

**Important comments on KERMA factors
and DPA cross-section data in ACE files
of JENDL-4.0, JEFF-3.2 and ENDF/B-VII.1**

**Chikara Konno¹⁾, Kenichi Tada¹⁾, Saerom Kwon²⁾,
Masayuki Ohta²⁾, Satoshi Sato²⁾**

1) Japan Atomic Energy Agency

2) National Institutes for Quantum Science and Technology

ND2016

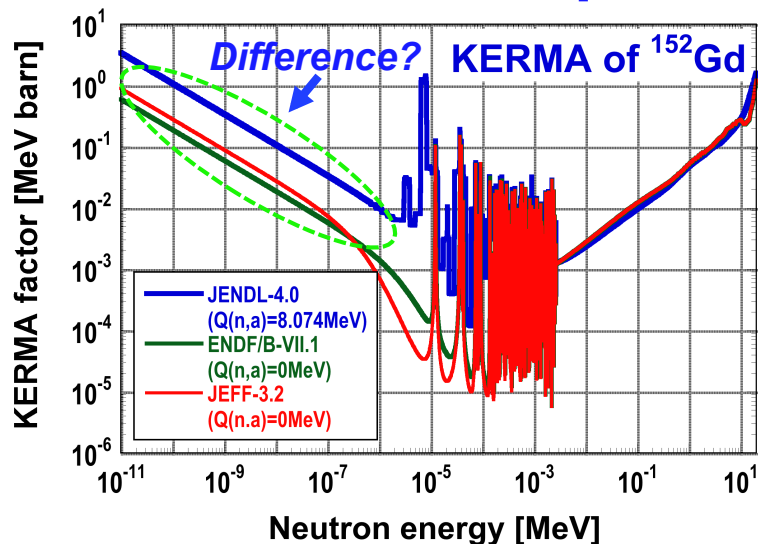
11-16 / 09 2016 Bruges Belgium



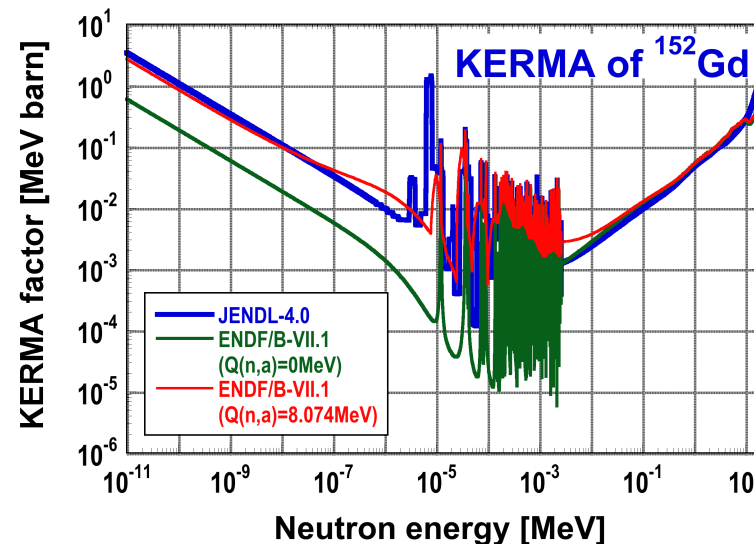
- ❑ **KERMA factors and DPA cross-section data** for calculating nuclear heating and damage in nuclear analyses are stored in ACE and MATXS files.
- ❑ It is known that KERMA factors of a lot of nuclei in the official ACE files are **not always correct** mainly because of inconsistent energy-balance.
- ❑ So far we pointed out that KERMA and DPA data are **different** among JENDL-4.0, ENDF/B-VII.1 and JEFF-3.2 even for **nuclei with consistent energy-balance**.
 - ① Nuclear data issues
 - ✓ Incorrect Q value in nuclear data
 - ✓ Huge gas production cross section data
 - ② NJOY issues
 - ✓ ^1H of ENDF/B-VII.1 (this bug fixed)
 - ✓ mt=102 data in file 6 (new NJOY bug?)



