To the next major FENDL

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- Issues of FENDL-3.2b (=FENDL-3.2c)
- Issue on analysis of FNG tungsten experiment
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Introduction

- At the 2023 FENDL meeting we noted the following issues.
  - Iron : JENDL-5 is better than FENDL-3.2b (=FENDL-3.2c).
  - ^{63}Cu : JENDL-5 is better than FENDL-3.2b (=FENDL-3.2c).
  - ESS beryllium $S(\alpha,\beta)$ data considering crystallite domain size improve overestimation for low energy neutrons in beryllium experiment.
- Last year we examined an issue which F4E group encountered in analyzing FNG tungsten experiment.
- Here we introduce them briefly and propose additional requests to the next FENDL.

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- Issues of FENDL-3.2b (=FENDL-3.2c)
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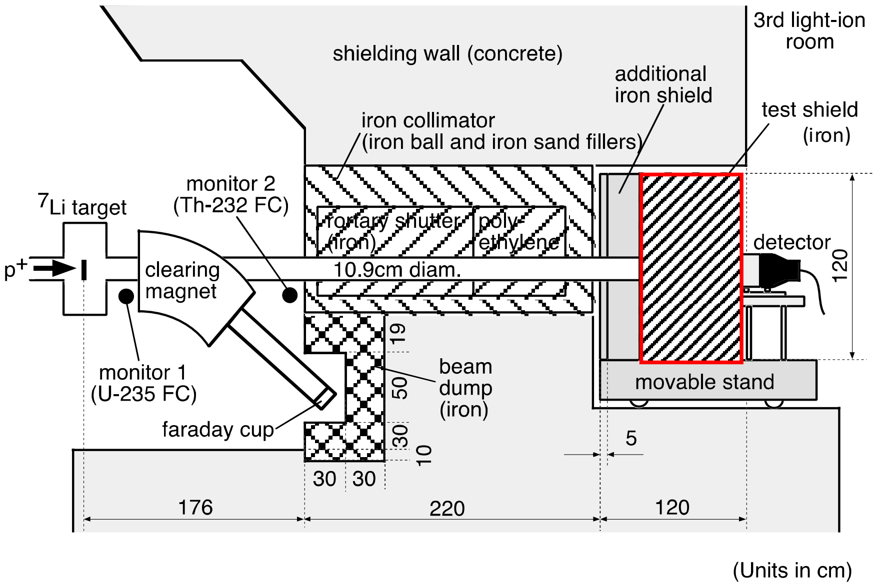
- Summary

TIARA iron experiment -(1)

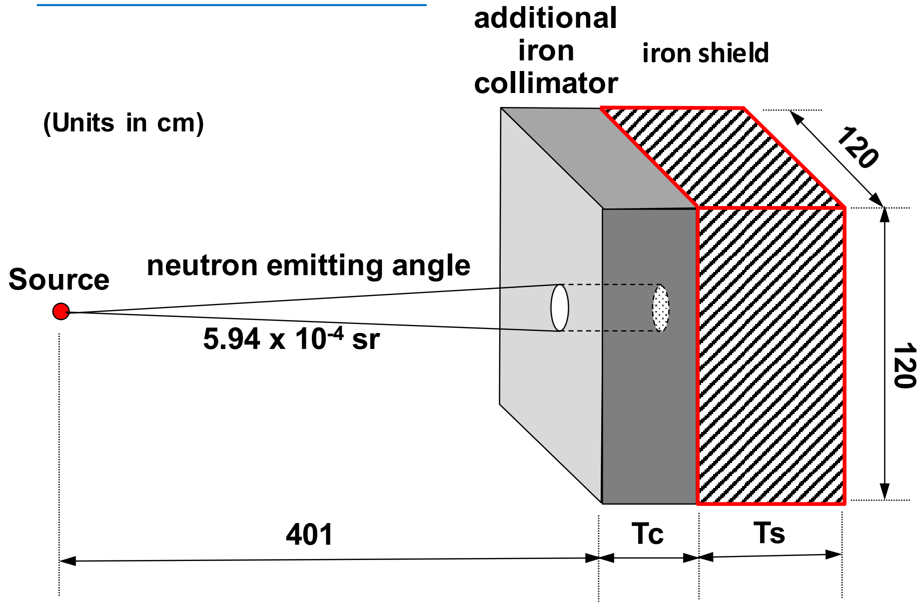
Experimental configuration



- 43 and 68 MeV of protons were bombarded on the Li-7 target.
- The generated neutrons, 40 and 65 MeV, were collimated and entered on the iron test shield.
- The neutron spectrum above 5 MeV was measured by scintillators.

See the following report for more details about the experiments and analyses:
H. Nakashima et al., JAERI-Data/Code 96-005, 1996

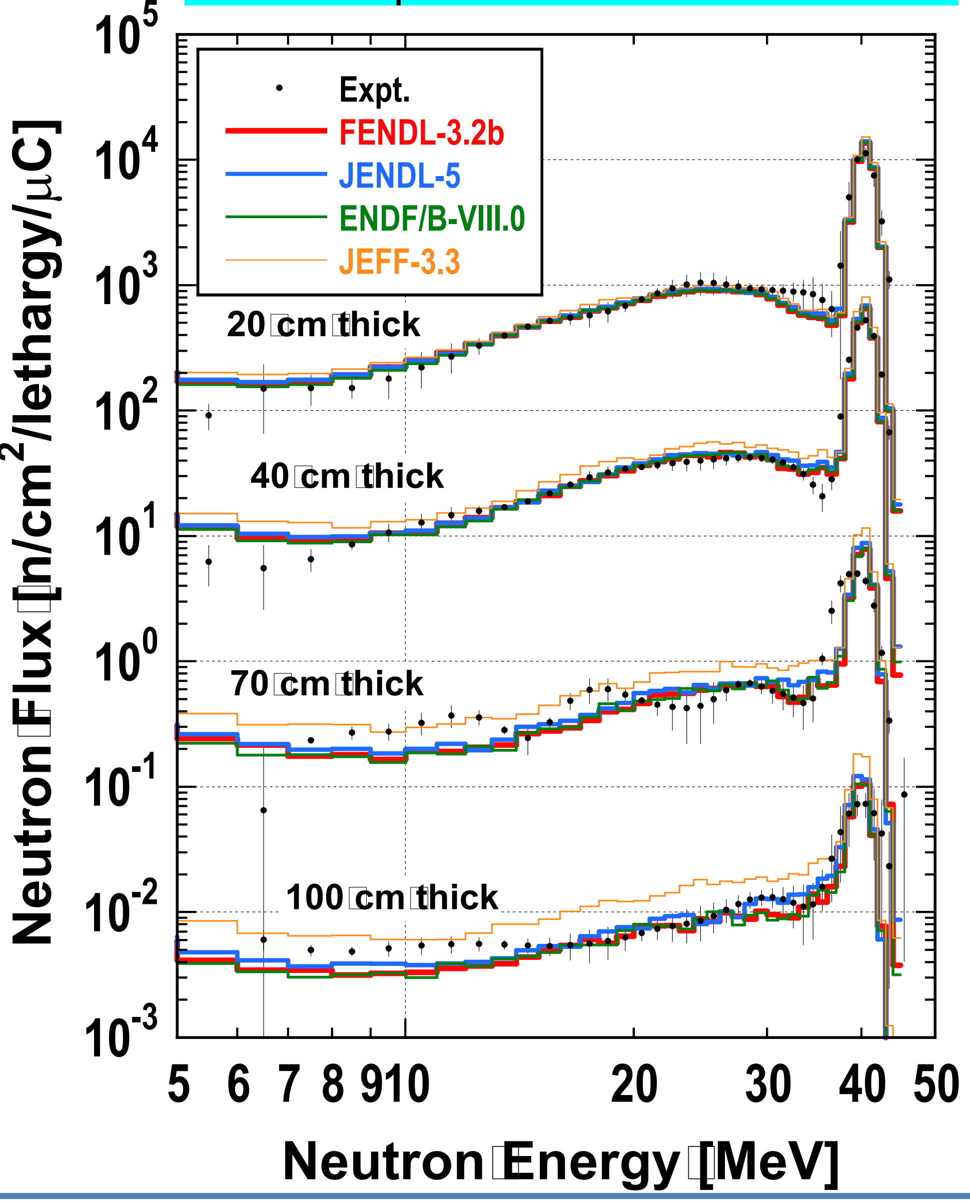
Calculation model



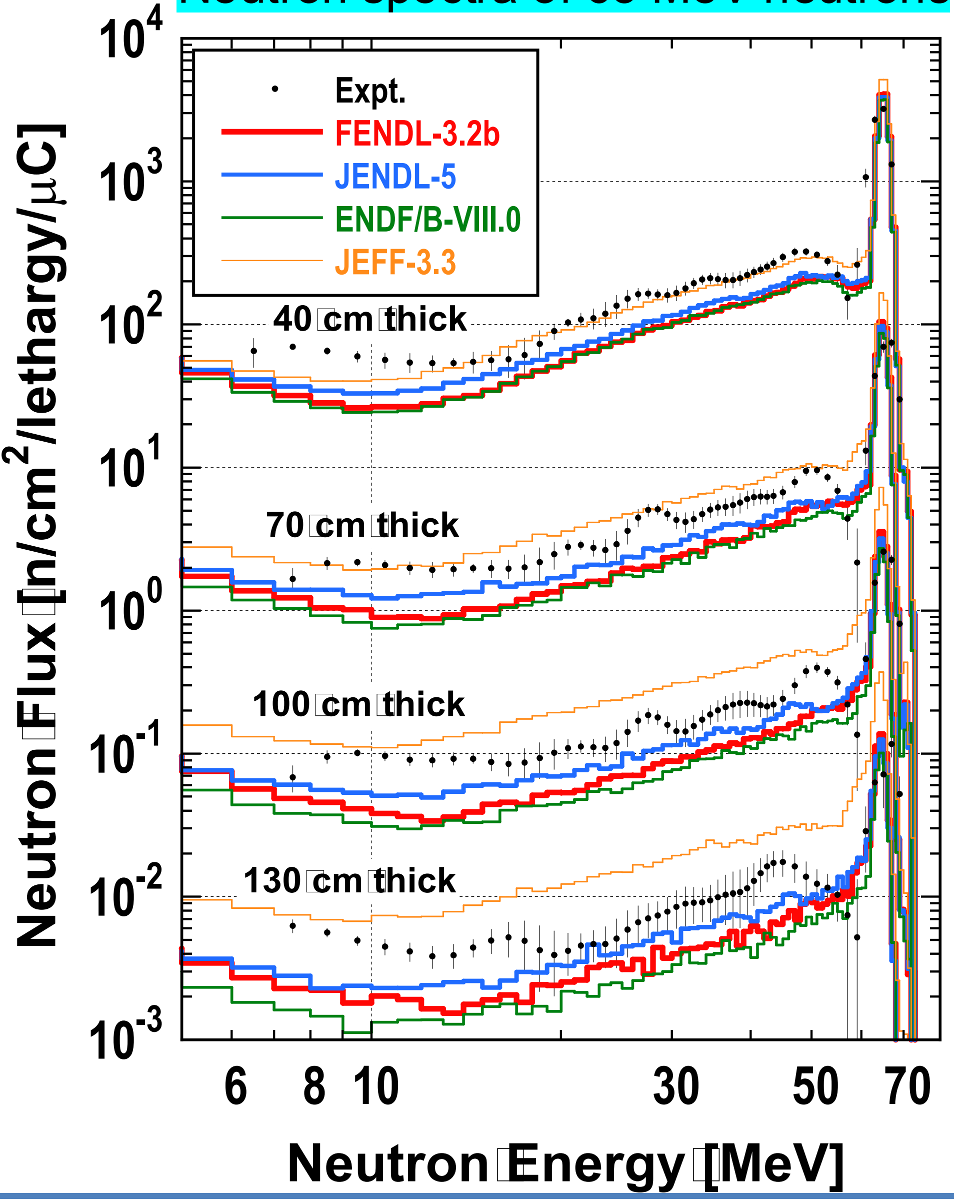
- Code: MCNP6.2
- Libraries:
  - FENDL-3.2b (iron = FENDL-3.2c)
  - JENDL-5
  - ENDF/B-VIII.0
  - JEFF-3.3
- The measured neutron spectrum was used as the source neutron in MCNP.

