+06	-41.61	1.39E+06	1.39E+06	1.06E+03	2.08E-02
2.00E+03	2.38E+06	-41.71	1.39E+06	1.38E+06	1.06E+03	2.08E-02
6.00E+03	2.38E+06	-42.45	1.37E+06	1.37E+06	1.08E+03	2.09E-02
1.00E+04	2.39E+06	-43.11	1.36E+06	1.36E+06	1.10E+03	2.10E-02
2.00E+04	2.39E+06	-44.24	1.34E+06	1.33E+06	1.13E+03	2.13E-02
6.00E+04	2.43E+06	-43.60	1.37E+06	1.37E+06	1.17E+03	2.22E-02
1.00E+05	2.47E+06	-44.06	1.38E+06	1.38E+06	1.24E+03	2.32E-02
2.00E+05	2.57E+06	-45.92	1.39E+06	1.39E+06	1.33E+03	2.55E-02
4.00E+05	2.77E+06	-46.42	1.48E+06	1.48E+06	1.54E+03	3.03E-02
6.00E+05	2.96E+06	-46.78	1.58E+06	1.57E+06	1.71E+03	3.50E-02
8.00E+05	3.16E+06	-46.82	1.68E+06	1.68E+06	1.88E+03	3.97E-02
1.00E+06	3.35E+06	-46.44	1.79E+06	1.79E+06	2.11E+03	4.45E-02
1.40E+06	3.74E+06	-44.87	2.06E+06	2.06E+06	2.47E+03	5.40E-02
1.80E+06	4.13E+06	-43.76	2.32E+06	2.32E+06	2.80E+03	8.71E+02
2.20E+06	4.52E+06	-2.77	4.40E+06	2.49E+06	3.13E+03	1.90E+06

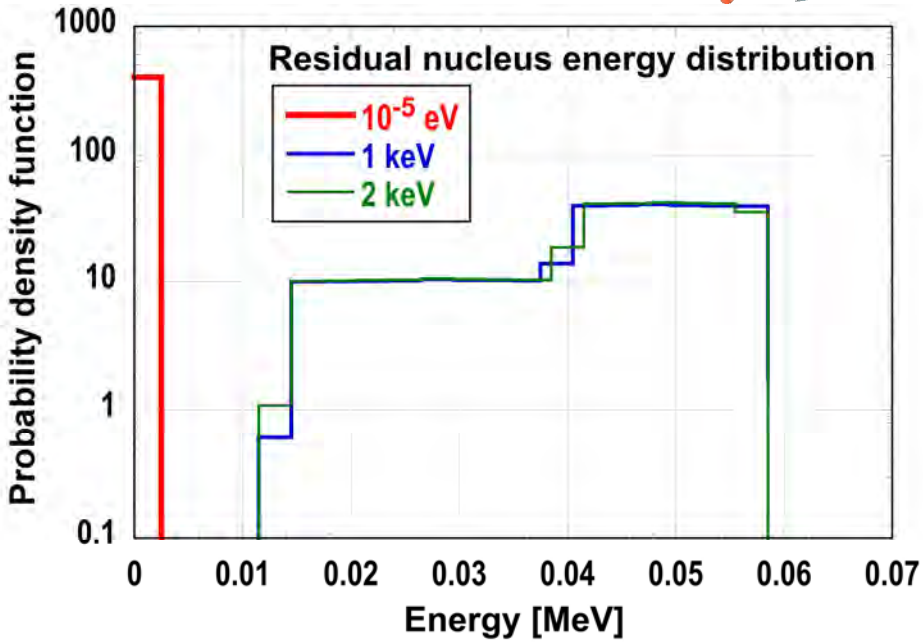
PSYCHE output for (n,p) reaction

- For neutrons of 10^{-5} eV, energies of proton and residual nucleus (^{40}Ar) are small.
- For neutrons up to 1.8 MeV, gamma energies are too small.

Energy distribution check of (n,p) reaction



Probability density function (energy distribution) of secondary proton in the (n,p) reaction

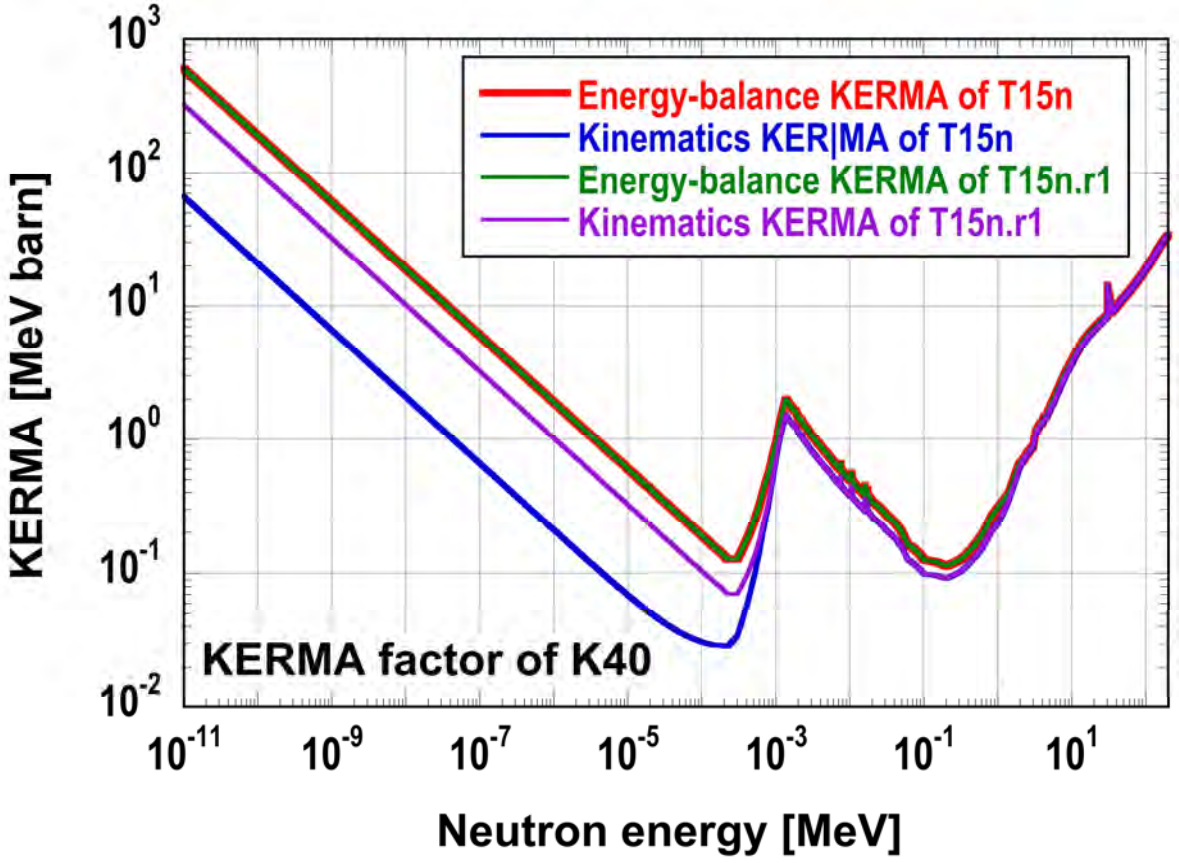


Probability density function (energy distribution) of residual nucleus in the (n,p) reaction

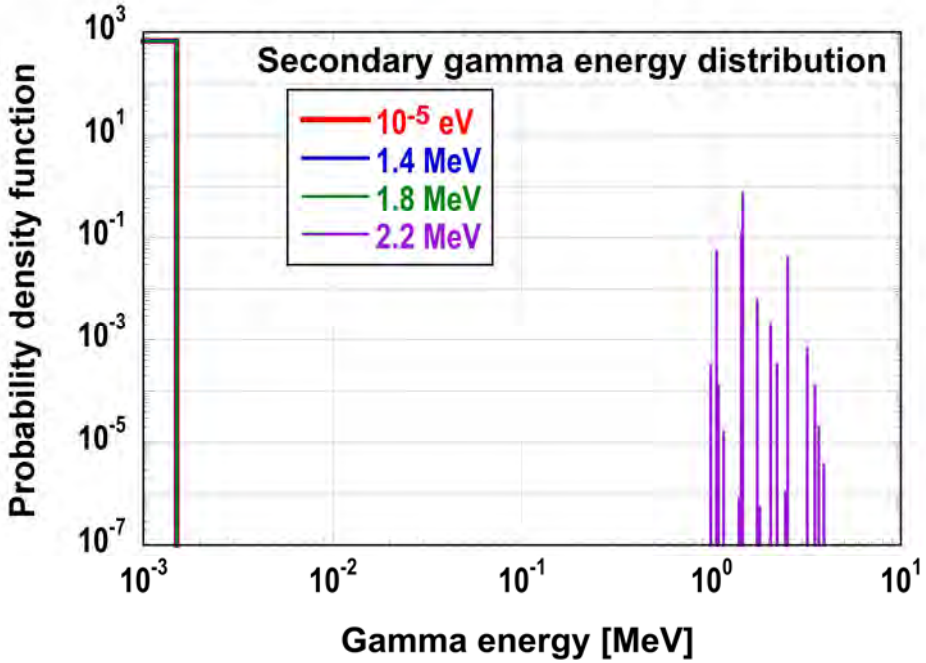
- **Energy distribution** data between 10^{-5} eV and 1 keV are deduced with **linear-linear interpolation**.
- **Energy distribution** data of proton and residual nucleus (^{40}Ar) for neutrons of 10^{-5} eV in the (n,p) reaction are small. They should be replaced to those for neutrons of 1 keV.