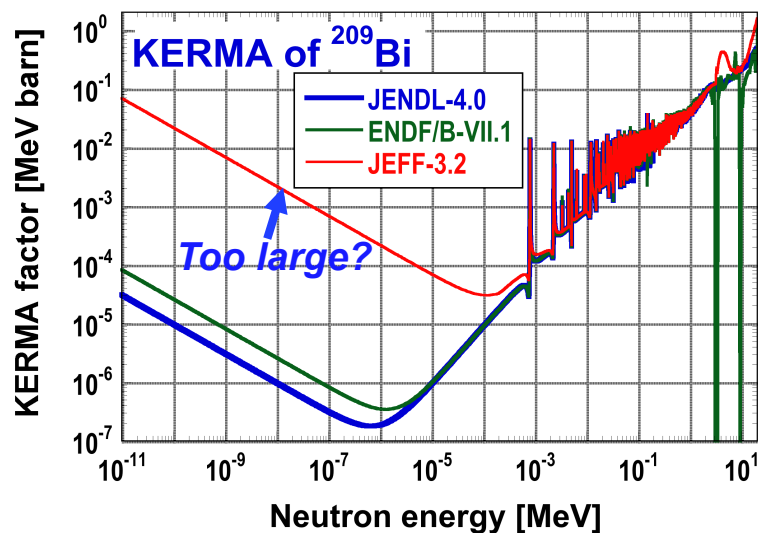
Example of inconsistent Q value



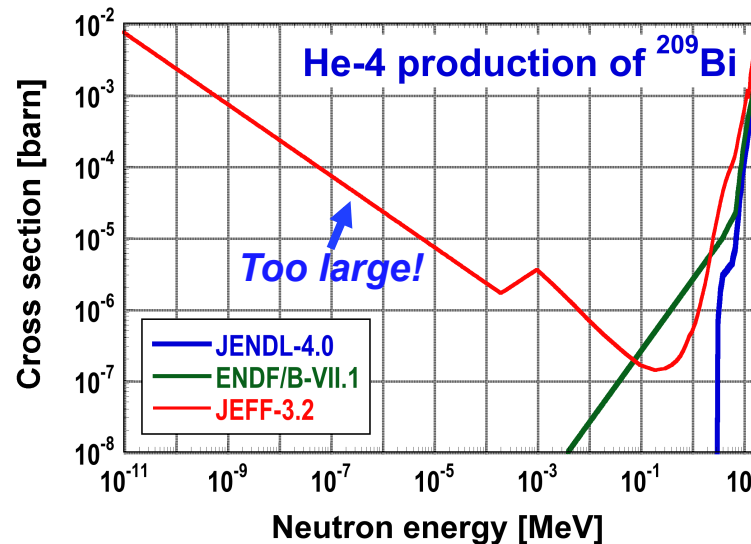
Q value mod.



Example of huge gas production cross section



He-4 prod. diff.

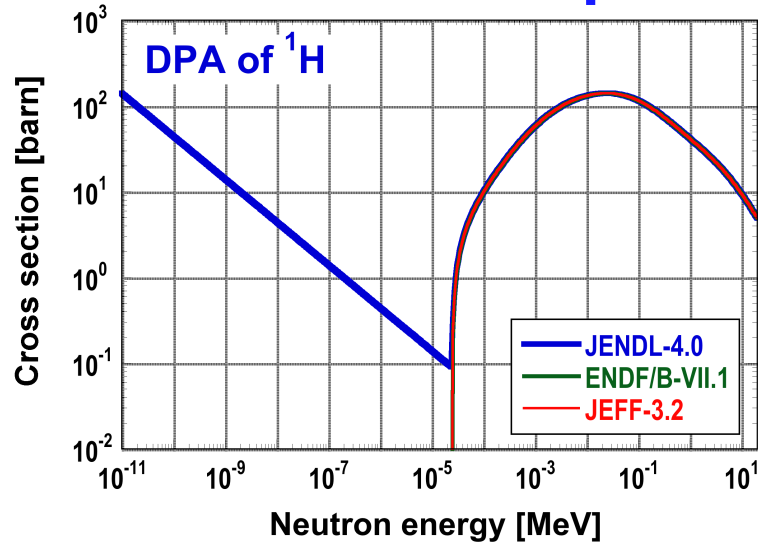


Introduction -(3)

