Nuclear heating and damage data in JENDL-5 neutron ACE file

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Introduction

- JENDL-5 was released in 2021.
- The neutron ACE file of JENDL-5 was produced with mainly FRENDY2, while the data on nuclear heating and damage were done with the NJOY2016.65 code modified for JENDL-5, and it was released as one of ACE-J50 (https://rpg.jaea.go.jp/main/en/ACE-J50/) in 2022.
- The neutron ACE file of JENDL-5 has nuclear heating and damage data which are used in PHITS calculations.
- Here the nuclear heating and damage data in the neutron ACE file of JENDL-5 are introduced in detail for PHITS users.

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Nuclear heating and damage data in ACE file #6

- Neutron ACE files have heating numbers and damage production energy cross sections as the nuclear heating and damage data.

$$\textit{Heating number} = (\textit{KERMA factor}) / \sigma_{tot}$$

KERMA : Kinetic Energy Released in MAterials

σ_{tot} : total cross section

$$\textit{DPA cross section} = \frac{0.8 * Td}{2 * Ed} \quad (\textit{NRT-dpa})$$

DPA : Displacement Per Atom

Td : damage production energy cross section

Ed : atomic displacement energy

- KERMA factors and damage production energy cross sections were produced with HEATR module of NJOY.

How to calculate KERMA factors

- KERMA factors are calculated with two methods.
  - **Energy balance method**
    - ✓ KERMA factors are calculated from differences of energies before and after reactions.
    - ✓ When energies before and after reactions are not conserved, KERMA factors with energy balance method can be negative or too large.
    - ✓ Original NJOY stores heating numbers from KERMA factors with this method to ACE files.
  - **Kinematics method**
    - ✓ KERMA factors are calculated from energy provided to residual nuclei, which are estimated with kinematics.
    - ✓ This method produces upper KERMA factors but no negative or too large ones.

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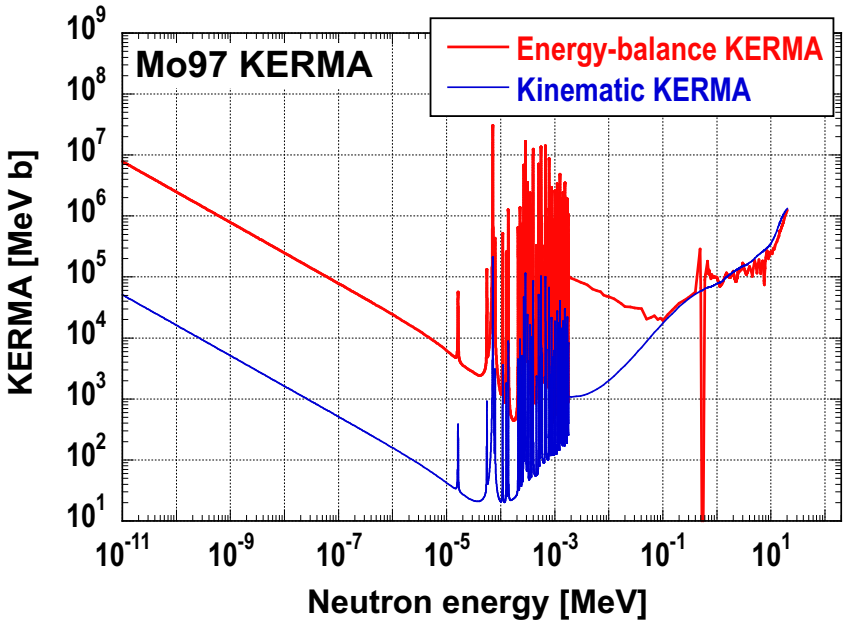
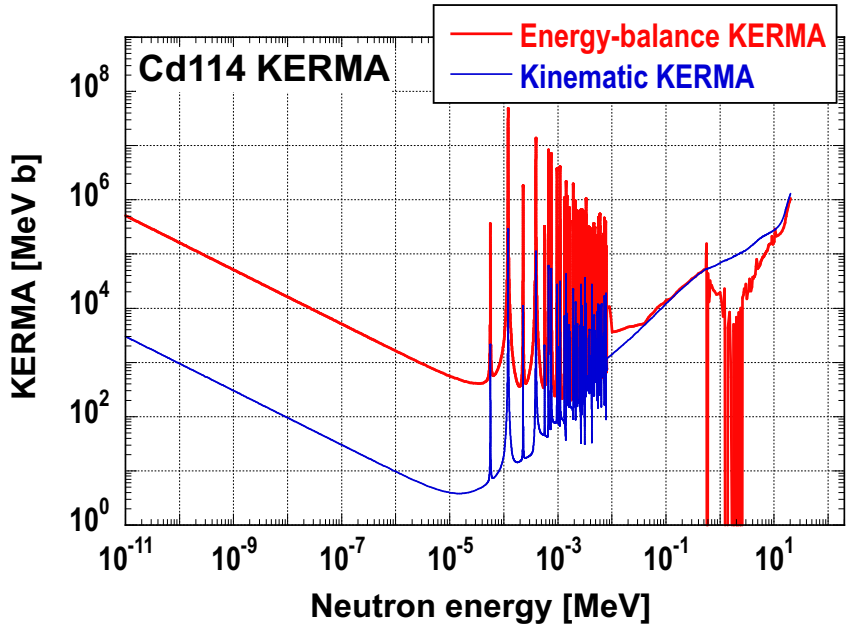
Neutron file of JENDL-4.0 -(1)