Revision 1 of T15n ^{40}K

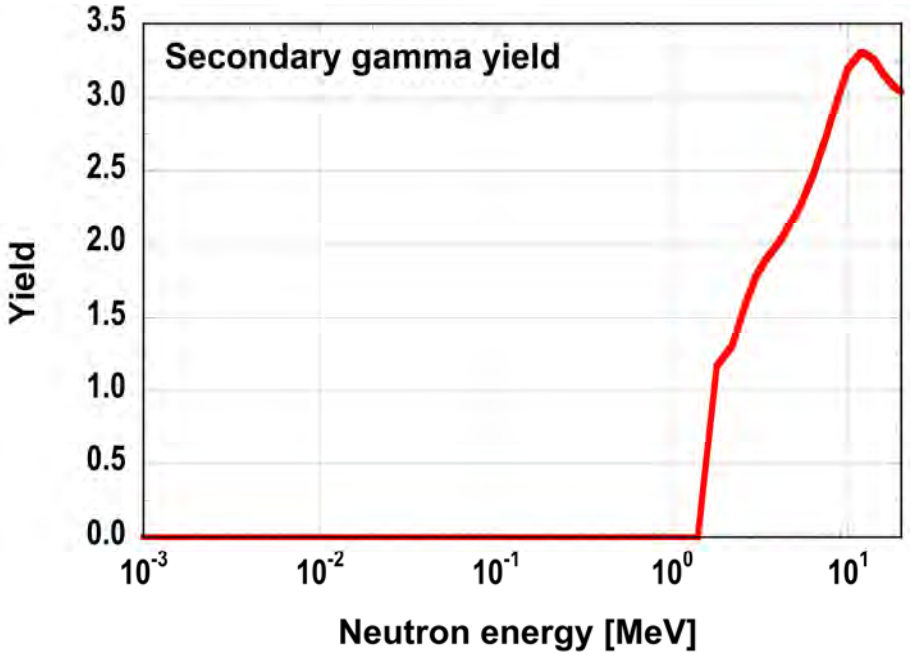
- I modified energy distribution data of proton and residual nucleus in the (n,p) reaction (T15n.r1).
- Kinematics KERMA of T15n.r1 is close to energy-balance KERMA, but is still smaller.



Gamma data check of (n,p) reaction



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

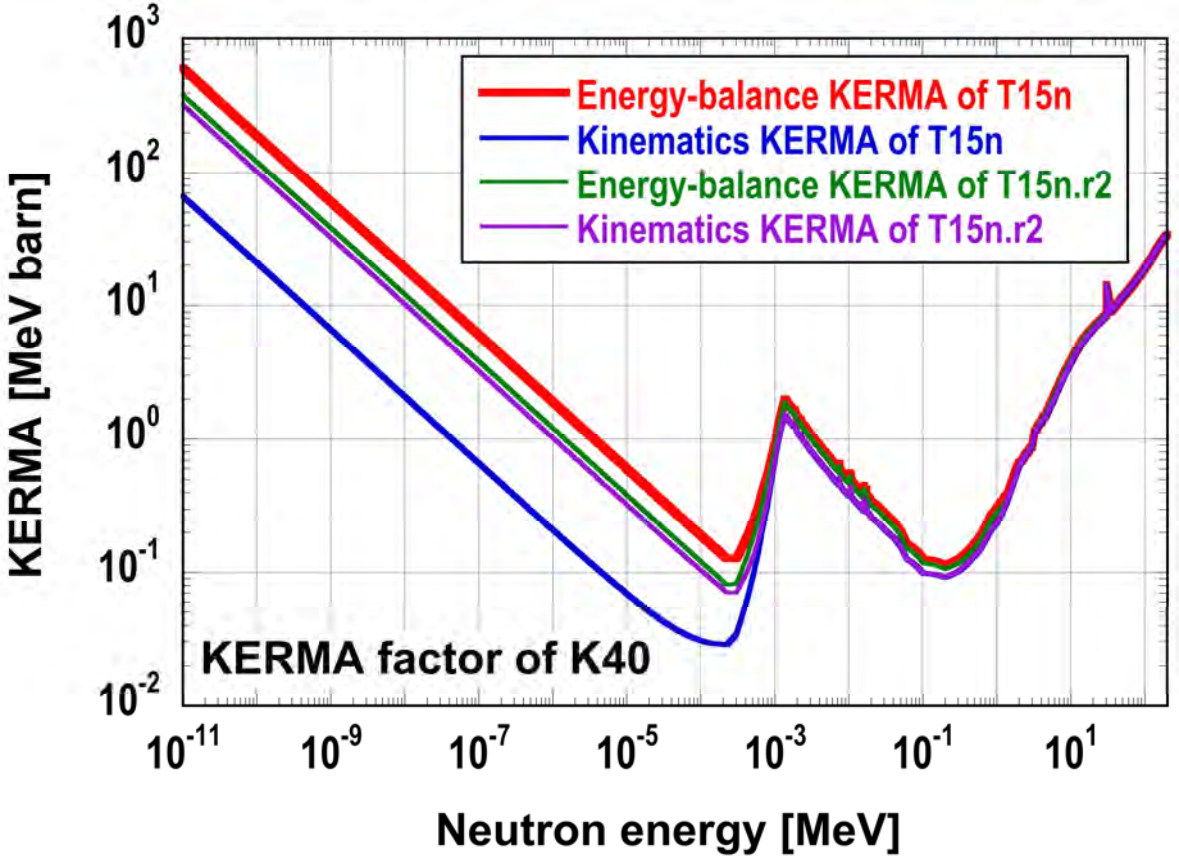


Secondary gamma yield in the (n,p) reaction

- Gamma energy distribution data for neutrons less than 2.2 MeV are too small. They should be replaced to those for neutrons of 2.2 MeV.
- Gamma yields for neutrons less than 1.8 MeV are too small. They should be modified to keep energy-balance.