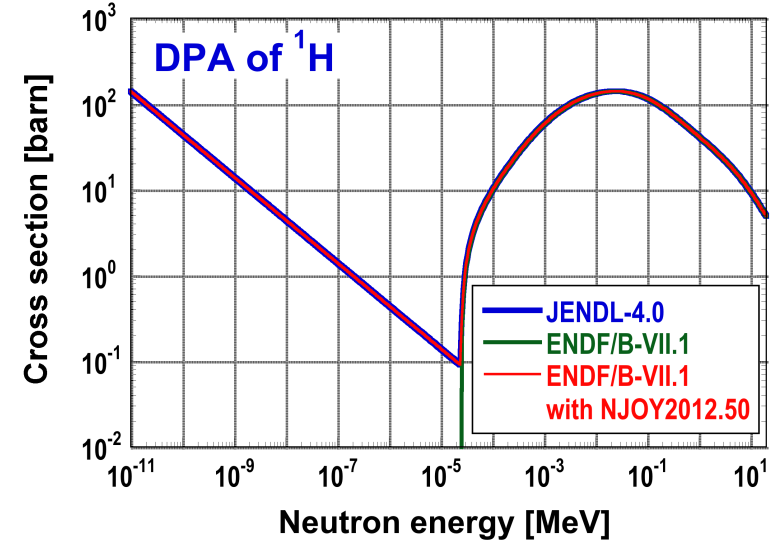
#4



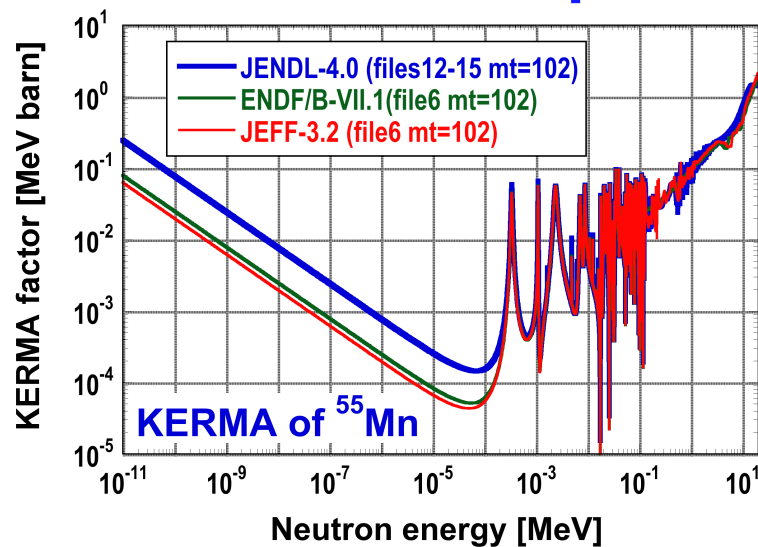
Example of ^1H of ENDF/B-VII.1



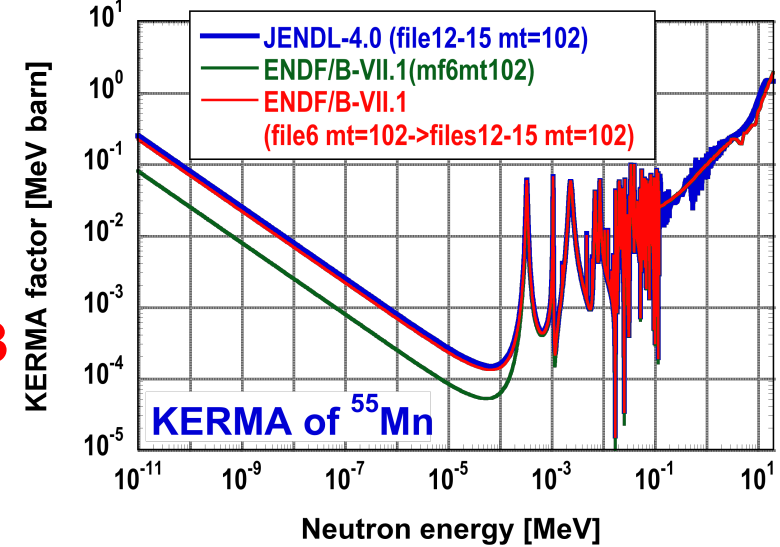
➔
NJOY
revision



Example of mt=102 data in file 6



➔
file6 to
files12-13



Objective

#5



- We continue this study and examine **KERMA** factors and **DPA** cross section data in the latest official ACE files of JENDL-4.0, ENDF/B-VII.1 and JEFF-3.2 **in more detail.**