- The energies before and after reactions are **not conserved** in a lot of neutron files of **JENDL-4.0**.

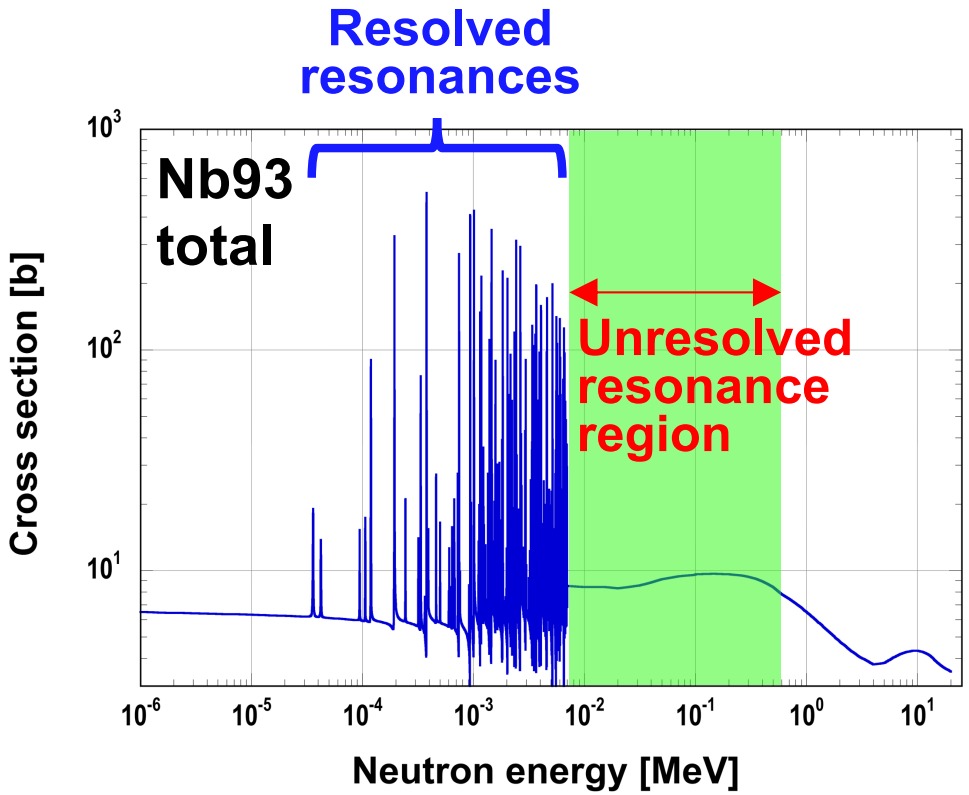


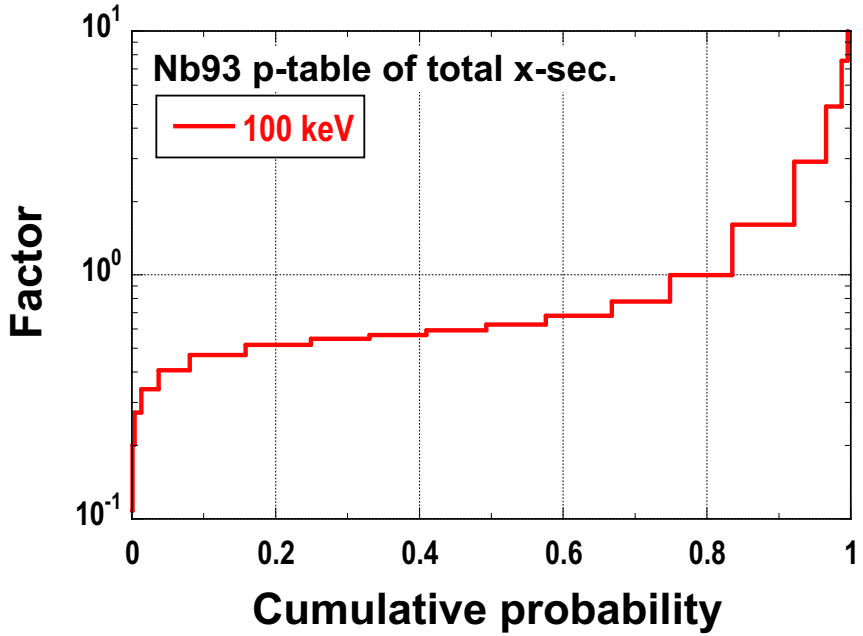