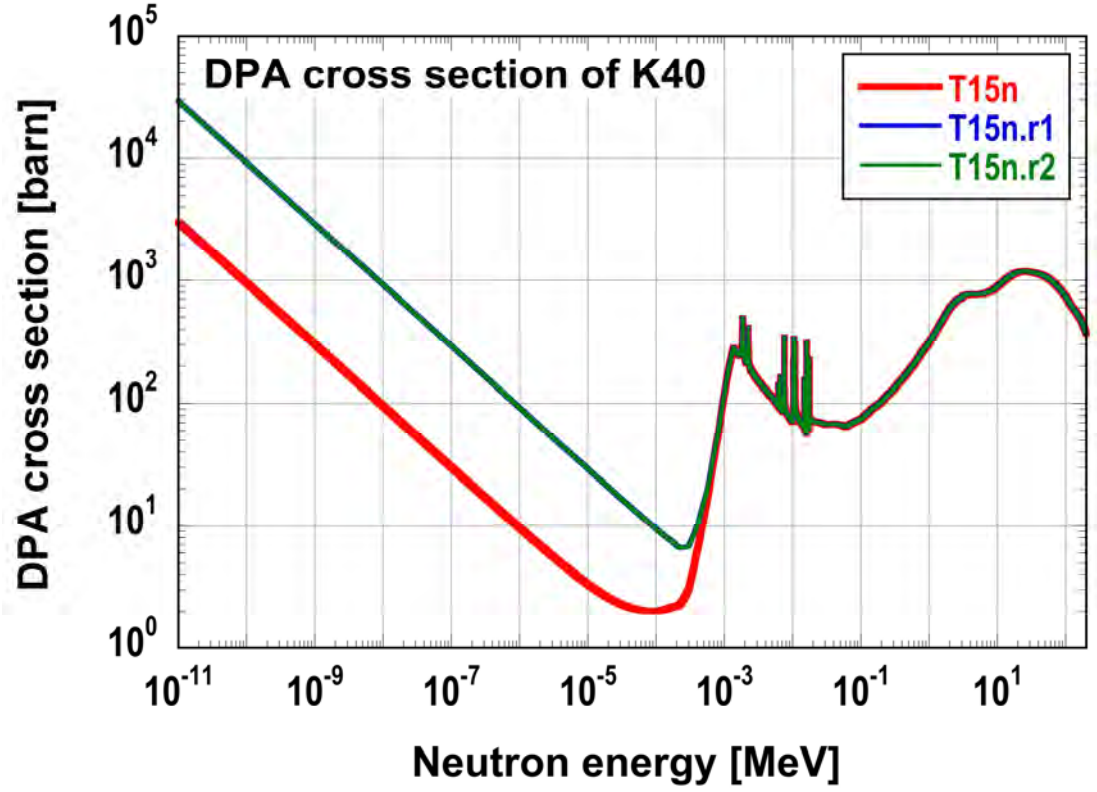
Revision 2 of T15n ^{40}K

- I also modified energy distribution and yield data of gamma in the (n,p) reaction of T15n.r1 (T15n.r2).
- Kinematics KERMA is slightly smaller than energy-balance KERMA in T15n.r2, which is due to the (n,α) reaction data.
- Energy-balance KERMA of T15n is larger than that of T15n.r2, because it includes gamma energies in the (n,p) reaction.

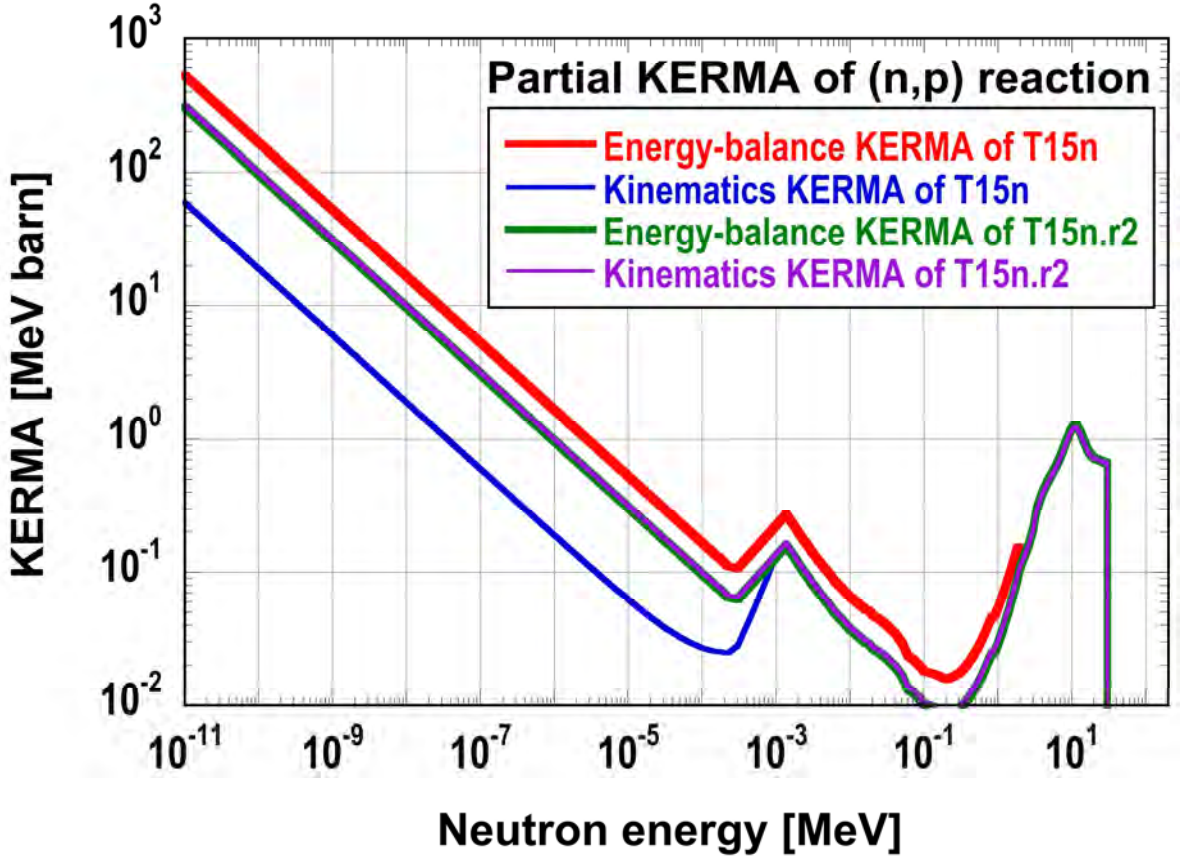


DPA of ^{40}K -(1)

- The DPA cross-section data in T15n do not include energies of proton and residual nucleus in the (n,p) reaction below 1 keV.
- The DPA cross-section data of T15n.r1 and T15n.r2 are the same because they are probably calculated by kinematics method, which does not consider gamma data in File 6.



Partial KERMA of revised (n,p) reaction



- Partial **energy-balance** and **kinematics** KERMAs of the (n,p) reaction in **T15n.r2** are the **same**. They are different from those in T15n.

Energy-balance check of revised (n,p) reaction

ENERGY BALANCE SUMMARY: Q = 2.37533E+06

TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

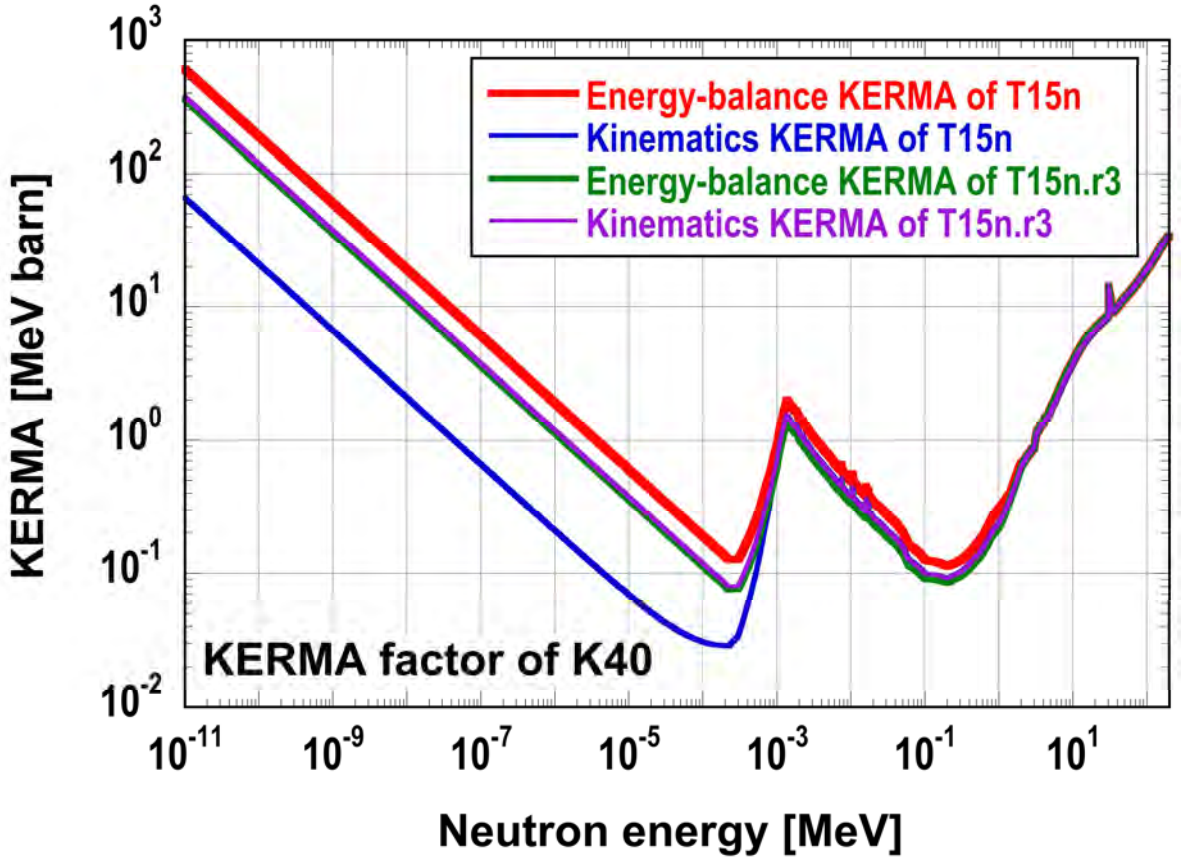
E	AVAIL	%DIFF	SUM	01001	18040	00000
1.00E-05	2.38E+06	0.08	2.38E+06	1.39E+06	1.06E+03	9.90E+05
1.00E+03	2.38E+06	0.06	2.38E+06	1.39E+06	1.06E+03	9.90E+05
2.00E+03	2.38E+06	-0.03	2.38E+06	1.38E+06	1.06E+03	9.91E+05
6.00E+03	2.38E+06	-0.76	2.36E+06	1.37E+06	1.08E+03	9.93E+05
1.00E+04	2.39E+06	-1.40	2.35E+06	1.36E+06	1.10E+03	9.95E+05
2.00E+04	2.39E+06	-2.50	2.34E+06	1.33E+06	1.13E+03	1.00E+06
6.00E+04	2.43E+06	-1.72	2.39E+06	1.37E+06	1.17E+03	1.02E+06
1.00E+05	2.47E+06	-2.04	2.42E+06	1.38E+06	1.24E+03	1.04E+06
2.00E+05	2.57E+06	-3.58	2.48E+06	1.39E+06	1.33E+03	1.09E+06
4.00E+05	2.77E+06	-3.50	2.67E+06	1.48E+06	1.54E+03	1.19E+06
6.00E+05	2.96E+06	-3.36	2.86E+06	1.57E+06	1.71E+03	1.29E+06
8.00E+05	3.16E+06	-2.96	3.06E+06	1.68E+06	1.88E+03	1.38E+06
1.00E+06	3.35E+06	-2.20	3.28E+06	1.79E+06	2.11E+03	1.48E+06
1.40E+06	3.74E+06	0.03	3.74E+06	2.06E+06	2.47E+03	1.68E+06
1.80E+06	4.13E+06	0.02	4.13E+06	2.32E+06	2.80E+03	1.81E+06
2.20E+06	4.52E+06	-2.77	4.40E+06	2.49E+06	3.13E+03	1.90E+06