- For all the nuclei (**497** nuclei) included in **JENDL-4.0**, **ENDF/B-VII.1** and **JEFF-3.2**, we extracted the total cross section data, **average heating numbers** and **damage energy production data** from the latest **official ACE files**.
 - JENDL-4.0 : AceLibJ40 by JAEA (NJOY99.336+)
 - ENDF/B-VII.1 : MCNP data by LANL (NJOY99.393)
 - JEFF-3.2 : ACE file by OECD/NEA (NJOY99.393+)

- We converted the average heating numbers to **KERMA factors** and the damage energy production data to **DPA cross section data** and plotted the KERMA and DPA data for comparison.
 - ✓ $\text{KERMA} = (\text{average heating number}) \times (\text{total cross section})$
 - ✓ $\text{DPA} = 0.8 \times (\text{damage energy production data}) / (2 \times (\text{displacement energy}))$

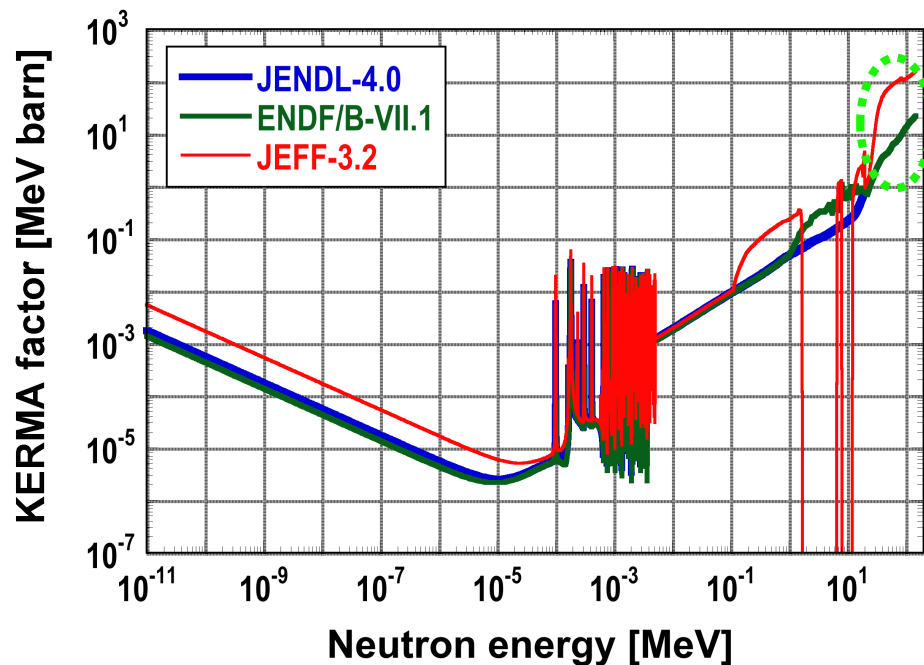


- ❑ It is newly found out that KERMA and DPA data of **a lot of nuclei** are **different** among JENDL-4.0, ENDF/B-VII.1 and JEFF-3.2.
- ❑ Reasons for most of the differences of KERMA and DPA data among the nuclear data libraries are successfully **categorized** as the followings.
 - 1) Huge secondary particle production yield
 - 2) No secondary gamma data
 - 3) Secondary gamma data in files 12-15 mt=3
 - 4) mt=103-107 data without mt=600s-800s data in file 6