- Thus heating numbers from KERMA factors with **kinematics method** were stored to all the neutron ACE files of JENDL-4.0 by using modified **NJOY99**.

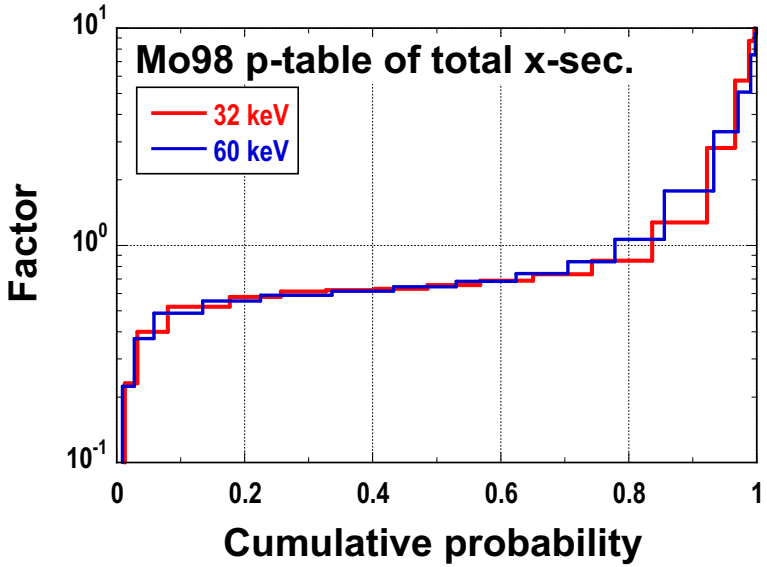
Neutron file of JENDL-4.0 -(2)