TIARA iron experiment -(2)

Neutron spectra of 40 MeV neutrons



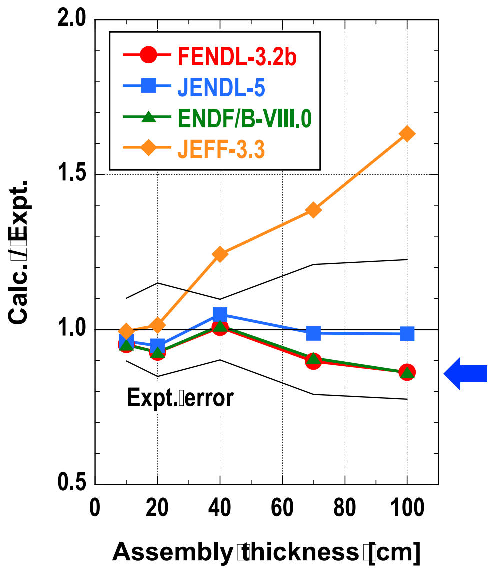
Neutron spectra of 65 MeV neutrons



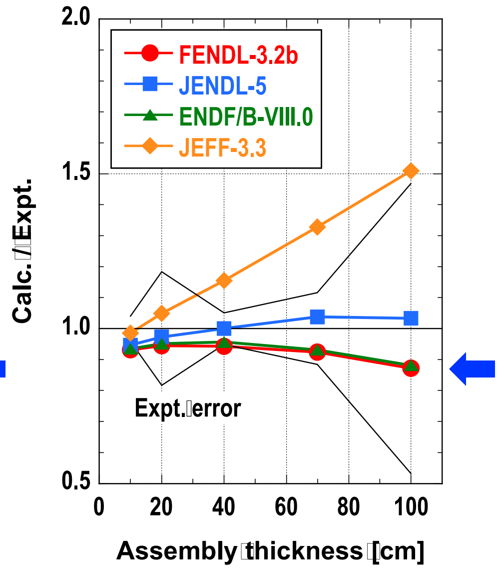
TIARA iron experiment -(3)

40 MeV neutron expt.

Cont. (10 – 35 MeV)

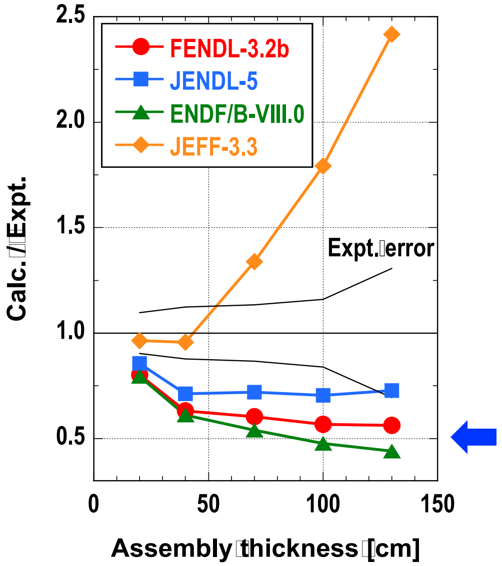


Peak (35 – 45 MeV)

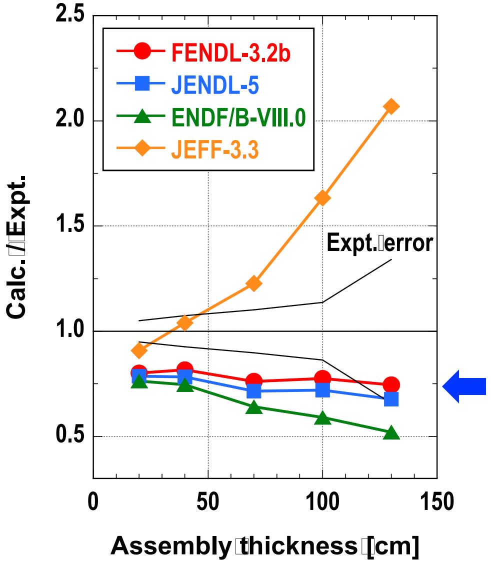


65 MeV neutron expt.

Cont. (10 – 60 MeV)



Peak (60 – 70 MeV)

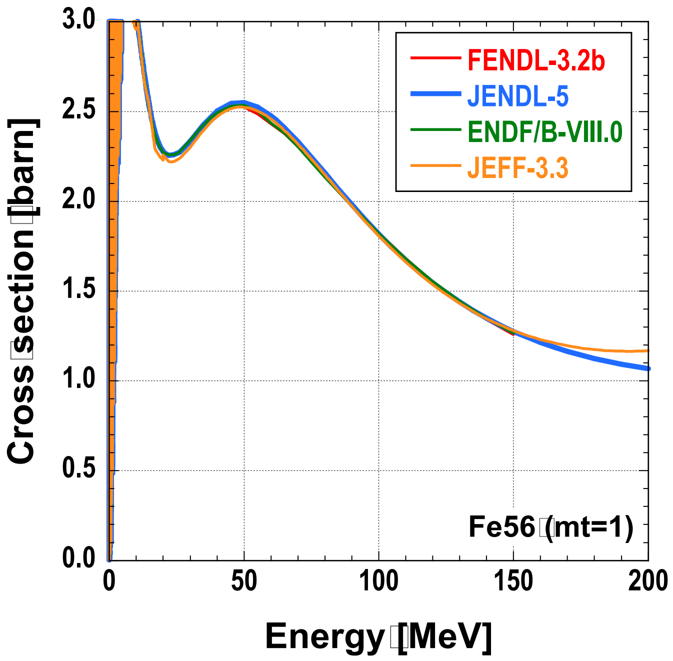


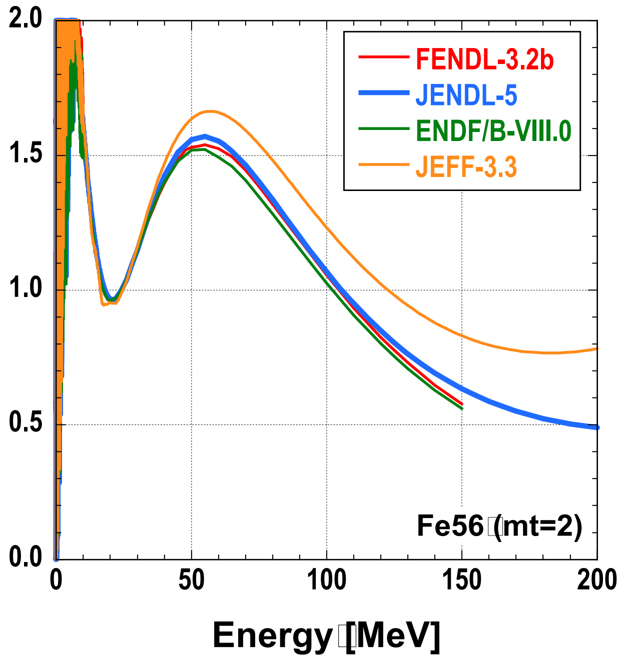
JENDL-5 is better than FENDL-3.2b.

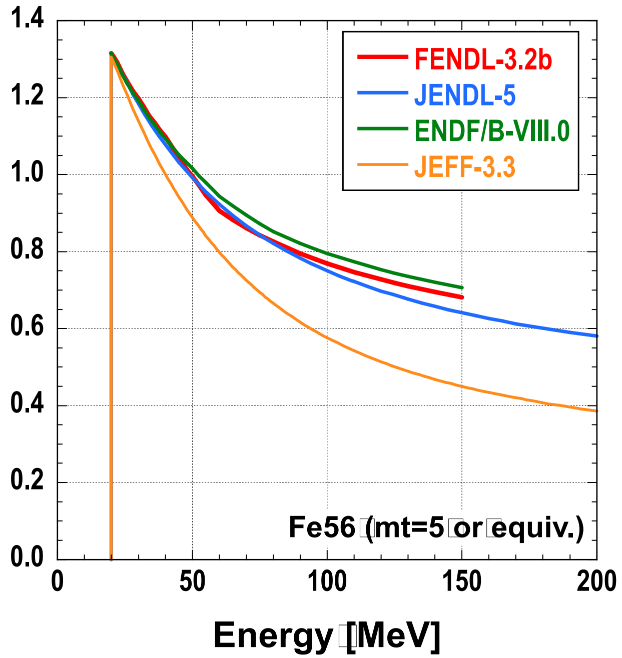
TIARA iron experiment -(4)

Possible reasons of the different calculation results

- Elastic scattering cross section (mt=2)
- Non-elastic scattering cross section (mt=5 or “total – elastic” : mt=5 equiv.)







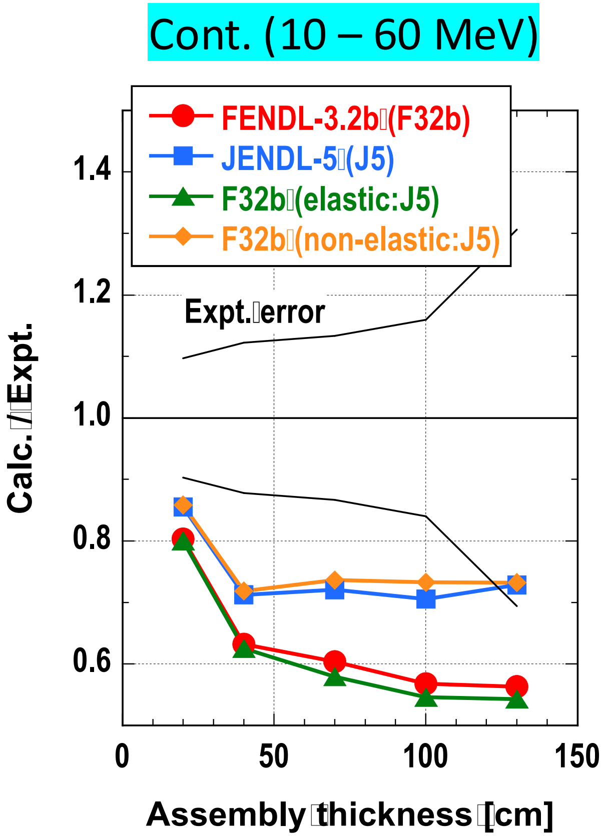
We examine reasons of the large C/E differences by replacing elastic scattering or non-elastic scattering data of Fe56 to those in JENDL-5.

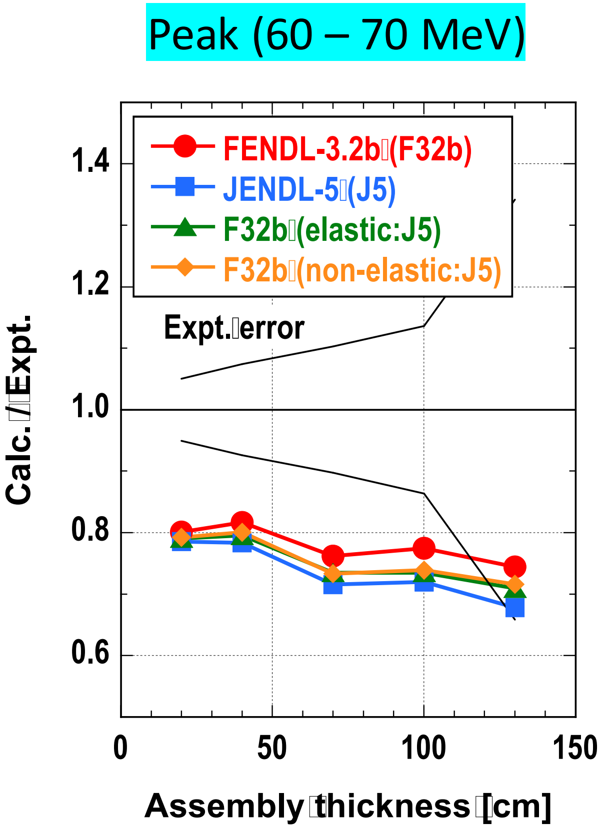
TIARA iron experiment -(5)

Modified Fe56 files of FENDL-3.2b

- Replaced elastic scattering data (mt=2) by those in JENDL-5 **F32b (elastic:J5)**
- Replaced non-elastic scattering data ("total – elastic") by those in JENDL-5 **F32b (non-elastic:J5)**