PSYCHE output for (n,p) reaction of TENDL-2015.r2

- **Revised (n,p) reaction data generally keep energy-balance.**

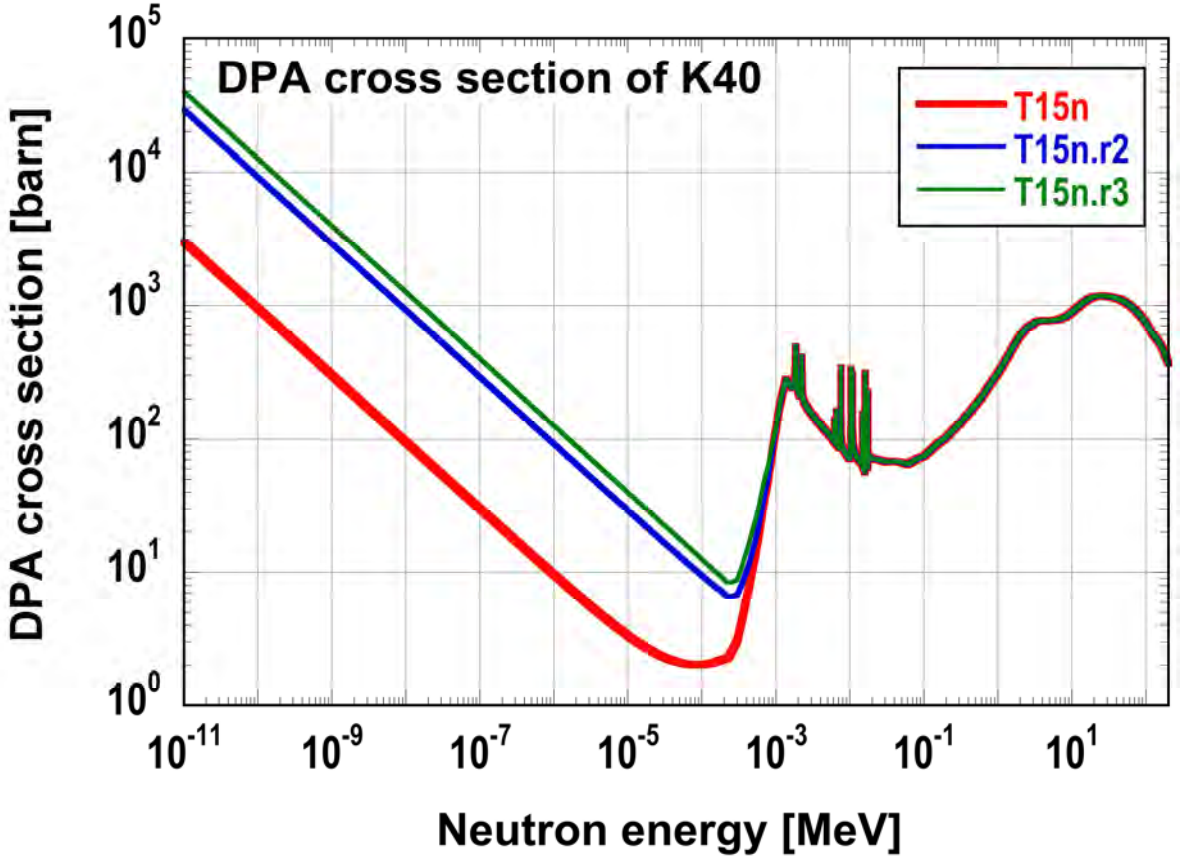
Revision 3 of T15n ^{40}K

- I also did the same procedure to the (n,α) reaction of T15n.r2 ^{40}K as the (n,p) reaction. (T15n.r3).
- The kinematics KERMA factor in T15n.r3 is the same as the energy-balance KERMA factor in T15n.r3.



DPA of ^{40}K -(2)

- The DPA cross-section of T15n.r3 is slightly larger than that of T15n.r2 below 1 keV because it includes revised energy of alpha and residual nucleus.



File 6 data issue

- I investigated reasons why the kinematics KERMA factor is much smaller than the energy-balance KERMA factor in lower neutron energy by using the ^{40}K data of T15n in more detail.
- I specified that the File 6 data (energy distribution data of proton, alpha, residual nucleus and gamma, and gamma yield data) of the (n,p) and (n,α) reactions in ^{40}K of T15n seem to be incorrect, which causes incorrect KERMA and DPA data.
- T15n and/or the next TENDL neutron sub-library should be re-checked based on this study.