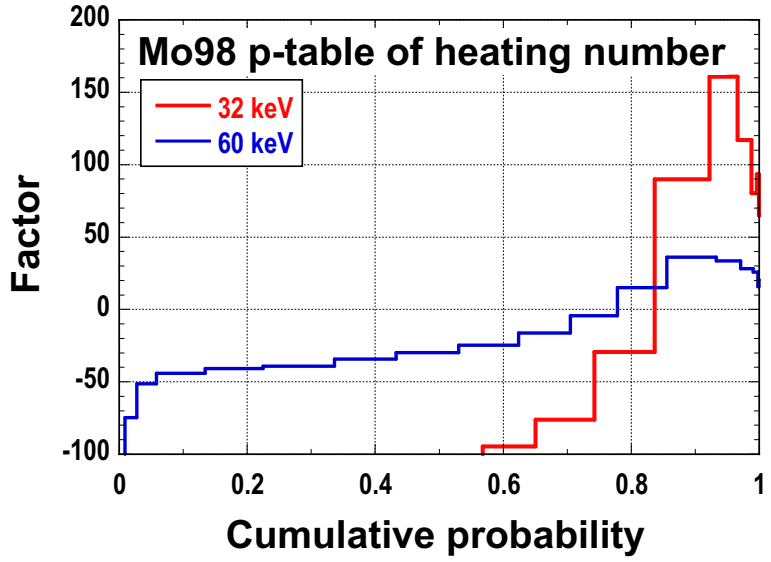
- However the modification of NJOY99 was not adequate, which often produced negative probability table (p-table) of heating number.
- p-table is used for self-shielding correction in unresolved resonance region.





Neutron file of JENDL-4.0 -(3)





- ACE files with **negative p-table** produce "**NaN**" (Not a number) in PHITS heating calculations.
- Thus **all p-table data were deleted** from neutron ACE files of JENDL-4.0 with negative p-table.

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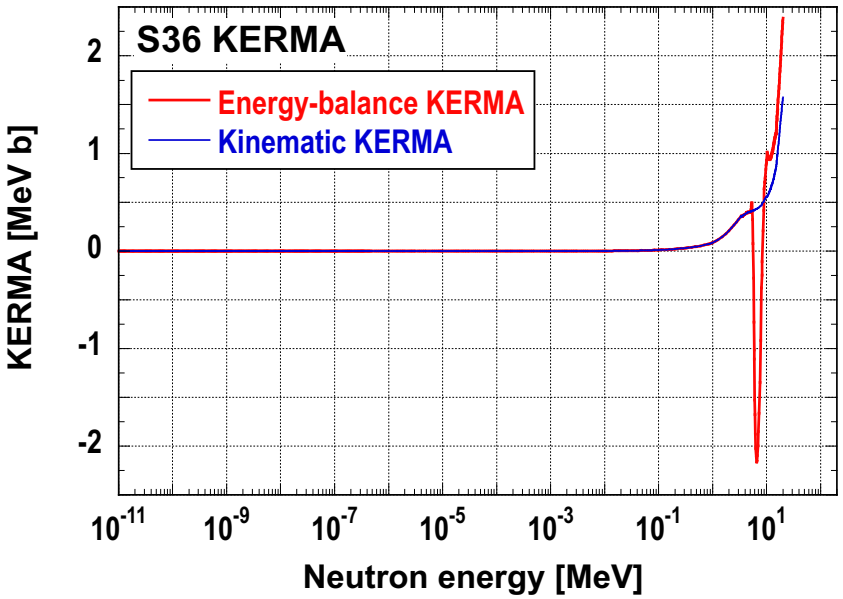
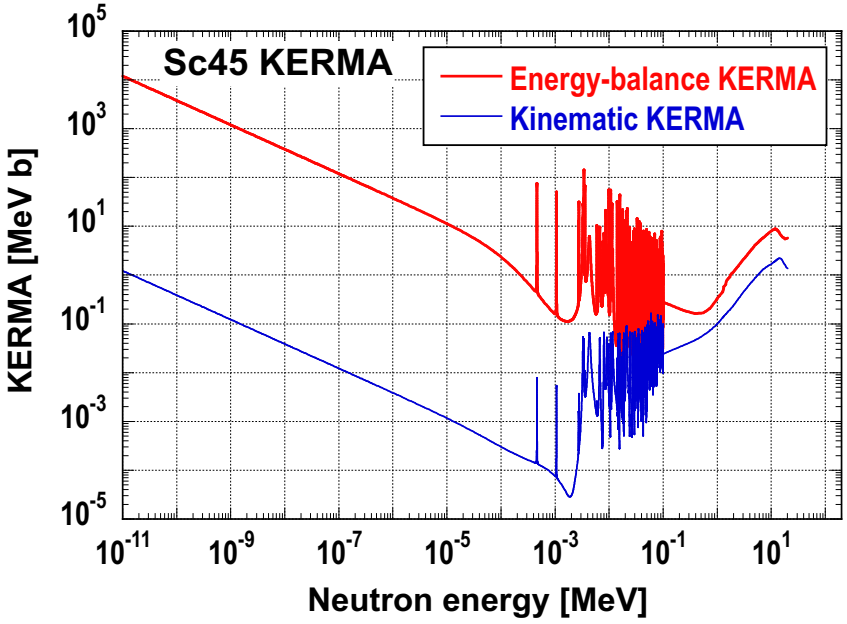
Neutron file of JENDL-5 -(1)