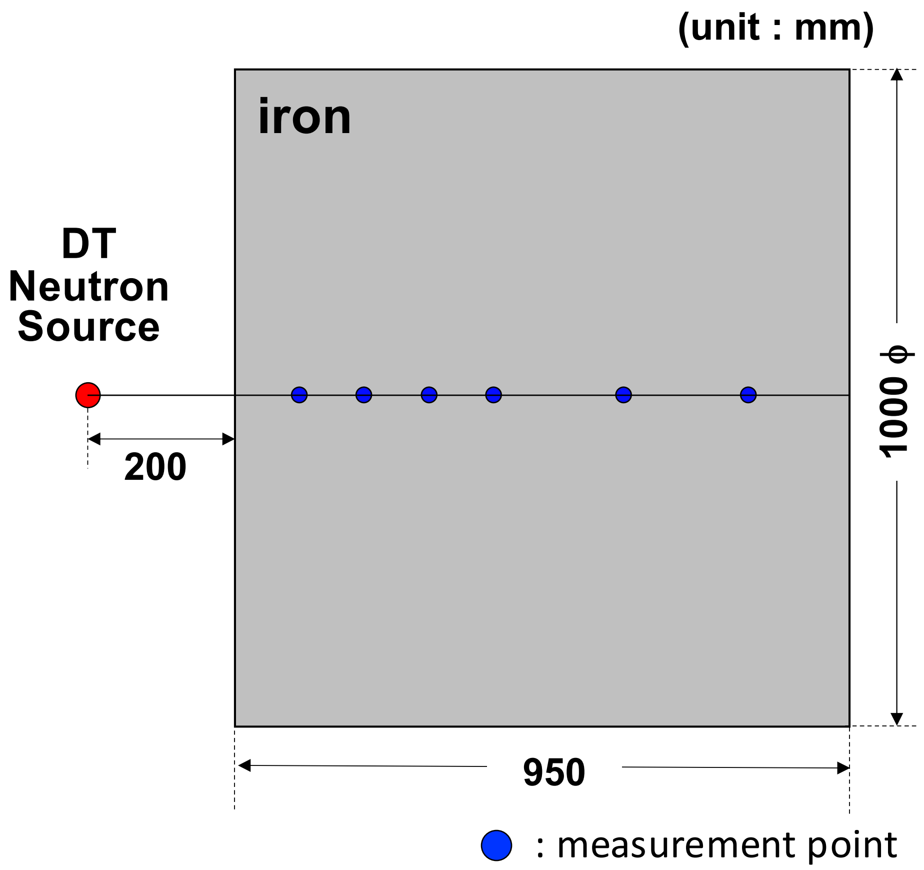
65 MeV Neutron

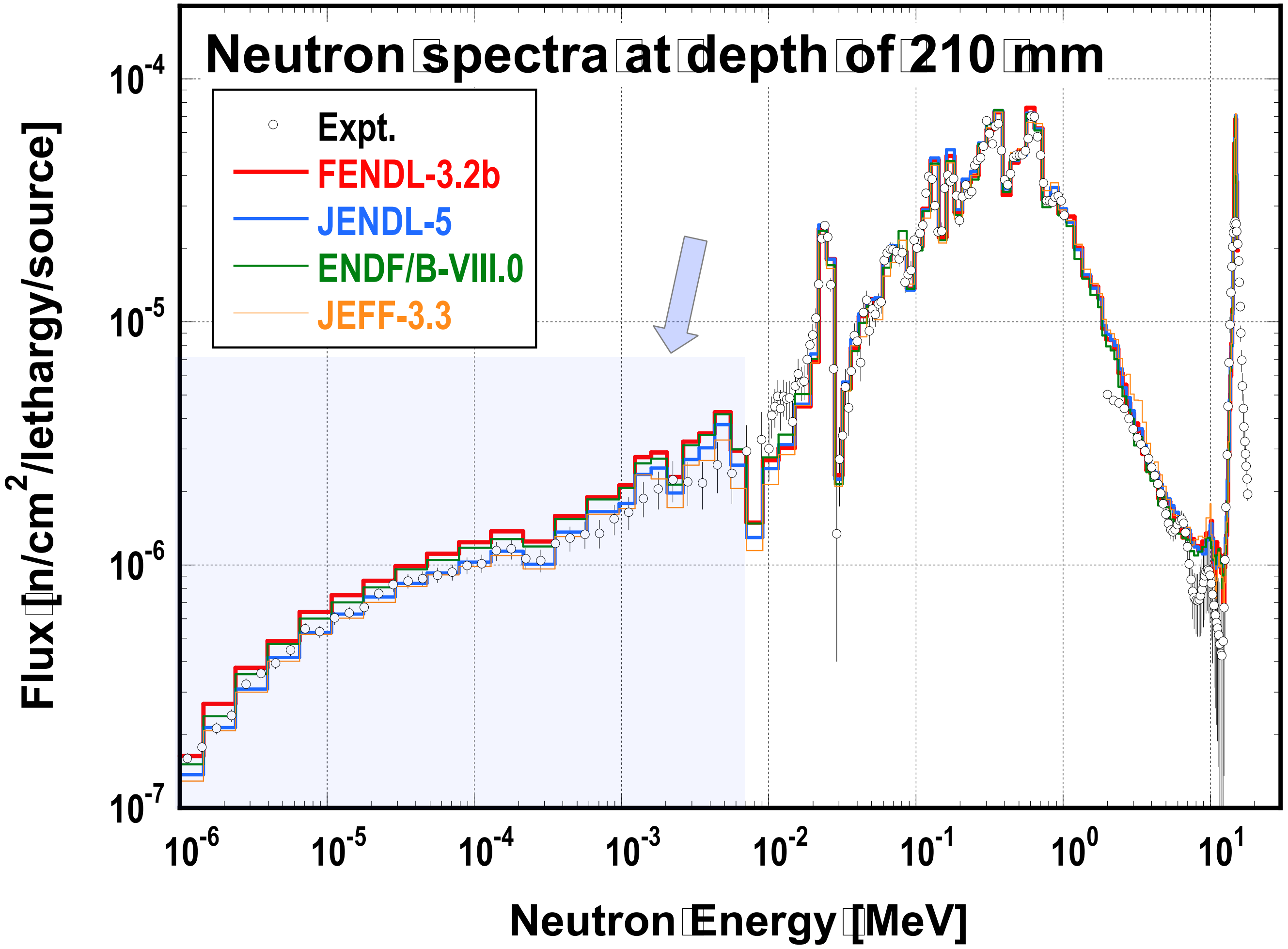




- Effect of elastic scattering data (mt=2) is small.
- Effect of non-elastic scattering data (mt=5) is large to continuum neutron fluxes.

FNS iron experiment -(1)

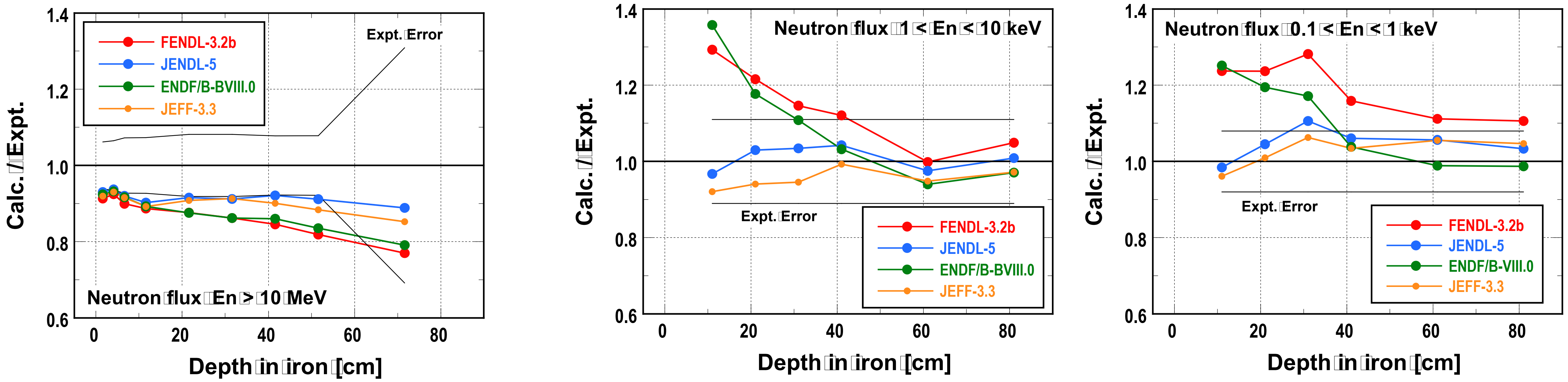




- Neutron spectra over almost the whole energy and reaction rates of several reactions were measured inside the iron assembly.

FENDL-3.2b and ENDF/B-VIII.0 overestimate the measured neutron spectrum below 10 keV!

FNS iron experiment -(2)

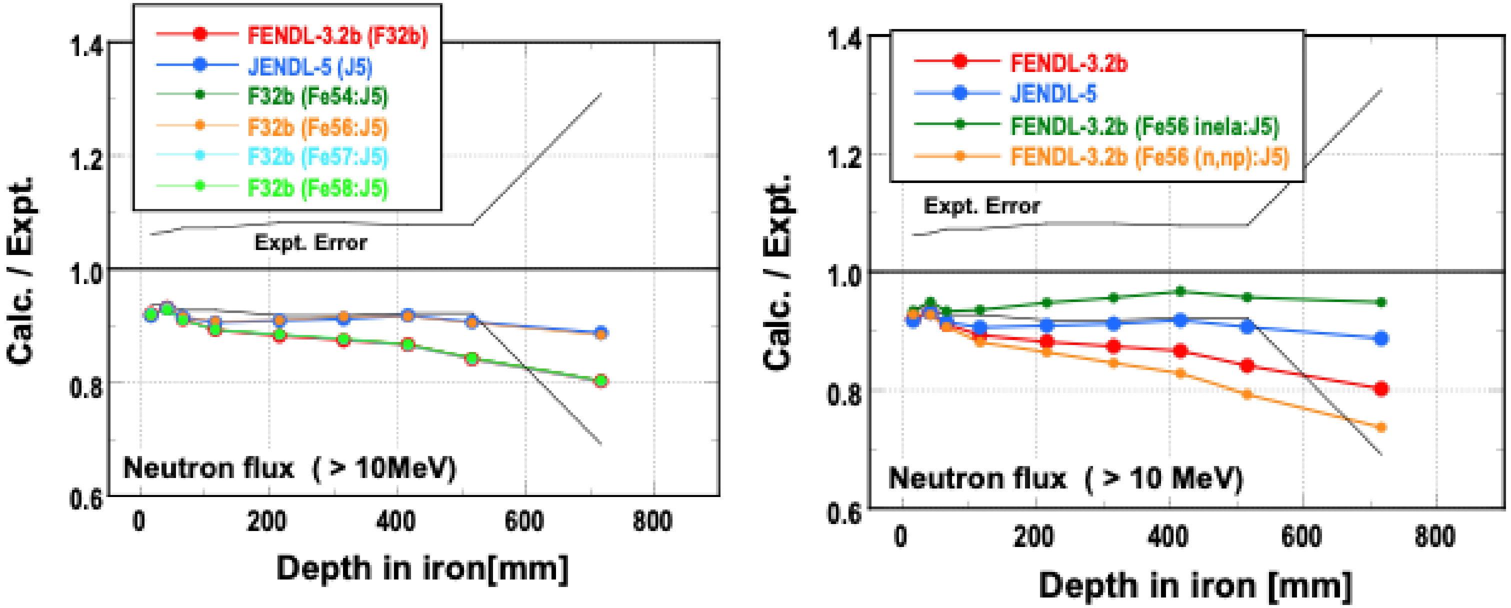


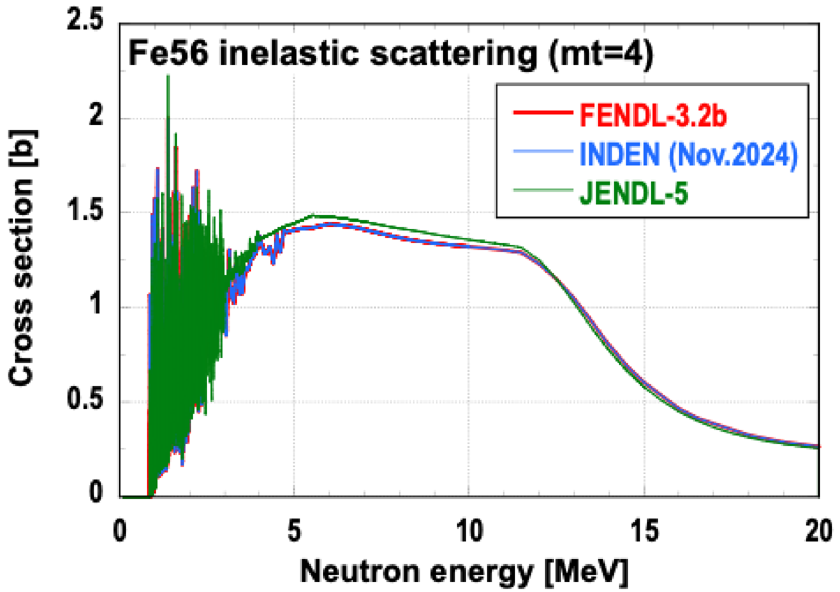
FENDL-3.2b and ENDF/B-VIII.0 tend to underestimate measured neutron flux above 10 MeV !