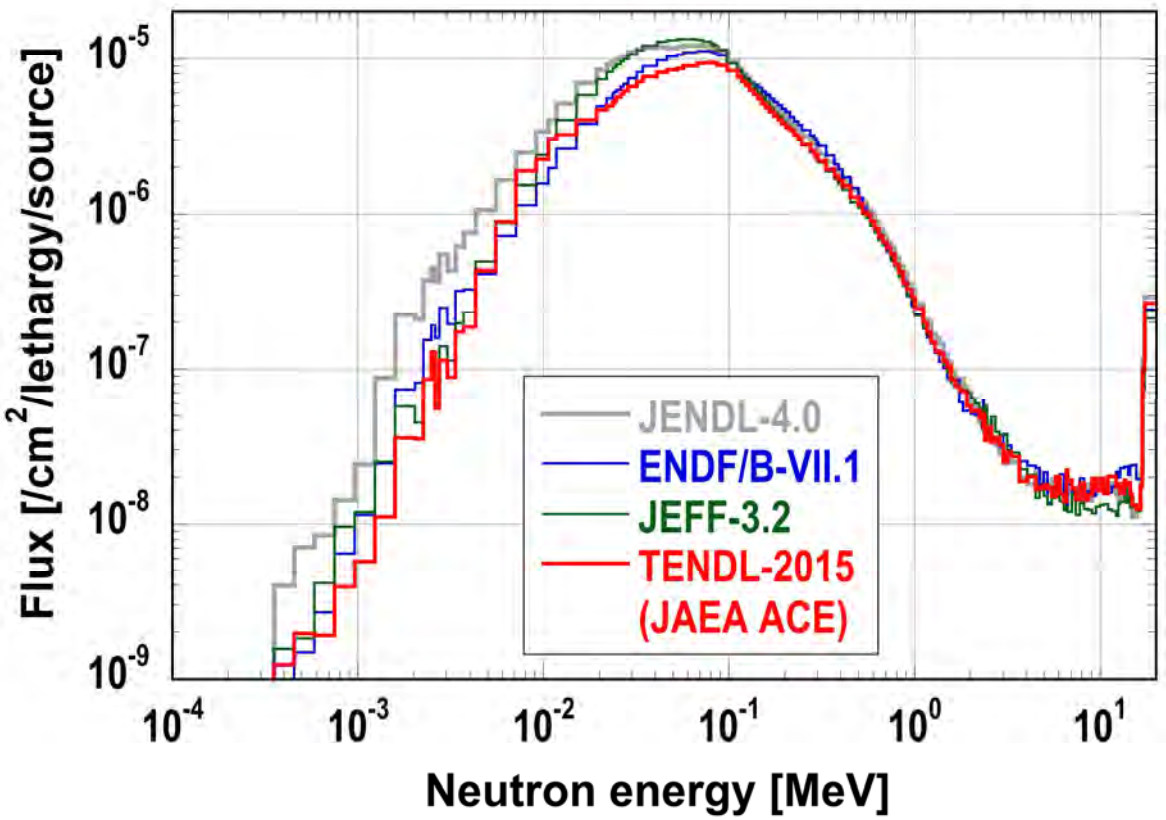
1. Introduction
2. TENDL-2015 ACE file issues
   - 2.1 Unresolved resonance data issue
   - 2.2 Gamma production data issue
3. TENDL-2015 issues
   - 3.1 High-energy gamma data issue
   - 3.2 File 6 data issue
4. **Summary**

Summary

- I found out that T15n and its official ACE file had the following issues.
  - No probability tables for unresolved resonance in the ACE files except for those of ^{235}U, ^{235m}U and ^{238}U
  - No gamma production data in the ACE files except for those of ^{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
  - No high-energy gamma peaks in the capture reaction of a lot of the T15n files
  - Inconsistent File 6 data of the (n,p) and (n,α) reactions in the T15n files
- The effects of these issues were demonstrated.
- T15n and its official ACE files should be revised and/or the next TENDL and its official ACE files should be produced based on this study.

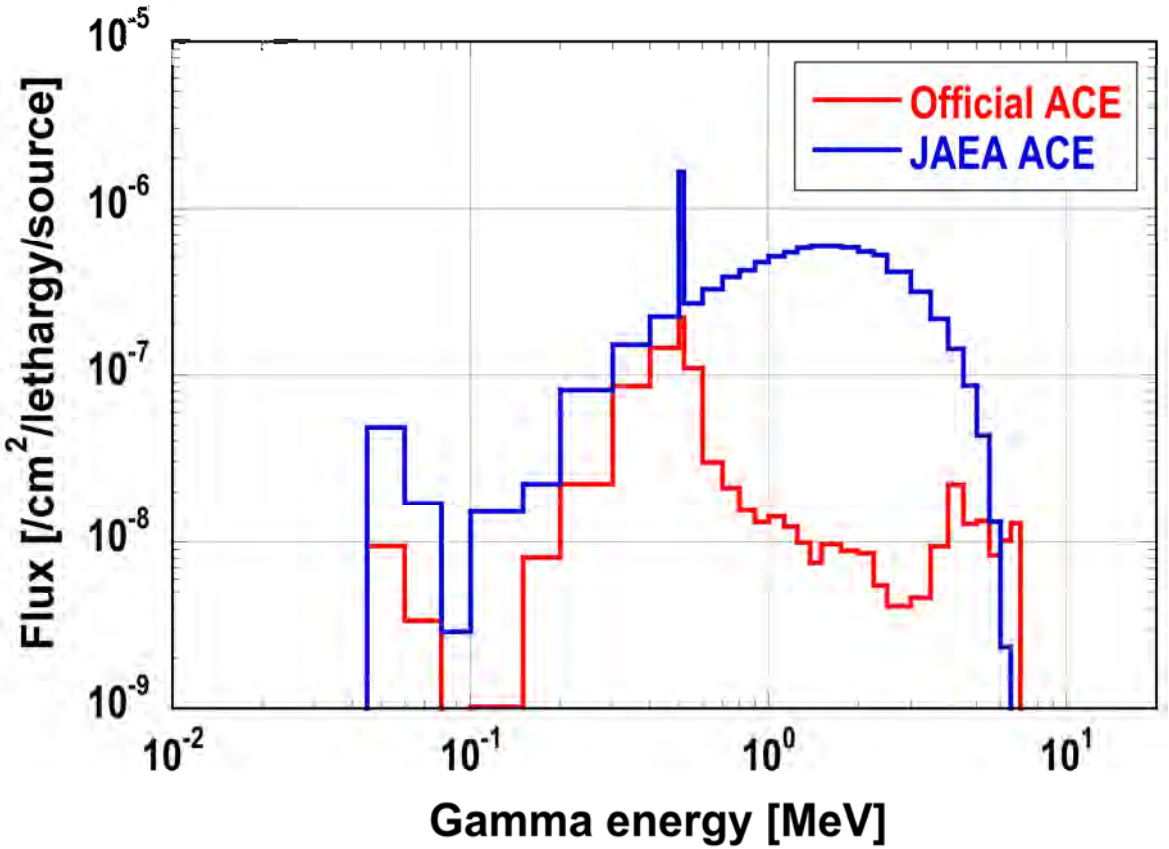
Thank you for your attention!

Neutron spectra -(2)



Neutron spectra at 50 cm from tungsten sphere center

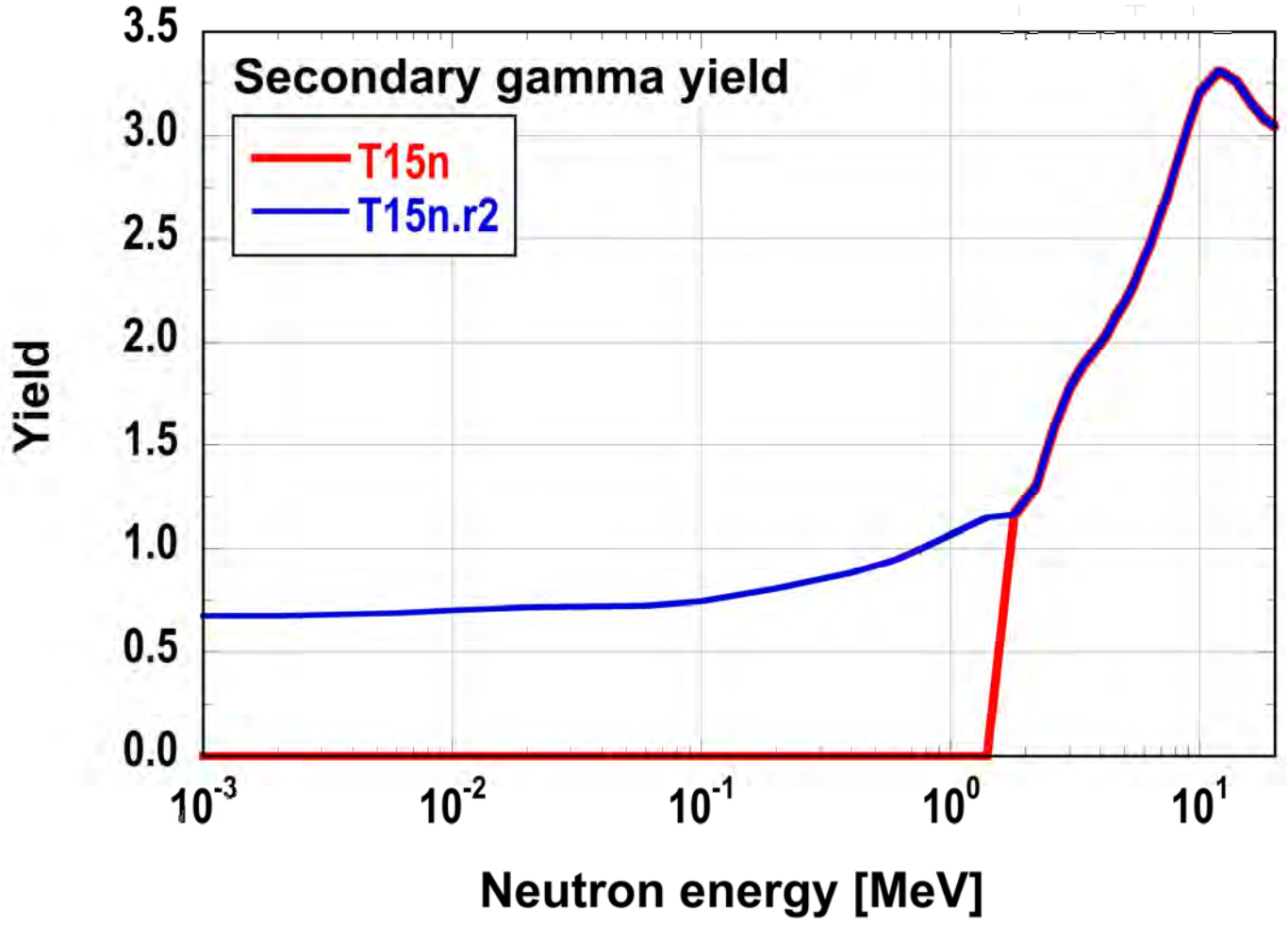
Gamma spectra -(2)