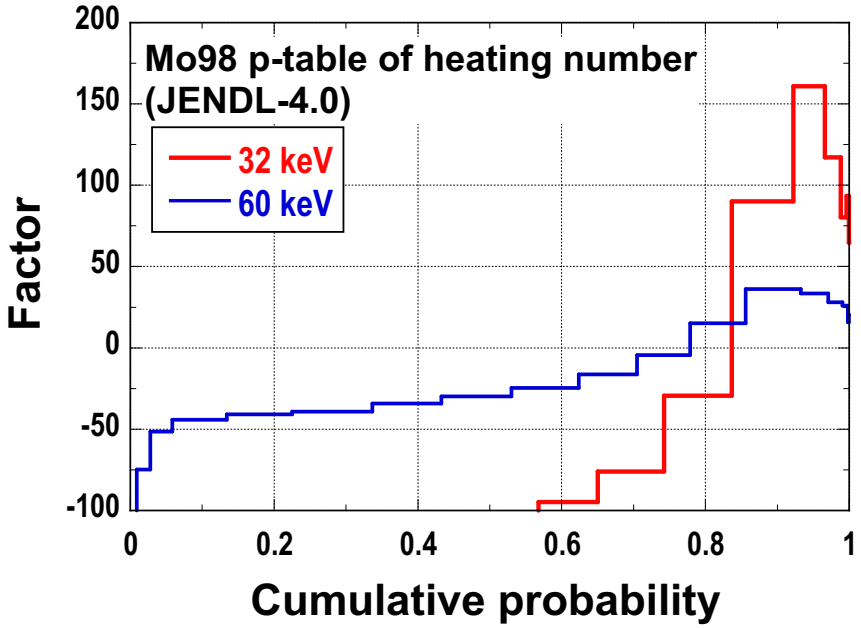
- Energies before and after reactions are **not conserved** in a lot of neutron files of **JENDL-5**.