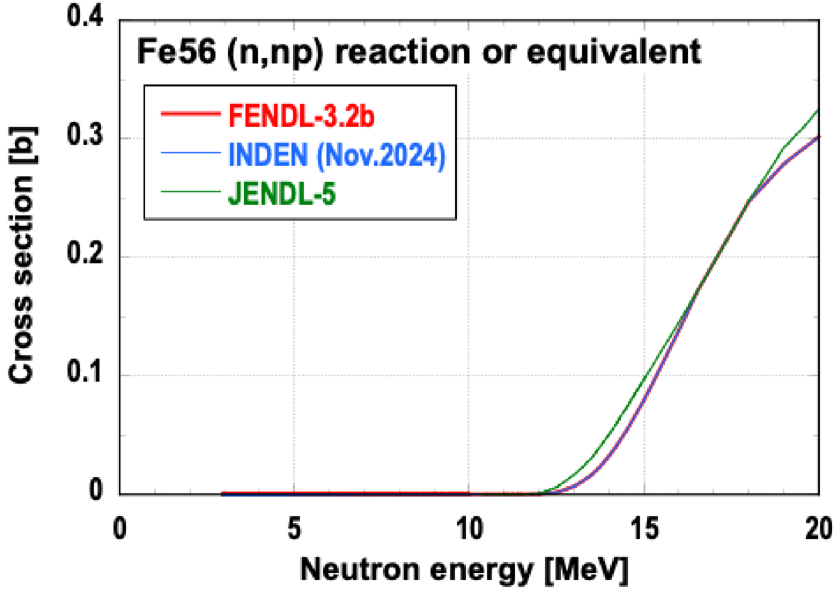
FENDL-3.2b and ENDF/B-VIII.0 tend to overestimate measured neutron flux below 10 keV up to depth of 60 cm!

Reasons of underestimation above 10 MeV

- **We compare the neutron fluxes between FENDL-3.2b and JENDL-5.**

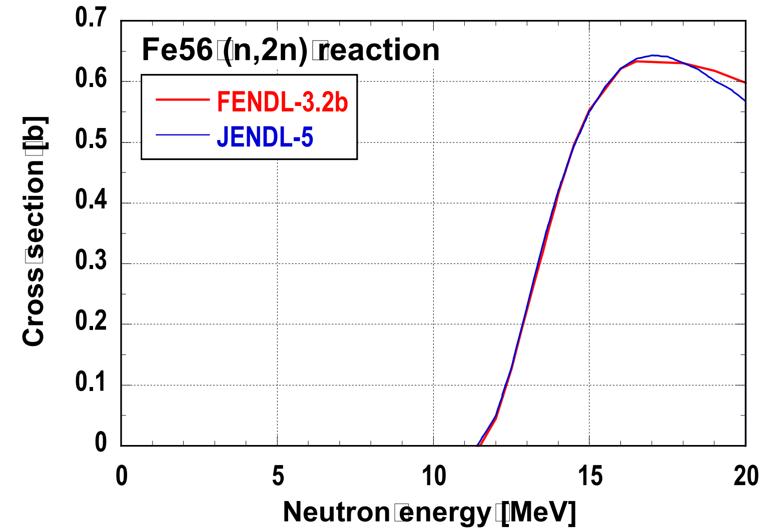


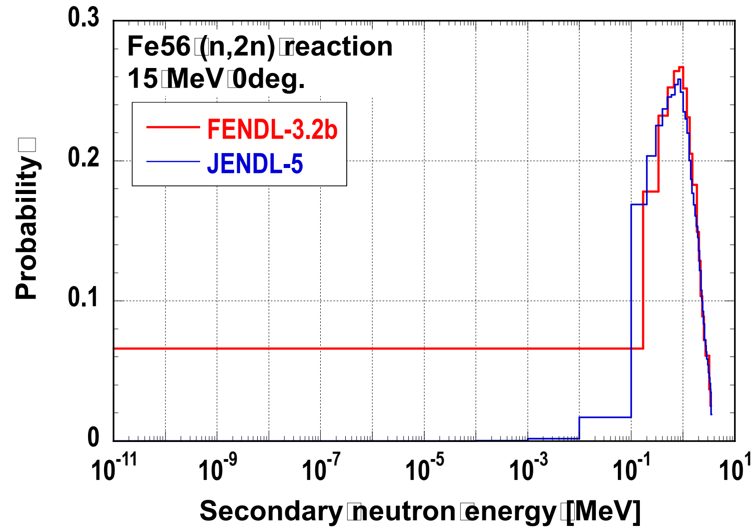


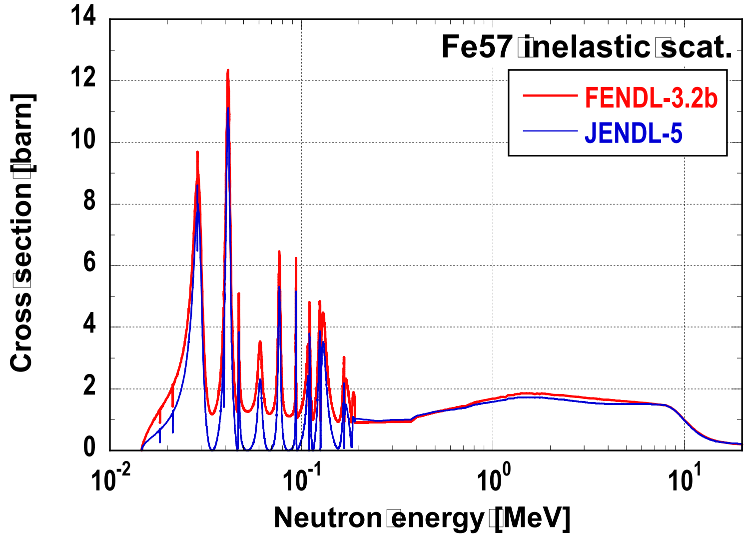


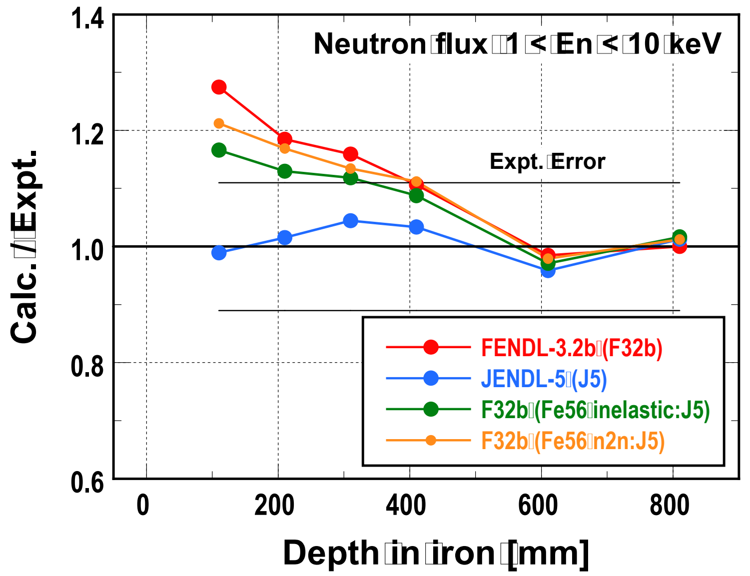
- FENDL-3.2b underestimates the measured neutron flux above 10 MeV.
- JENDL-5 shows the better agreement with the measured ones.
- ➢ **The inelastic scattering and (n,np) reaction data of ^{56}Fe cause the difference between FENDL-3.2b and JENDL-5.**