Gamma spectra at 50 cm from tungsten sphere center

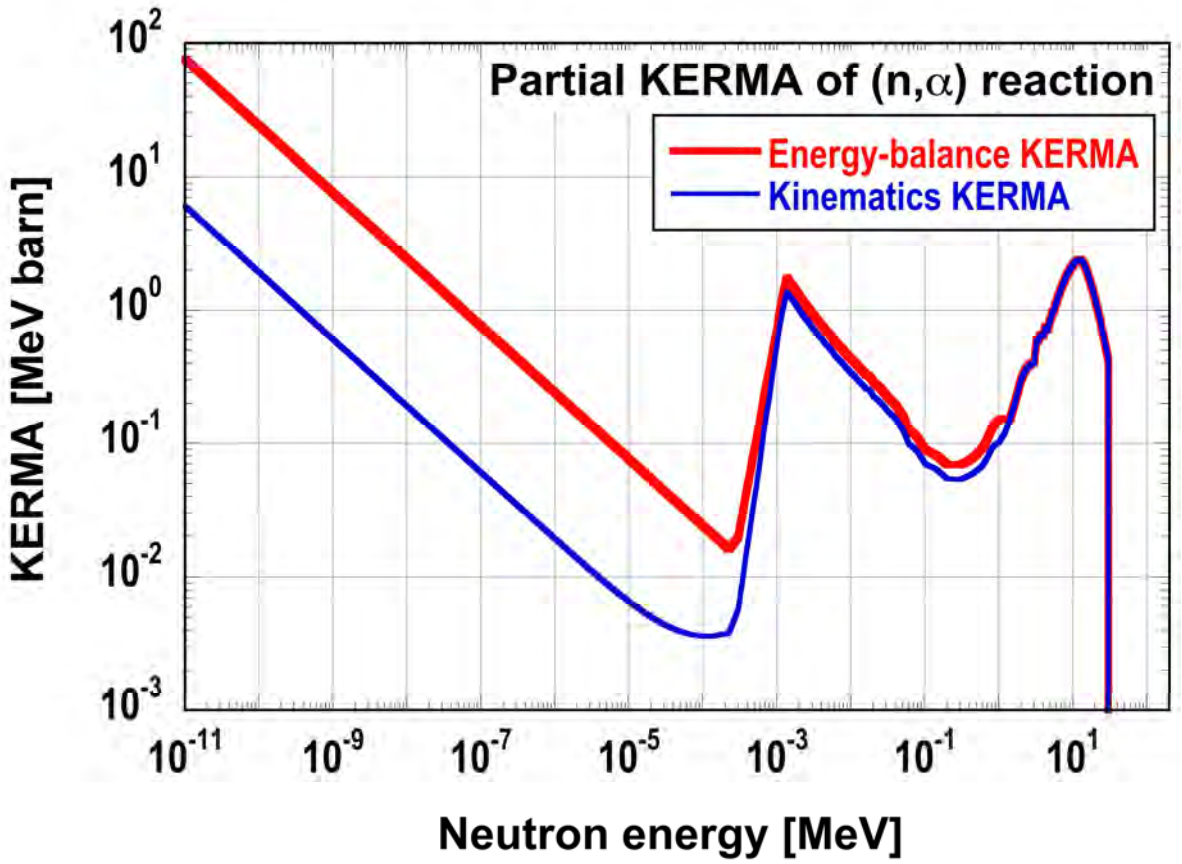
- The calculated gamma spectrum with the official ACE is very different from that with JAEA ACE.

Gamma yield of (n,p) reaction in ^{40}K



Yield of secondary gamma in (n,p) reaction

Partial KERMA of (n,α) reation



- Partial energy-balance KERMA of (n,α) reaction is larger than partial kinematics KERMA below 1 keV.
- Partial energy-balance or kinematics KERMA is wrong.

Energy-balance check of (n,α) reaction

ENERGY BALANCE SUMMARY: Q = 3.87244E+06

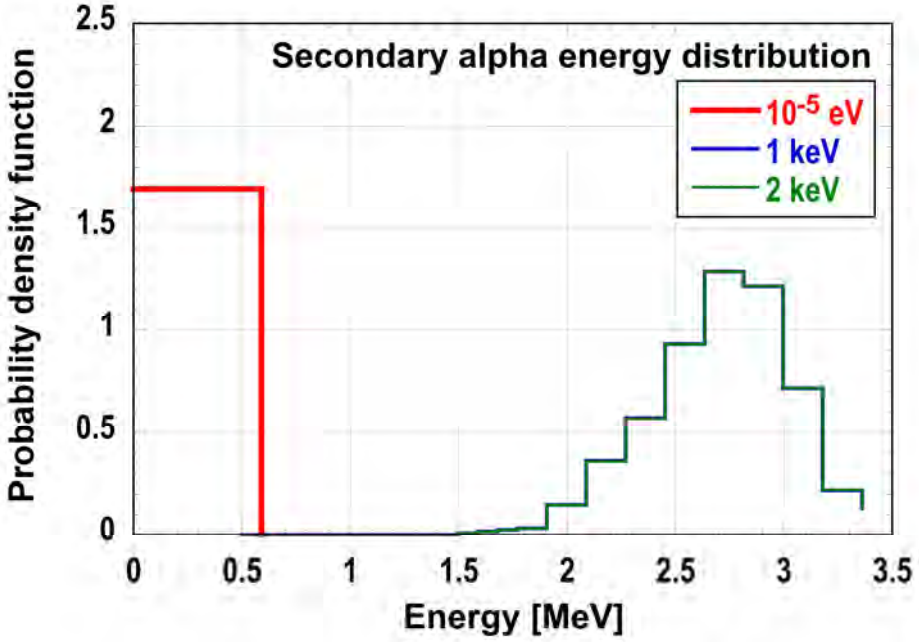
TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