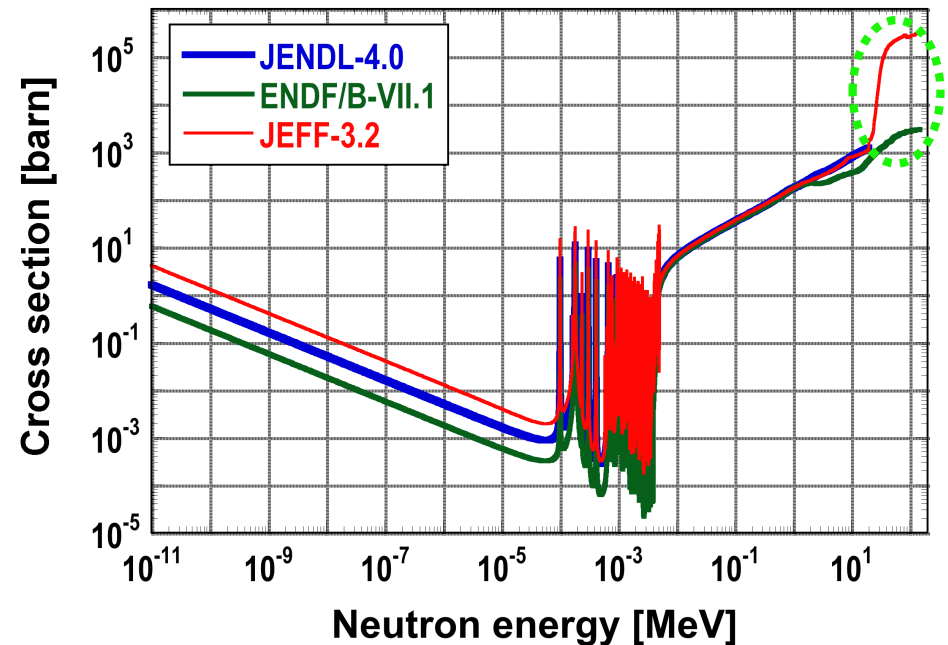
Huge secondary particle production yield -(1) #8



- The KERMA factors and DPA cross sections of ^{182}W , ^{183}W , ^{184}W and ^{186}W in JEFF-3.2 are extraordinarily large above 20 MeV.