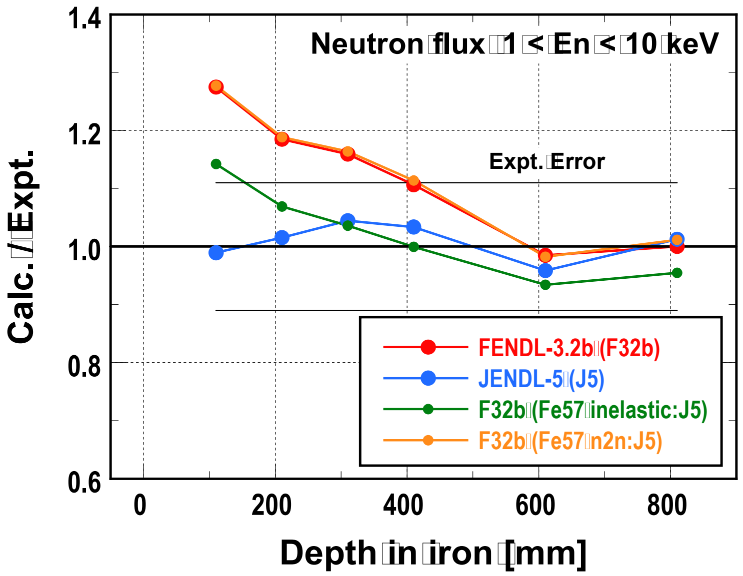
Reasons of overestimation below 10 keV





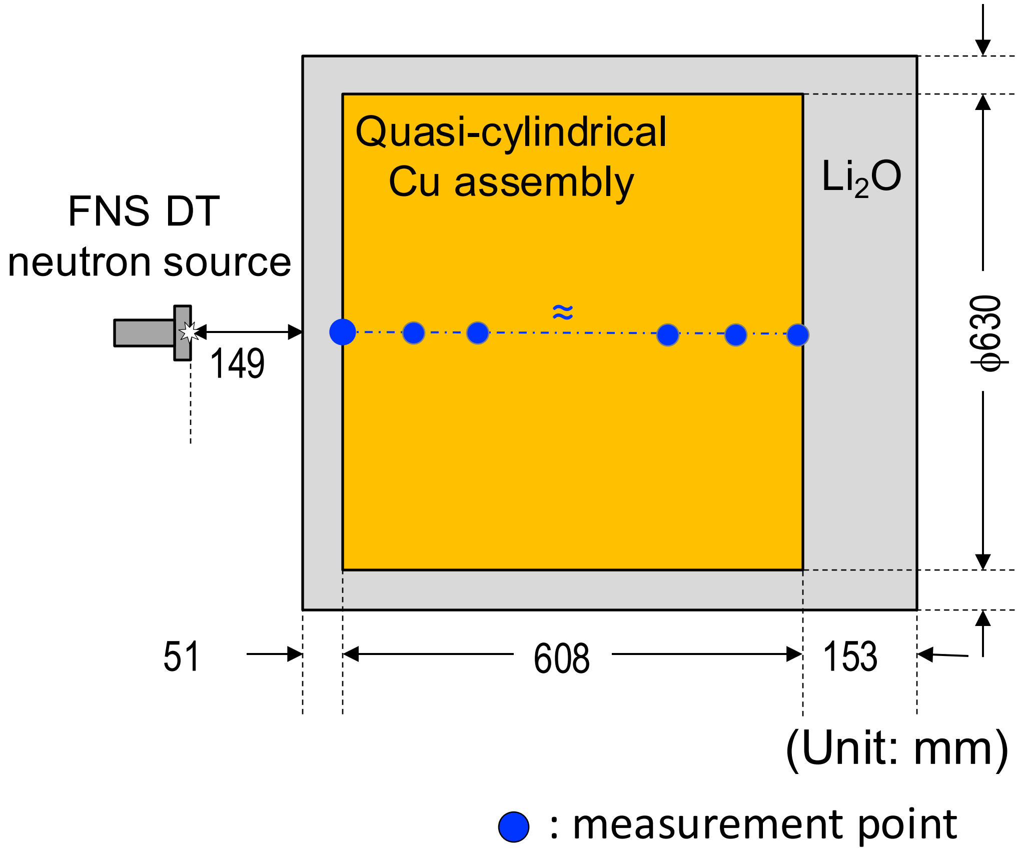


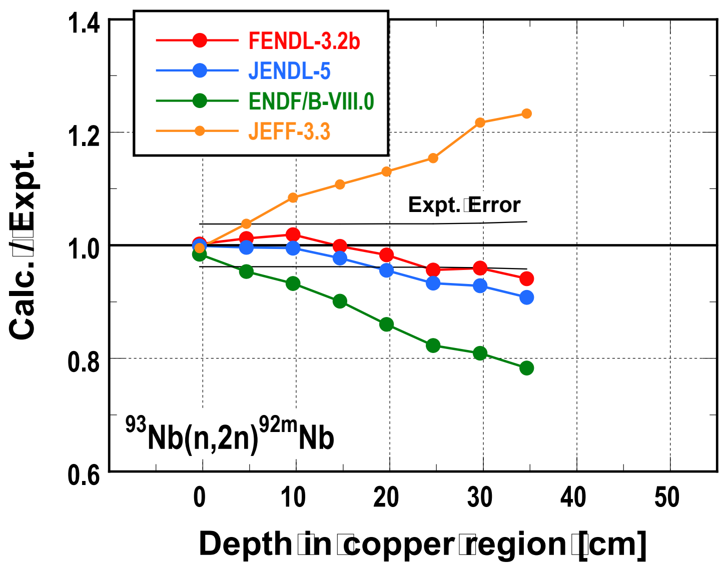


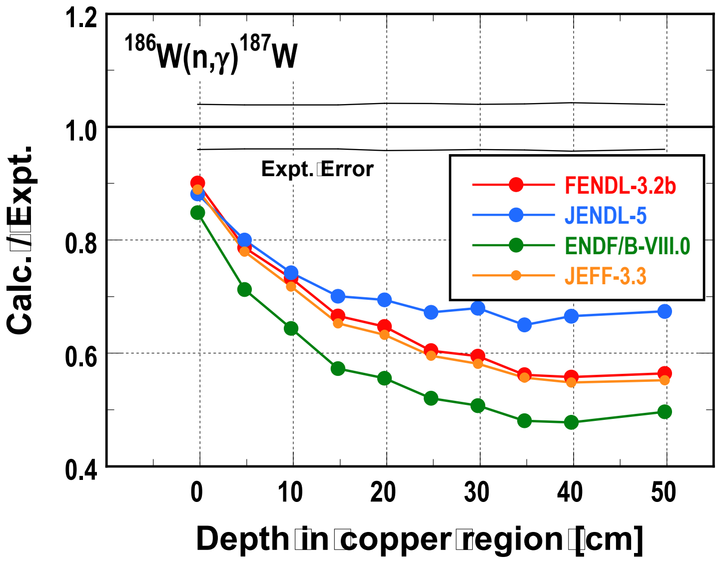


- Inelastic scattering and (n,2n) reaction data of Fe56 and inelastic scattering data of Fe57 in FENDL-3.2b cause the overestimation of neutron flux below 10 keV.

FNS copper experiment

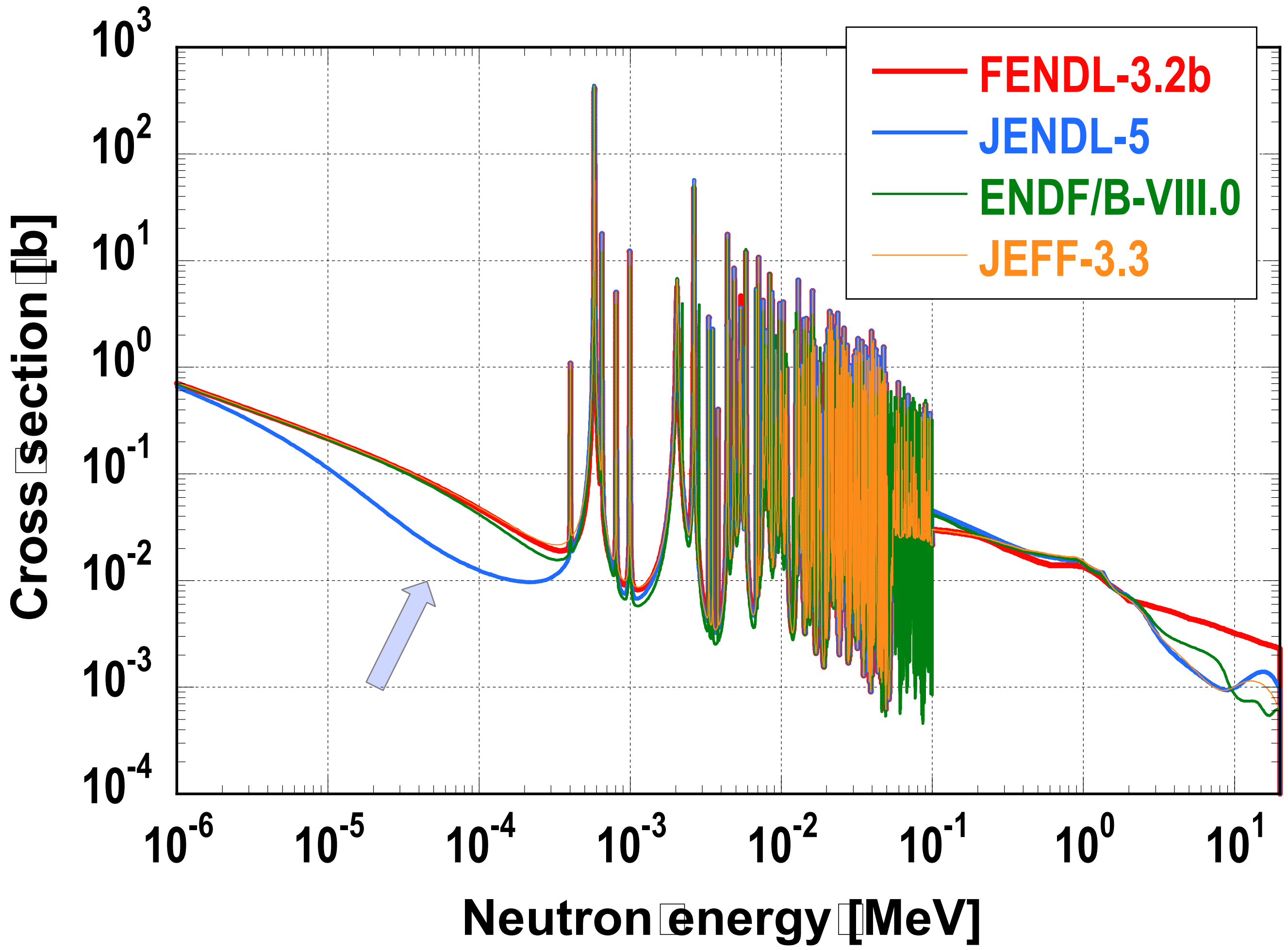






- *FENDL-3.2b (= FENDL-3.2c) is the best for neutrons over 10 MeV.*
- *FENDL-3.2b tends to underestimate as same as before. Only JENDL-5 shows the improvement due to ^{63}Cu.*

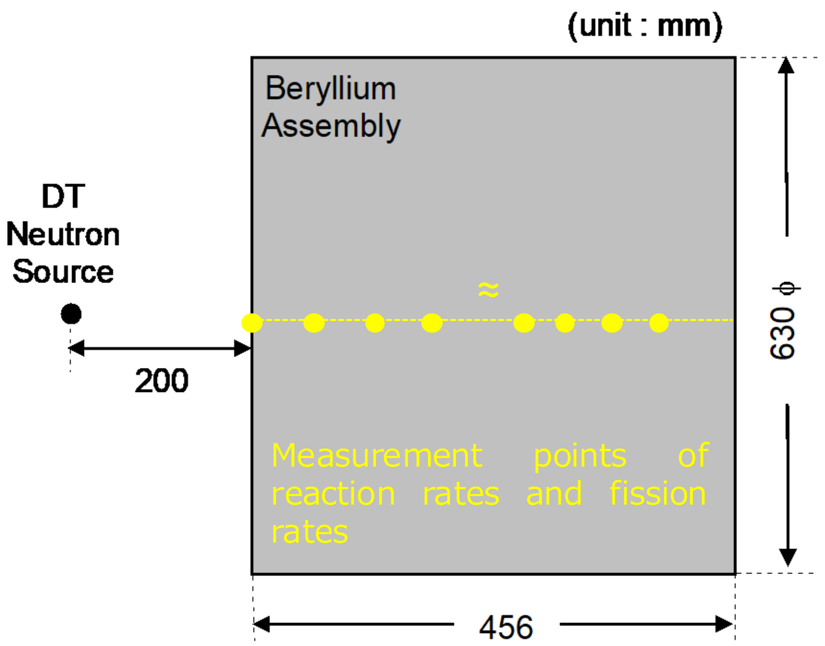
JENDL-5 ^{63}Cu capture cross section

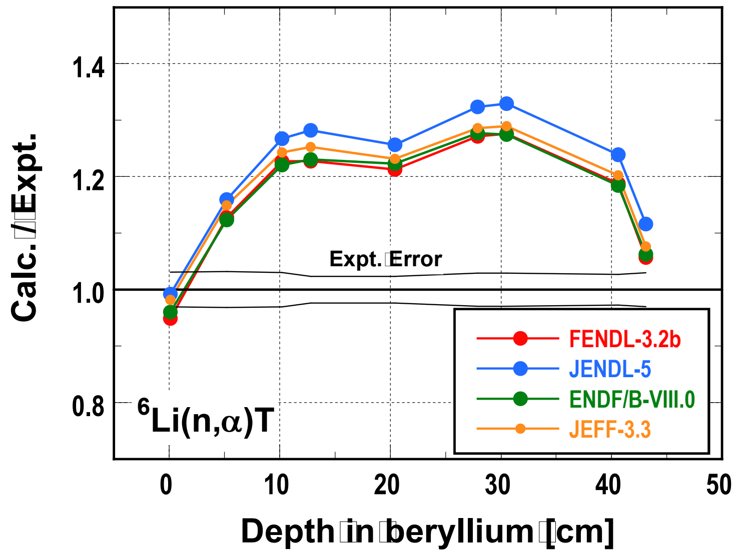


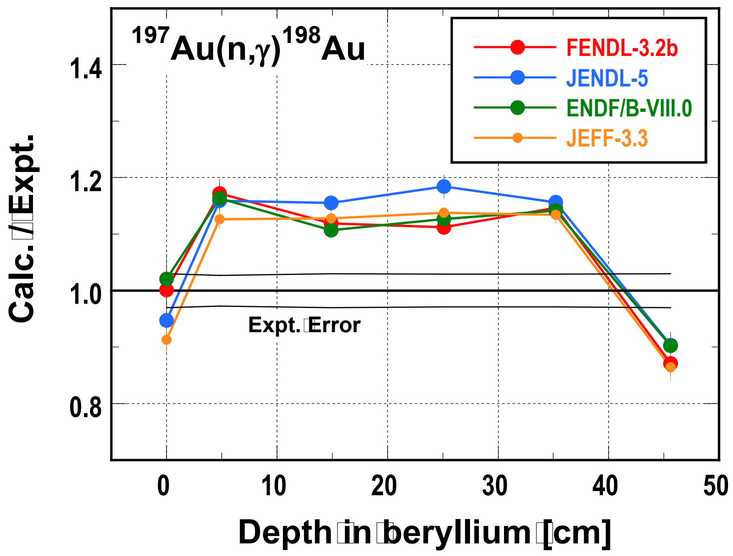
JENDL-5 is very different below 400 eV from other libraries.