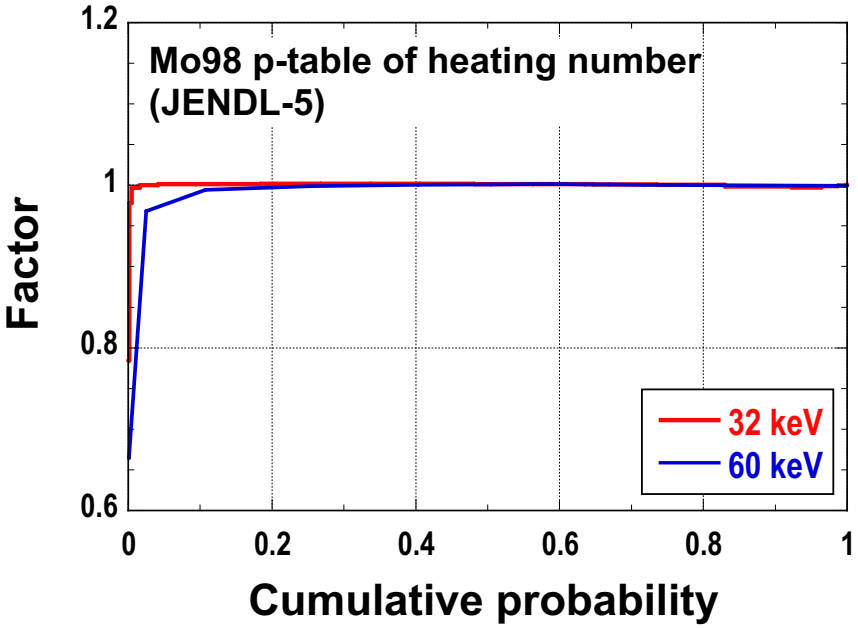




- Thus heating numbers from KERMA factors with **kinematic method** were stored to all the neutron ACE files of JENDL-5 by using adequately modified **NJOY2016.65**, which produced **no negative p-table**.

Neutron file of JENDL-5 -(2)





JENDL-4.0 Mo98

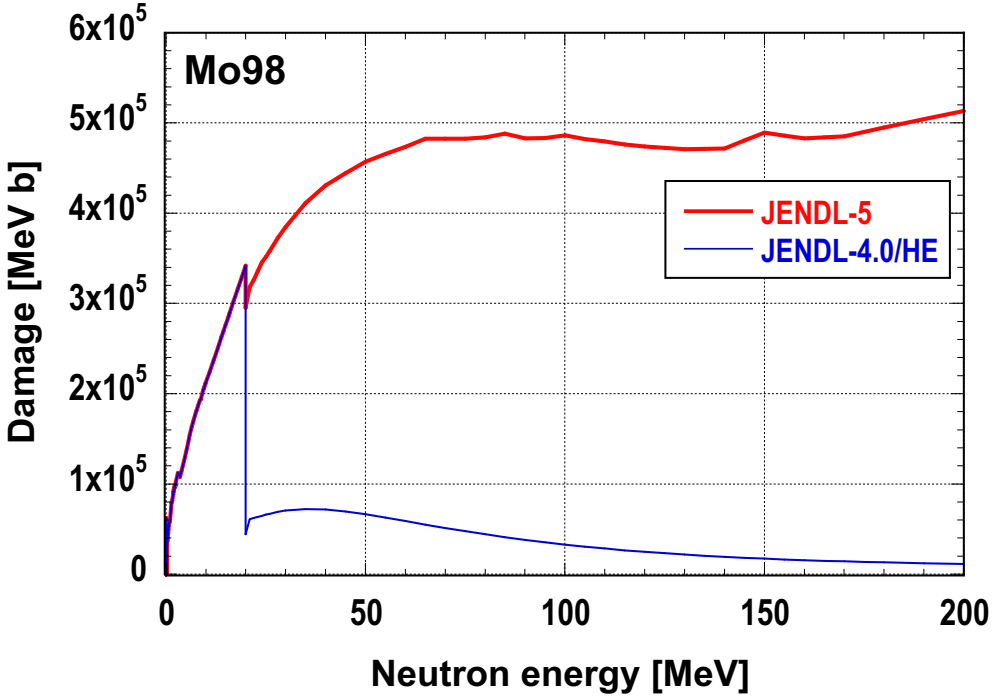
JENDL-5 Mo98

Neutron file of JENDL-5 -(3)

- It was pointed out that damage production energy cross sections in neutron ACE files of JENDL-4.0/HE dropped down above 20 MeV because of no energy distribution data of several residual nuclei above 20 MeV in JENDL-4.0/HE.

S. Kwon et al., J. Nucl. Sci. Technol., 57(2020), 344 – 351.

- JENDL-5 includes energy distribution data of all residual nuclei above 20 MeV, which solves the above issue.