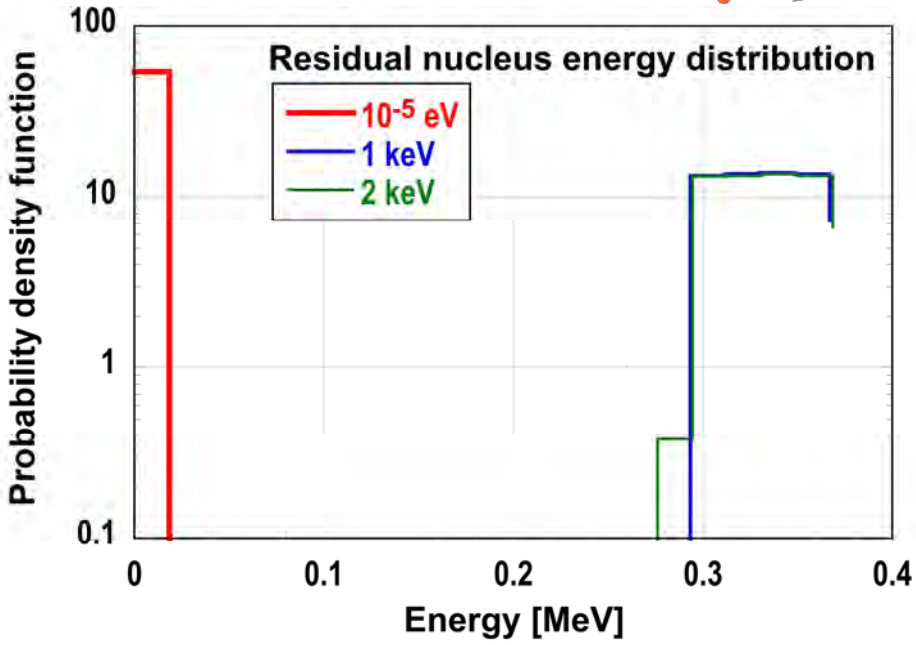
E	AVAIL	%DIFF	SUM	02004	17037	00000
1.00E-05	3.87E+06	-92.37	2.95E+05	2.95E+05	2.43E+02	2.46E-06
1.00E+03	3.87E+06	-30.02	2.71E+06	2.70E+06	8.69E+03	2.52E-06
2.00E+03	3.87E+06	-30.02	2.71E+06	2.70E+06	8.72E+03	2.59E-06
6.00E+03	3.88E+06	-30.01	2.71E+06	2.71E+06	8.79E+03	2.85E-06
1.00E+04	3.88E+06	-30.01	2.72E+06	2.71E+06	8.85E+03	3.11E-06
2.00E+04	3.89E+06	-30.03	2.72E+06	2.71E+06	8.90E+03	3.76E-06
6.00E+04	3.93E+06	-30.21	2.74E+06	2.73E+06	8.85E+03	6.36E-06
1.00E+05	3.97E+06	-30.44	2.76E+06	2.75E+06	9.05E+03	8.97E-06
2.00E+05	4.07E+06	-30.22	2.84E+06	2.83E+06	9.42E+03	1.55E-05
4.00E+05	4.26E+06	-31.74	2.91E+06	2.90E+06	1.00E+04	2.85E-05
6.00E+05	4.46E+06	-35.29	2.88E+06	2.87E+06	1.06E+04	4.15E-05
8.00E+05	4.65E+06	-37.53	2.91E+06	2.90E+06	1.12E+04	5.45E-05
1.00E+06	4.85E+06	-41.89	2.82E+06	2.80E+06	1.19E+04	6.92E+02
1.40E+06	5.24E+06	-9.23	4.75E+06	2.77E+06	1.31E+04	1.97E+06
1.80E+06	5.63E+06	-9.38	5.10E+06	3.14E+06	1.43E+04	1.94E+06

PSYCHE output for (n,α) reaction

- For neutrons of 10^{-5} eV, energies of alpha and residual nucleus (^{37}Cl) are small.
- For neutrons up to 1 MeV, gamma energies are too small.

Energy distribution check of (n,α) reaction



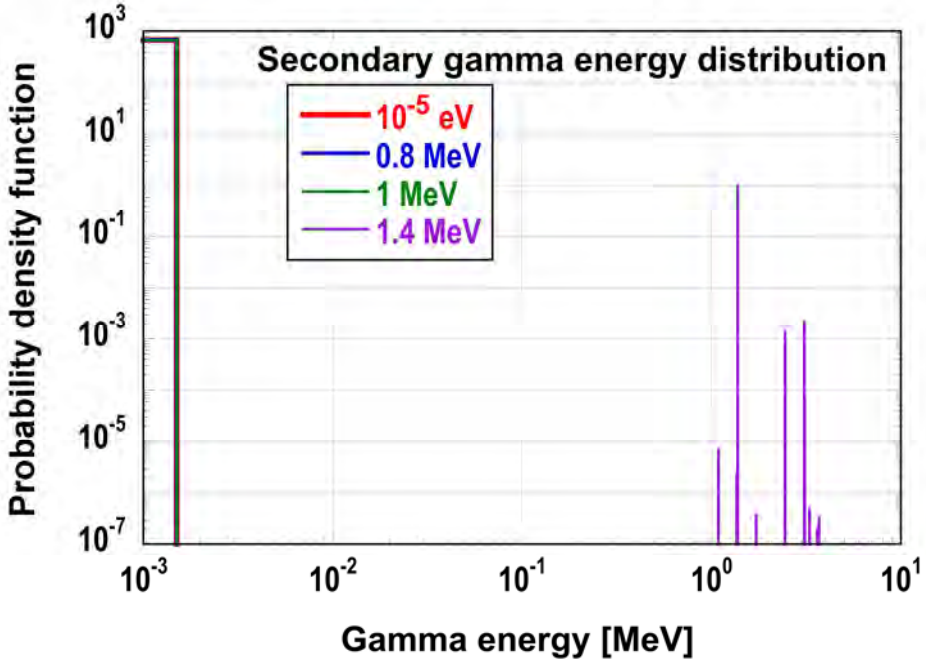


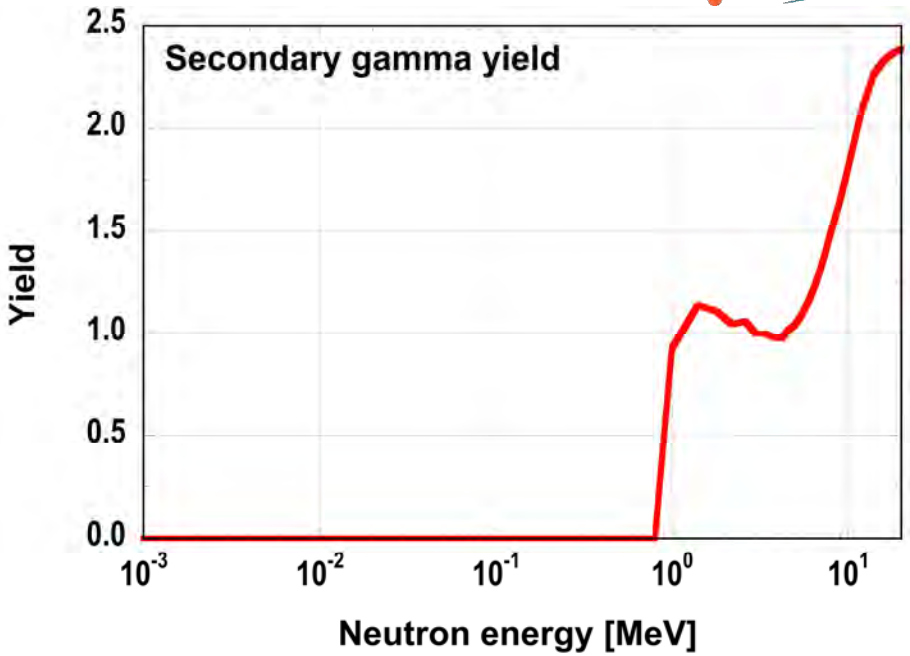
Probability density function (energy distribution) of secondary alpha in (n,α) reaction

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

- Energy distribution data between 10^{-5} eV and 1 keV are deduced with linear interpolation.
- Energy distribution data of alpha and residual nucleus (^{37}Cl) for neutrons of 10^{-5} eV in (n,α) reaction are smaller. They should be replaced to those for neutrons of 1 keV.