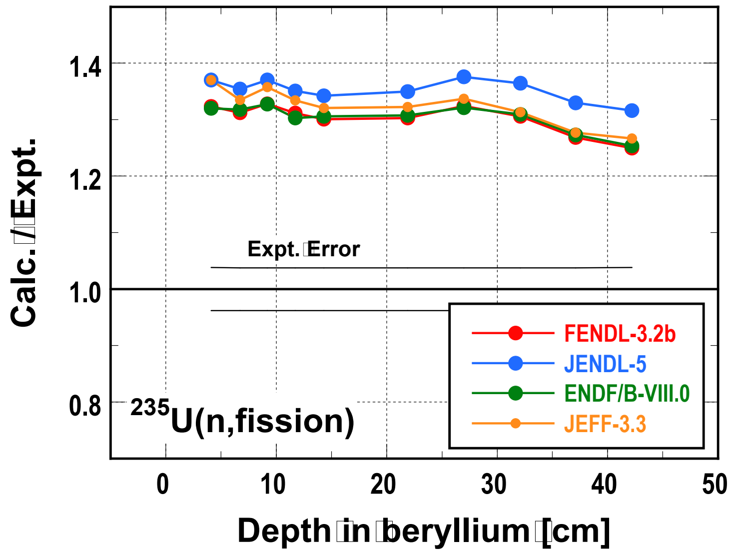
→ Improvement of $^{186}W(n,\gamma)^{187}W$ reaction rate

FNS beryllium experiment -(1)







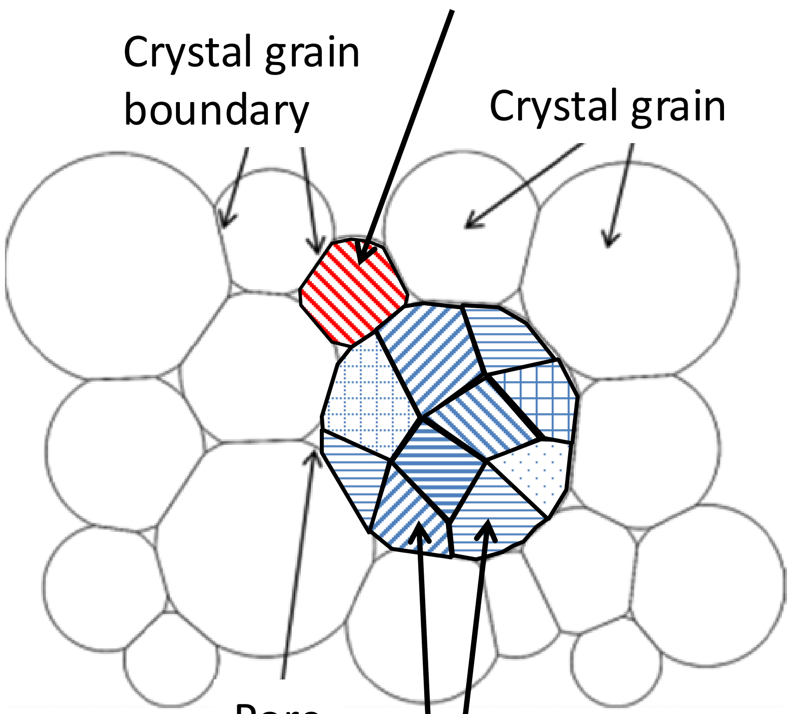


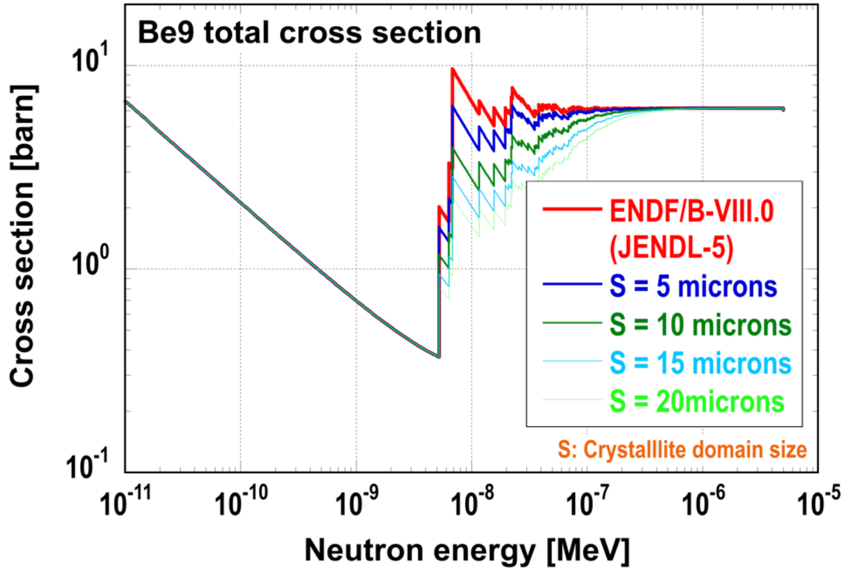
- All libraries cause overestimation of reaction rates sensitive to low energy neutrons!
  (FENDL-3.2c Be9 is the same as FENDL-3.2b Be9.)
- This has been not solved for a long time…

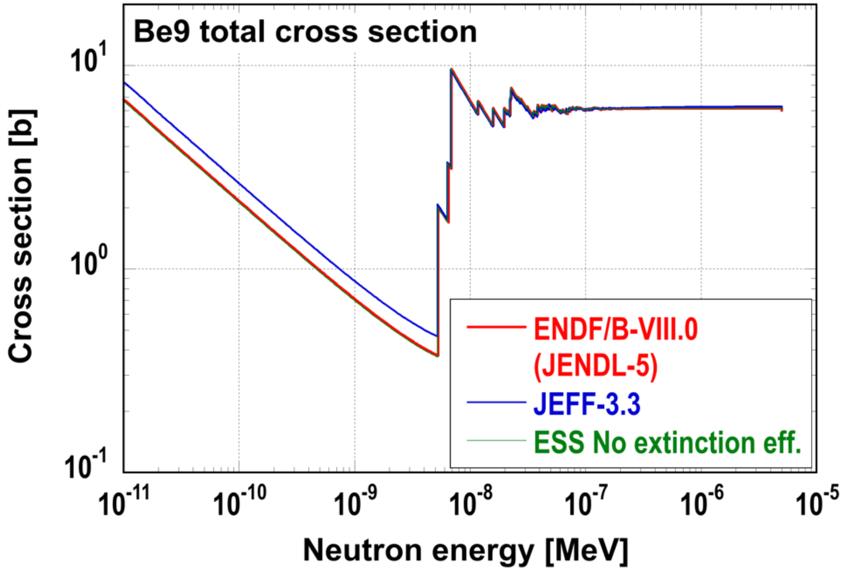
FNS beryllium experiment -(2)

Recently European Spallation Source (ESS) group produced beryllium thermal scattering law (TSL) data considering crystallite domain size*.

* • D. D. DiJulio et al., Impact of crystallite size on the performance of a beryllium reflector, *Journal of Neutron Research* 22, 275–279 (2020).
  • D. D. DiJulio et al., Thermal scattering libraries for cold and very-cold neutron reflector materials, *EPJ Web of Conferences* 284, 17013 (2023).

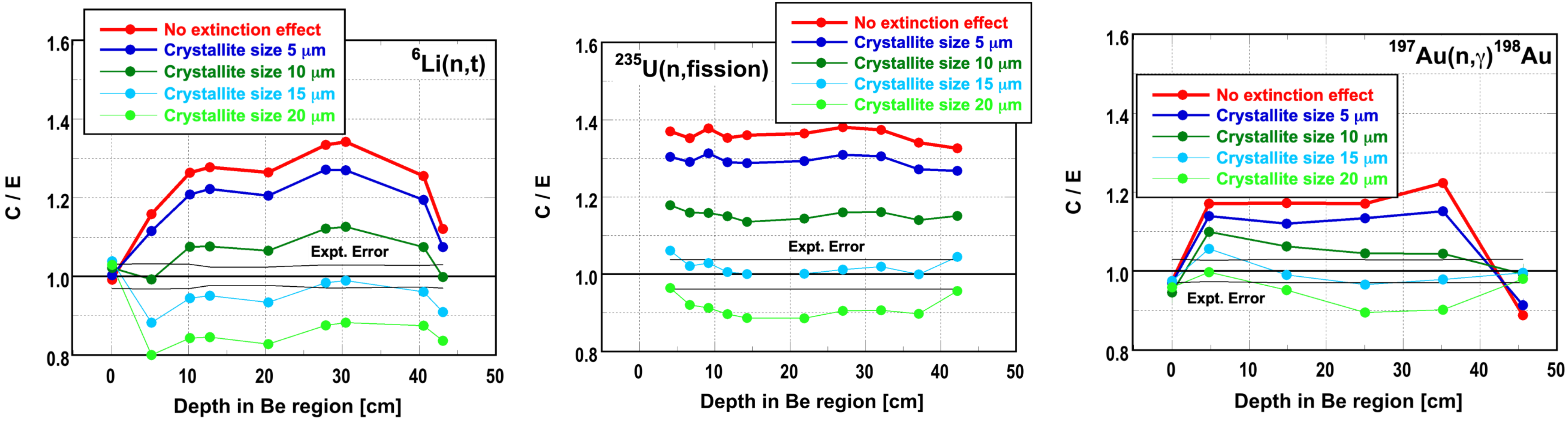






Cross sections of 0.005 - 0.4 eV are very different corresponding to crystallite domain size! (because of extinction effect)

FNS beryllium experiment -(3)



- Overestimation of reaction rates sensitive to lower energy neutrons decreases with increasing crystallite domain size!
- Data of 10 or 15 microns are the best!
- ESS data should be included in next FENDL.