KERMA factor of ^{184}W

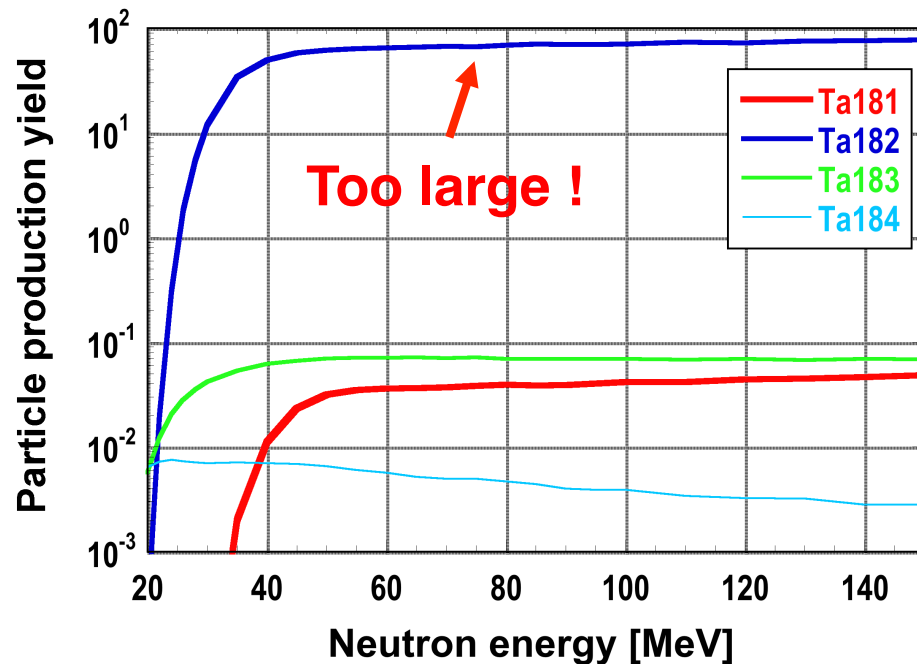


DPA X-sec. of ^{184}W

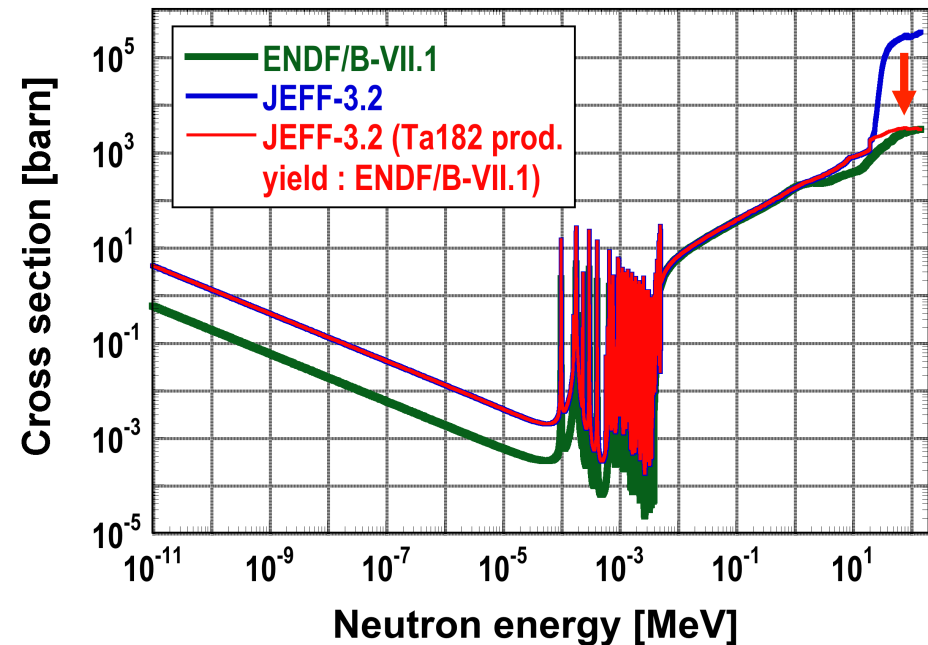
Huge secondary particle production yield -(2) #9



- ❑ Huge particle production yield data (e.g., ^{182}Ta in ^{184}W) are found.
- ❑ If these data are modified, this problem is resolved.



Ta isotope production yield of ^{184}W in JEFF-3.2



DPA X-sec. of ^{184}W

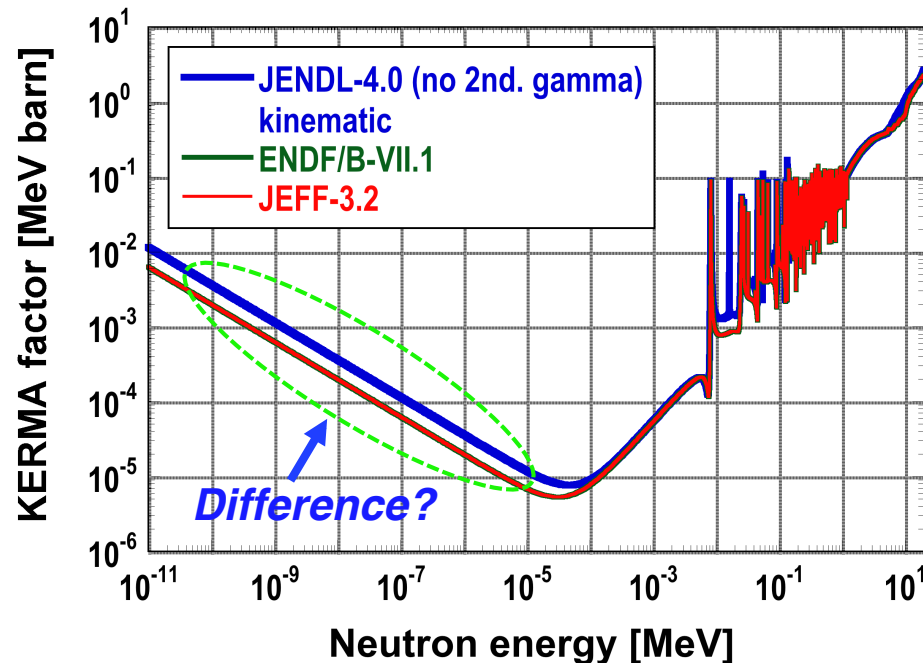
(Ta182 production yield in JEFF-3.2 is replaced with that in ENDF/B-VII.1.)