Gamma data check of (n,α) reaction



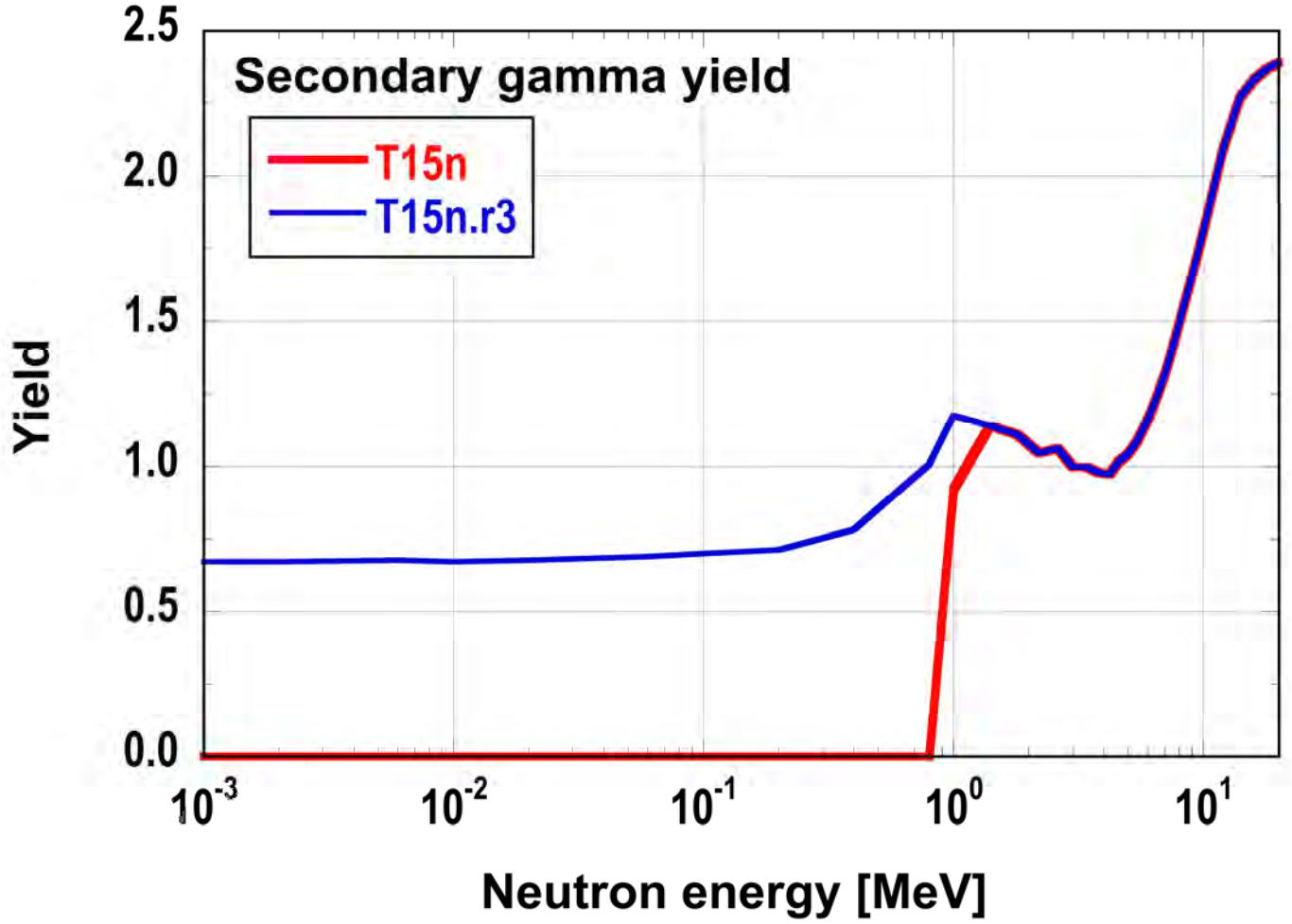


Probability density function (energy distribution) of secondary gamma in (n,α) reaction

Yield of secondary gamma in (n,α) reaction

- **Energy distribution** data of secondary gamma for neutrons less than **1.4 MeV** should be replaced to those for neutrons of 1.4 MeV.
- **Yield** data of secondary gamma for neutrons less than 1.4 MeV should be modified to keep energy-balance.

Gamma yield of (n,α) reaction in ^{40}K



Yield of secondary gamma in (n,α) reaction

Energy-balance check of revised (n,α) reaction

ENERGY BALANCE SUMMARY: Q = 3.87244E+06

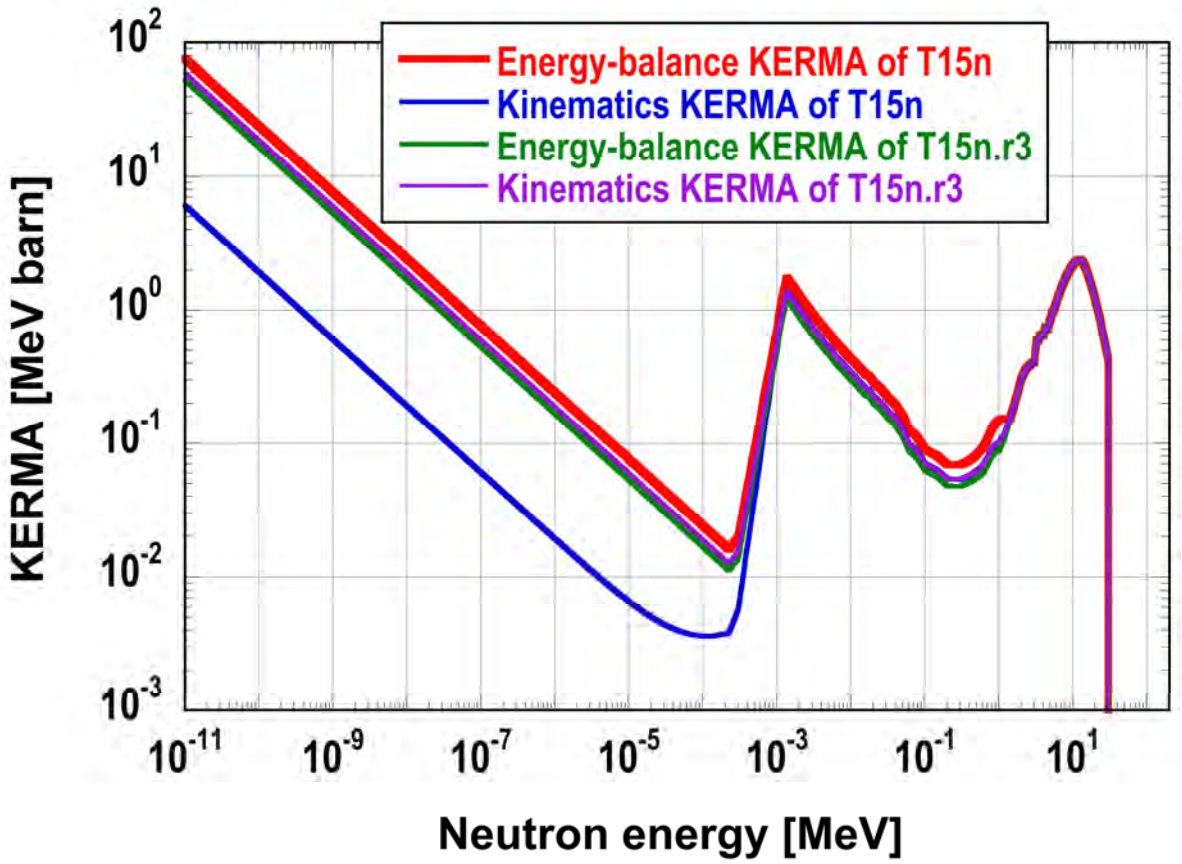
TOTAL SECONDARY ENERGY BY EMITTED PARTICLE (CM)

E	AVAIL	%DIFF	SUM	02004	17037	00000
1.00E-05	3.87E+06	0.01	3.87E+06	2.70E+06	8.69E+03	1.16E+06
1.00E+03	3.87E+06	0.00	3.87E+06	2.70E+06	8.69E+03	1.16E+06
2.00E+03	3.87E+06	0.02	3.88E+06	2.70E+06	8.72E+03	1.16E+06
6.00E+03	3.88E+06	0.07	3.88E+06	2.71E+06	8.79E+03	1.17E+06
1.00E+04	3.88E+06	0.12	3.89E+06	2.71E+06	8.85E+03	1.17E+06
2.00E+04	3.89E+06	0.21	3.90E+06	2.71E+06	8.90E+03	1.18E+06
6.00E+04	3.93E+06	0.46	3.95E+06	2.73E+06	8.85E+03	1.21E+06
1.00E+05	3.97E+06	0.66	4.00E+06	2.75E+06	9.05E+03	1.23E+06
2.00E+05	4.07E+06	1.93	4.15E+06	2.83E+06	9.42E+03	1.31E+06
4.00E+05	4.26E+06	2.34	4.36E+06	2.90E+06	1.00E+04	1.45E+06
6.00E+05	4.46E+06	0.56	4.48E+06	2.87E+06	1.06E+04	1.60E+06
8.00E+05	4.65E+06	-0.06	4.65E+06	2.90E+06	1.12E+04	1.74E+06
1.00E+06	4.85E+06	0.05	4.85E+06	2.80E+06	1.19E+04	2.03E+06
1.40E+06	5.24E+06	-9.23	4.75E+06	2.77E+06	1.31E+04	1.97E+06
1.80E+06	5.63E+06	-9.38	5.10E+06	3.14E+06	1.43E+04	1.94E+06

PSYCHE output for (n,α) reaction of TENDL-2015.r3

- Revised (n,α) reaction data generally keep energy-balance.

Partial KERMA of revised (n,α) reaction



- Partial energy-balance and kinematics KERMAs of (n,α) reaction in T15n.r3 are almost the same. They are different from those in T15n.