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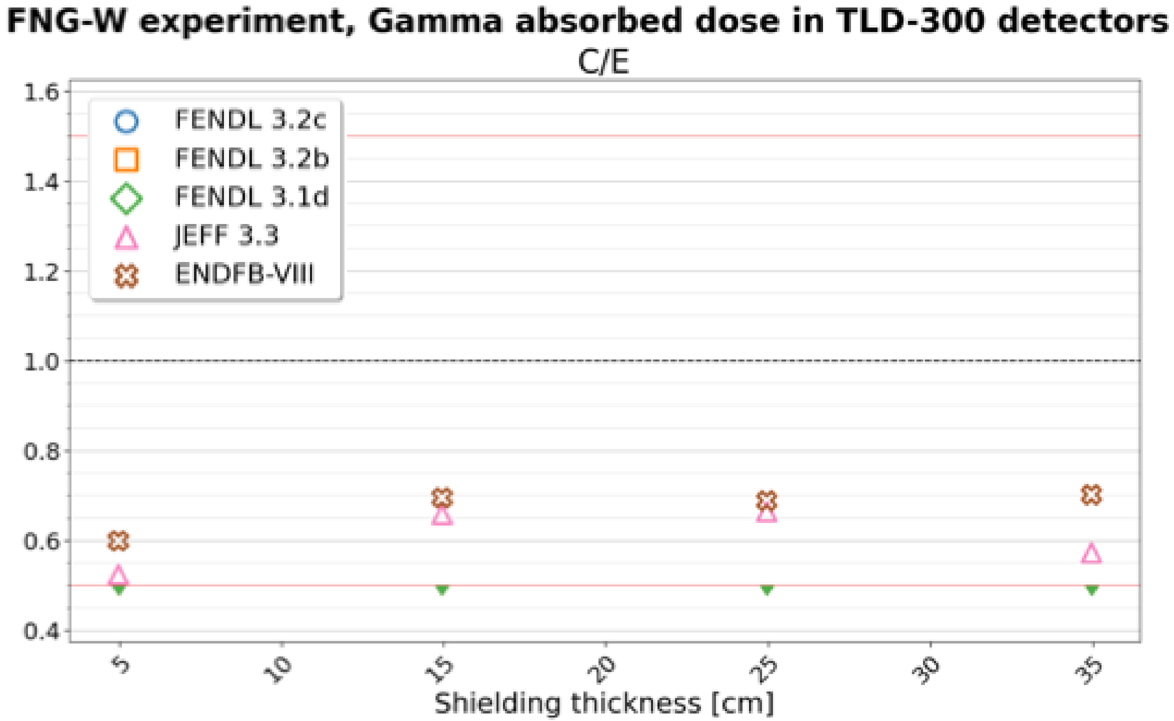
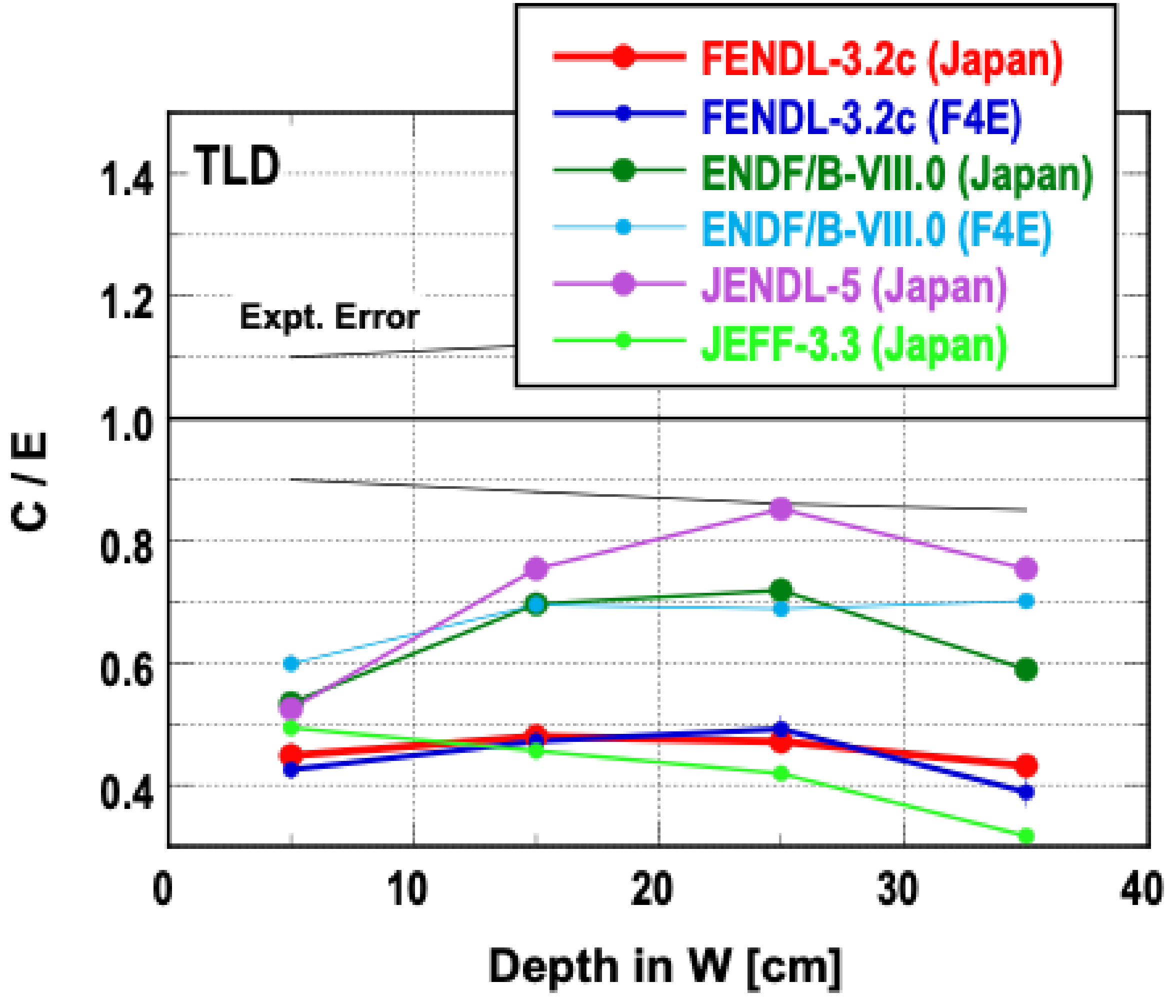
F4E analysis of FNG tungsten experiment

- Last year Dr. Laghi, F4E, reported FENDL is significantly worse (~0.4 C/E) than JEFF and ENDF (~0.6 C/E) in gamma heating of the FNG W experiment with MCNP input in SINBAD.
- Dr. Fabbri provided us the MCNP input file which Dr. Laghi used.
- Thus, we examined this issue.
  - ➢ Code : MCNP6.2
  - ➢ ACE file
    - ✓ Official FENDL-3.2c ACE file
    - ✓ Official ENDF/B-VIII.0 ACE file
    - ✓ Official JEFF-3.3 ACE file
    - ✓ Official JENDL-5 ACE file
    - ✓ Photo-atomic : mcplib84



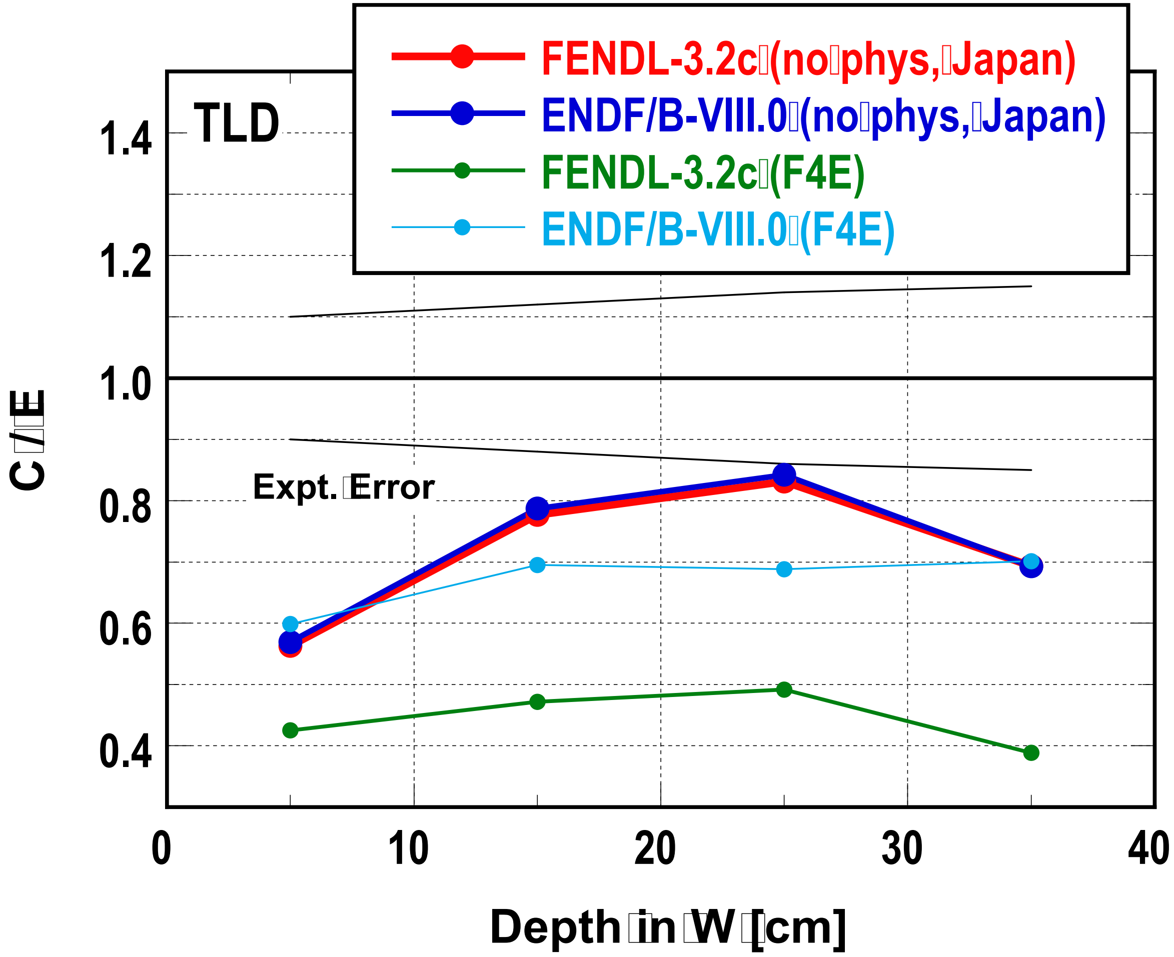
Results -(1)



C/E of gamma heating with CaF TLD

- Our calculated gamma heating data are similar to Dr. Laghi's ones.
- Our calculation with JENDL-5 is different from others.
- Our calculation with ENDF/B-VIII.0 stopped due to bad trouble "erg>emax 100 times in one collision.".
- Thus, we deleted "phys:n 16.0 0." because the first parameter emax (e.g. 16.0 in "phys:n 16.0 0.") might cause the bad trouble.

Results -(2)

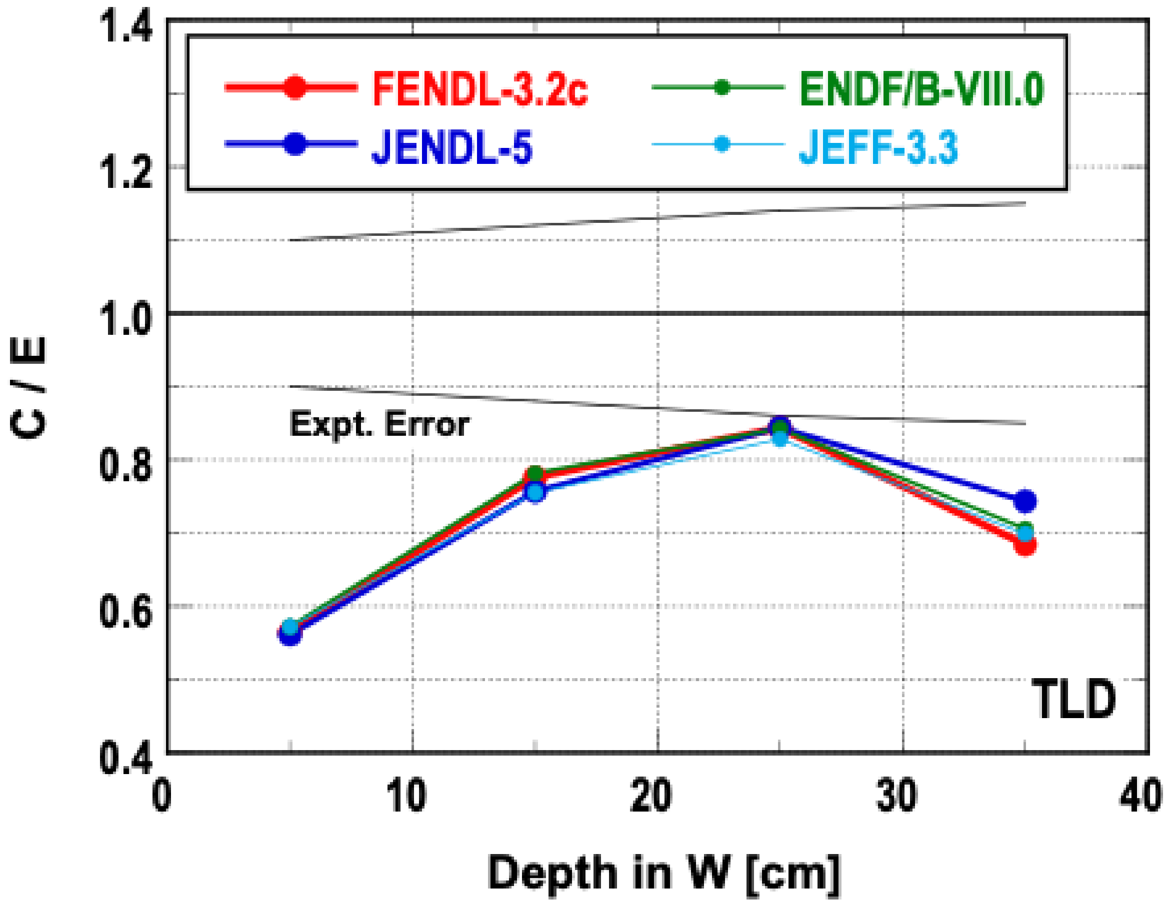


C/E of gamma heating with CaF TLD

- If "phys:n 16.0 0." was deleted, the calculated gamma heating data changed drastically.
- The difference between gamma heating data with FENDL-3.2c and ENDF/B-VIII.0 became very small.
- We are afraid that "phys:n 16.0 0." causes something wrong for tungsten data of FENDL-3.2c and ENDF/B-VIII.0.

"phys:n 16.0 0." causes something wrong.