Damage production energy cross section of ^{98}Mo

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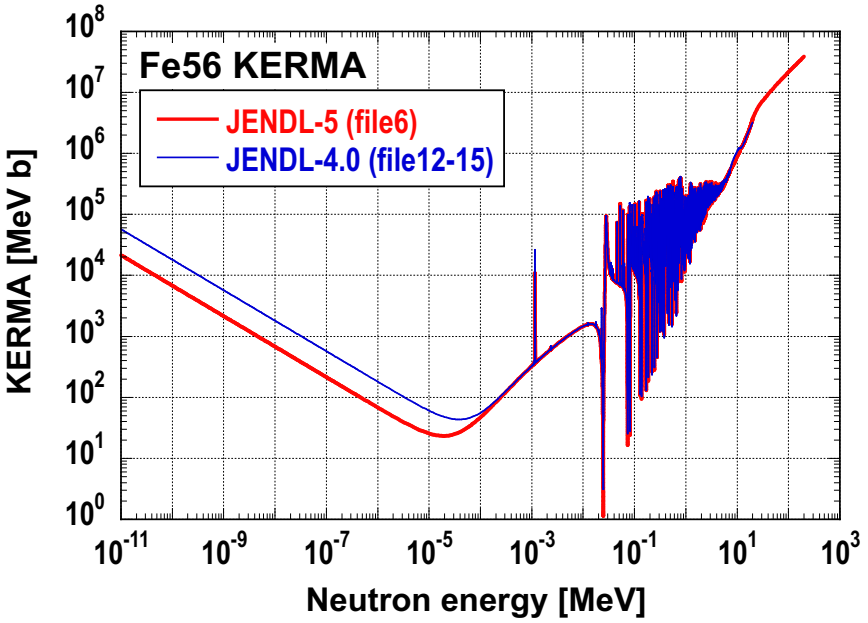
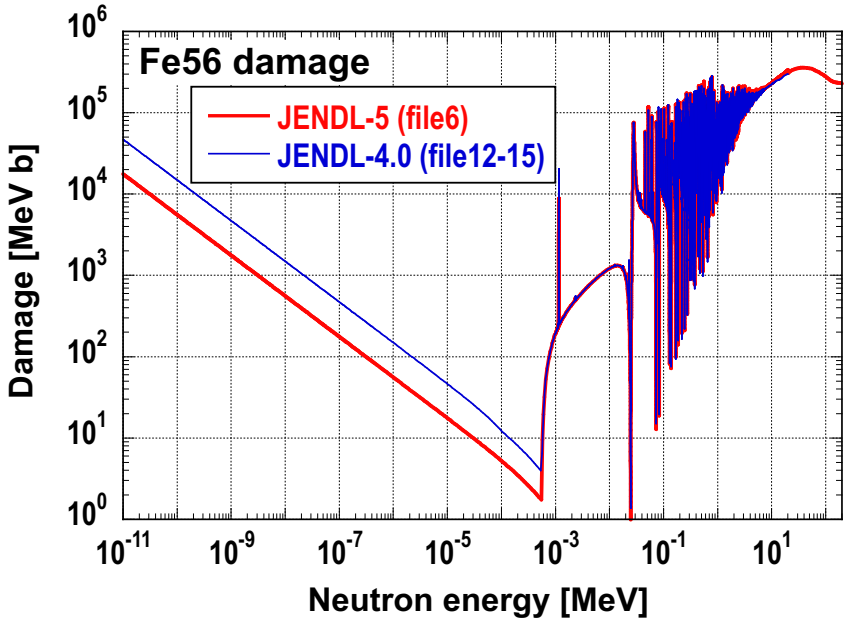
NJOY bug -(1)

❑ A fatal bug in HEATR module of NJOY

- KERMA factors and damage production energy cross sections of a lot of nuclei with gamma data of the capture reaction in Files 12-15 are different from those with gamma data of the capture reaction in File 6.