Results -(3)

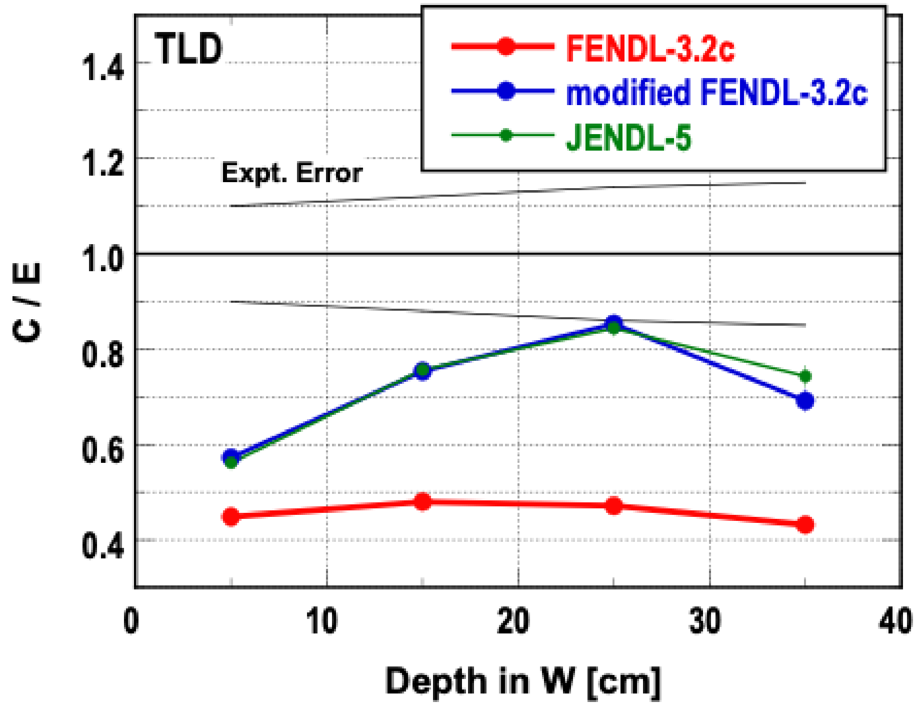


C/E of gamma heating with CaF TLD
(without ”phys:n 16.0 0.”)

- If ”phys:n 16.0 0.” is deleted, all the calculated gamma heating data are almost the same.
- JENDL-5 with ”phys:n 16.0 0.” is the same as JENDL-5 without ”phys:n 16.0 0.”
- Thus FENDL-3.2c, ENDF/B-VIII.0 and JEFF-3.3 seem to have some problems.
- After a lot of trials and errors we specified the reason.

Results -(4)

- The first two cross sections of MF3 MT28 (n,np) and MT41 (n,2np) data in W isotopes of FENDL-3.2c, ENDF/B-VIII.0 and JEFF-3.3 are 0.0 b as below.
- NJOY produces MT28 and MT41 cross sections from the second energy, though it does MT28 and MT41 energy distribution data from the first energy.
- Probably this situation caused the problem.
- Thus we changed the second cross section 0.0 b to a very small value (e.g. 10^{-20} b) in FENDL-3.2c.
- Then the modified FENDL-3.2 provides a good result even with ”phys:n 16.0 0.” .



C/E of gamma heating with CaF TLD (with ”phys:n 16.0 0.”)

W182 MF3 MT41

```
 7.418200+4 1.803850+2          0          0          0          07431 3 41
-1.467100+7-1.467100+7          0          0          1        237431 3 41
         23          2                                          7431 3 41
 1.475230+7 0.000000+0 1.700000+7 0.000000+0 1.800000+7 2.01513-127431 3 41
 1.900000+7 2.14401-10 2.000000+7 3.593950-9 2.200000+7 5.985370-67431 3 41
```

Results -(5)

- The issue can occur in a lot of nuclei of FENDL-3.2c.

  Ag109, Ar036, Ar038, Ar040, Ba130, Ba132, Ba134, Ba135, Ba136, Ba137
  Ba138, Bi209, Br079, Br081, C_013, Cd106, Cd111, Cd113, Ce136, Ce138
  Ce140, Ce142, Co059, Cr050, Cr052, Cr053, Cr054, Cs133, Er162, Er164
  Er166, Er167, Er168, Er170, F_019, Ga069, Ga071, Gd157, Gd160, Ge070
  Ge072, Ge073, Ge074, Ge076, Hf174, Hf176, Hf177, Hf178, Hf179, Hf180
  Lu175, Lu176, Mg024, Mg025, Mg026, Mo092, Mo094, Mo095, Mo096, Mo097
  Mo098, Mo100, Nb093, O_016, O_017, O_018, Pb204, Pb206, Pb207, Pb208
  Pt190, Pt192, Pt194, Pt195, Pt196, Pt198, Re185, Re187, S_032, S_033
  Sb121, Sb123, Sc045, Ta181, Th232, Ti047, Ti048, Ti049, Ti050, W_180
  W_182, W_183, W_184, W_186, Y_089, Zr090, Zr091, Zr092, Zr094, Zr096

Results -(6)

- Solutions for the issue
  1. *To delete 'Phys:n' data*
  2. *To change the second cross section 0.0 b to a very small value (e.g. 10^{-20} b) or to delete the first energy data of MF3 and MF6 in the case that the first two cross sections of MF3 are 0.0 b and to produce ACE files.*
  3. *To modify NJOY not to delete first energy data of MF3 or to delete the first energy data of MF6 in the case that the first two cross sections of MF3 are 0.0 b and to produce ACE files with the modified NJOY.*
  4. *To modify MCNP routine, where ACE data above emax are expunged.*

- We already demonstrate that the first and second solutions are good.
- We confirm that the third solution is also successful.
- We have not tested the fourth solution because the source code of MCNP6.2 is not available.
- We recommend to apply one of the above solutions to FENDL.

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Requests to next FENDL

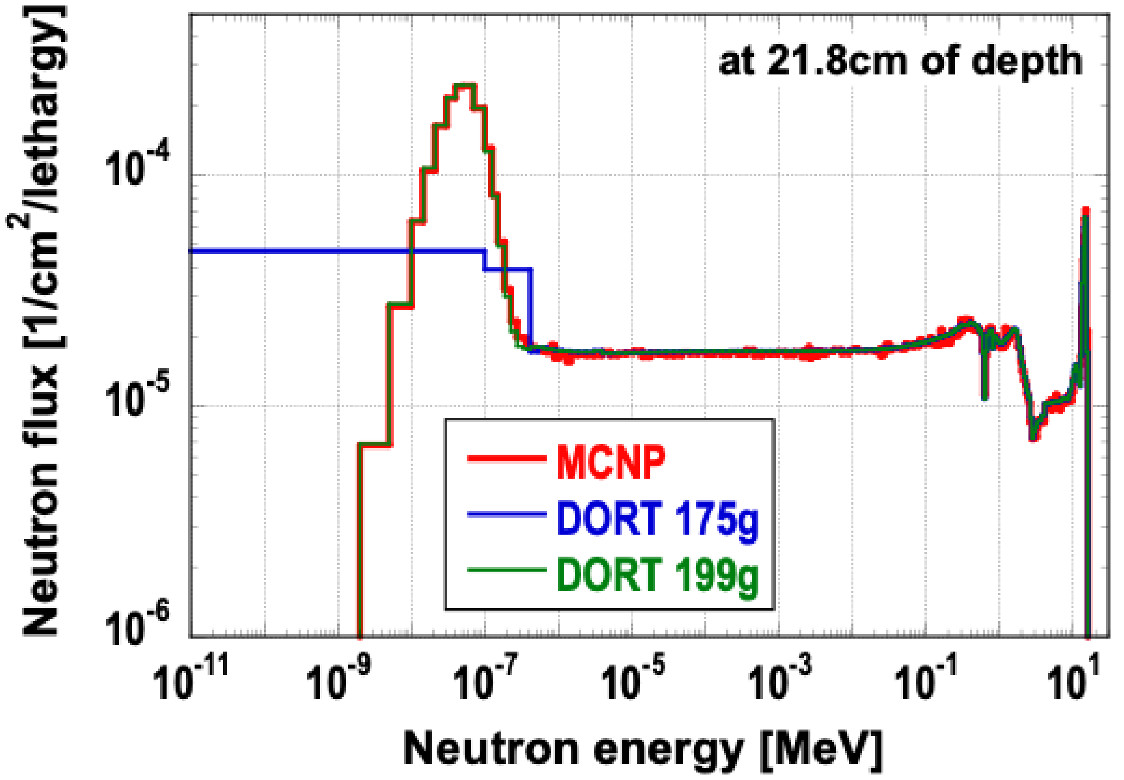
- To revise iron and copper data.
- To add S(α,β) data. (for Be, ESS S(α,β) data is recommended.)
- To revise ENDF-6 files or ACE files of nuclei where the first two cross sections of MF3 are 0.0 b.

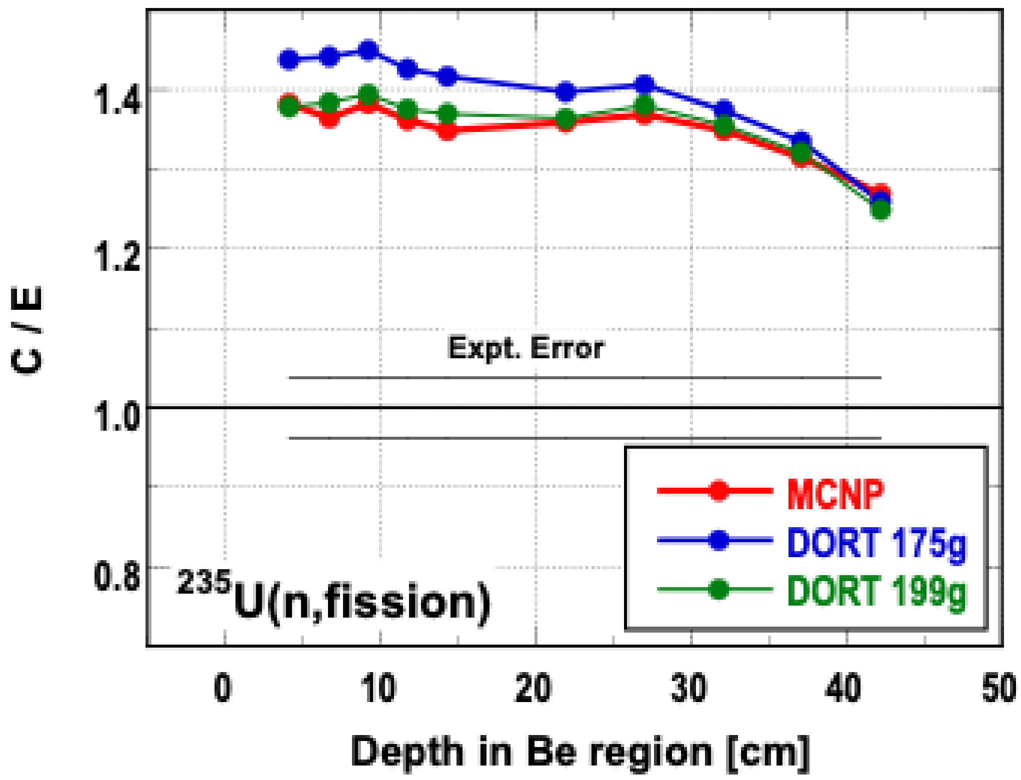
- To adopt 199 group structure below 19.64 MeV for MATXS files (the present FENDL MATXS files adopt 175 group structure below 19.64 MeV).

Effect of 199 group structure below 20 MeV

We analyzed FNS Be experiment by using FENDL-3.2c without TSL data.

- 175g : FENDL-3.2c MATXS (175 group structure below 19.64 MeV)
- 199g : a new FENDL-3.2c MATXS with 199 group structure below 19.64 MeV





DORT calculation result with 199 group is almost the same as MCNP one.

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Summary

QST

- We reviewed the issues presented at the 2023 FENDL meeting.
  - Iron : JENDL-5 is better than FENDL-3.2b (=FENDL-3.2c).
  - ^{63}Cu : JENDL-5 is better than FENDL-3.2b (=FENDL-3.2c).
  - ESS beryllium S(α,β) data considering crystallite domain size improve overestimation for low energy neutrons in the FNS beryllium experiment.
- We examined an issue which F4E group encountered in analyzing FNG tungsten experiment, which suggests that a lot of files in FENDL-3.2c include data which NJOY does not support.
- We proposed several requests to the next FENDL.

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