  C. Konno et al., Fusion Engineering and Design 109-111 (2016) 1649-1652.



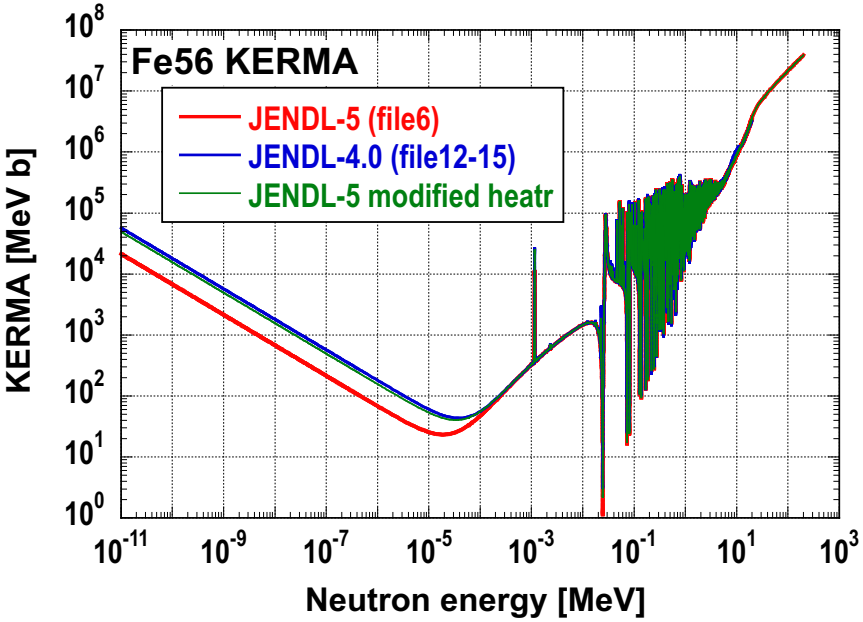


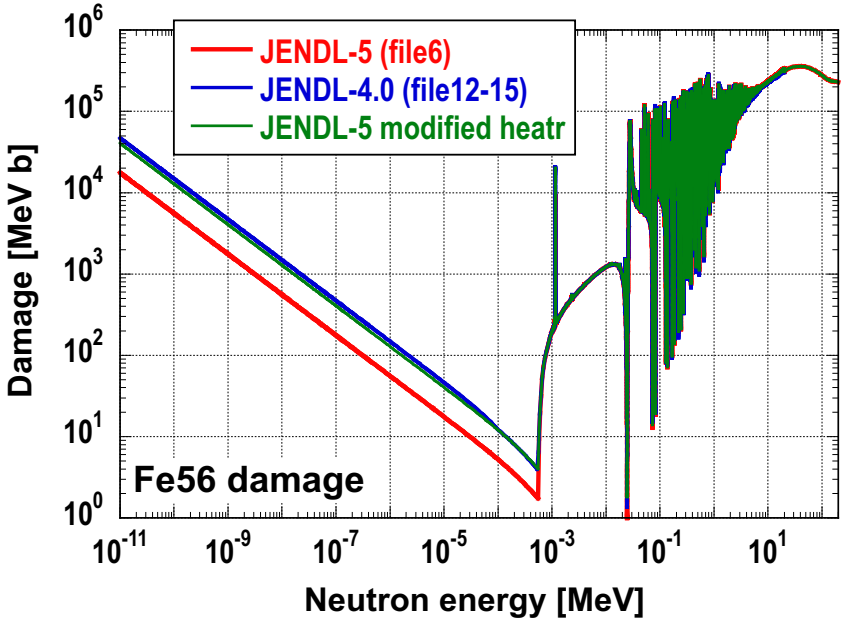
NJOY bug -(2)

- It was reported that **HEATR** module of NJOY has a fatal **bug** that it calculates KERMA factors and damage production energy cross sections **without multiplying secondary gamma yield** when **secondary gamma data** are stored **in File 6**.

  W. Yin et al., Annals of Nuclear Energy, 164 (2021) 108624.

❑ The bug in HEATR module of NJOY was fixed.





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Conclusion

- The nuclear heating and damage data in the neutron ACE file of JENDL-5 are explained.
- Neutron ACE files have heating numbers and damage production energy cross sections, not KERMA factors nor DPA cross sections.
- Heating numbers from KERMA factors with kinematics method were stored to all the neutron ACE files of JENDL-5.
- The JENDL-5 neutron ACE file has no negative p-tables of heating number in the JENDL-4.0 neutron ACE files.
- The JENDL-5 neutron ACE file is produced with the bug fixed NJOY2016.

Thank you for your attention!