No secondary gamma data -(1)

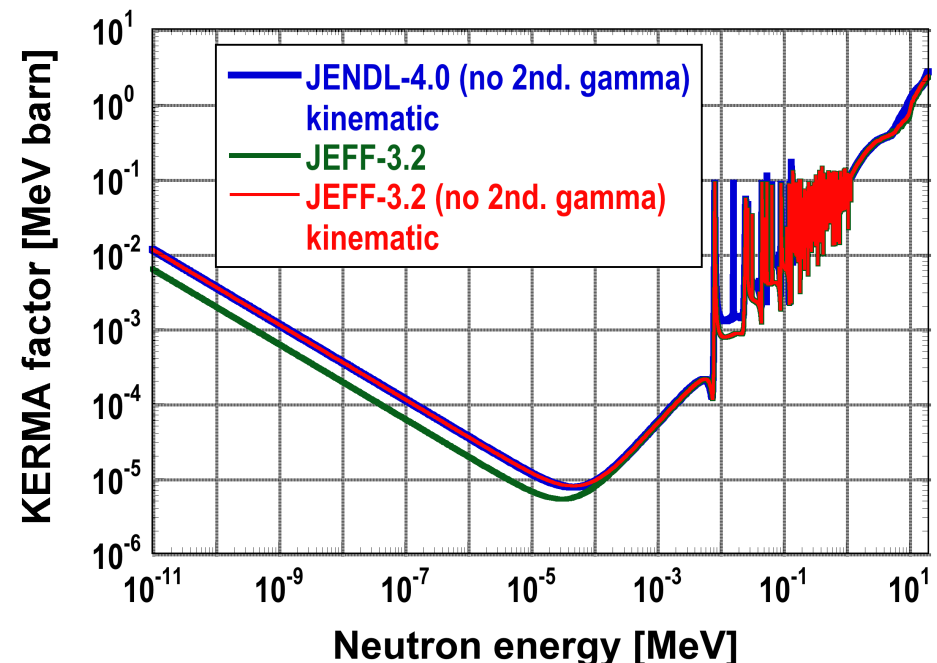
#10



- For nuclei without secondary gamma data, **kinematic KERMA factors** may be stored in ACE files as the second best (e.g., JENDL-4.0 ACE file). However the kinematic KERMA factor is **not correct**.



KERMA factor of ^{37}Cl



KERMA factor of ^{37}Cl

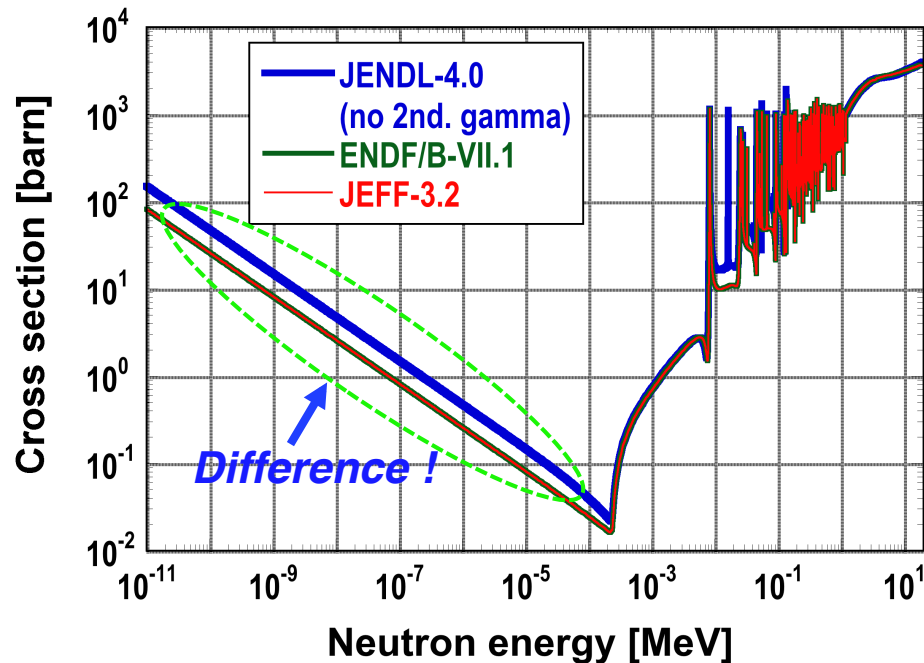
(Secondary gamma data in JEFF-3.2 are deleted.)

No secondary gamma data -(2)

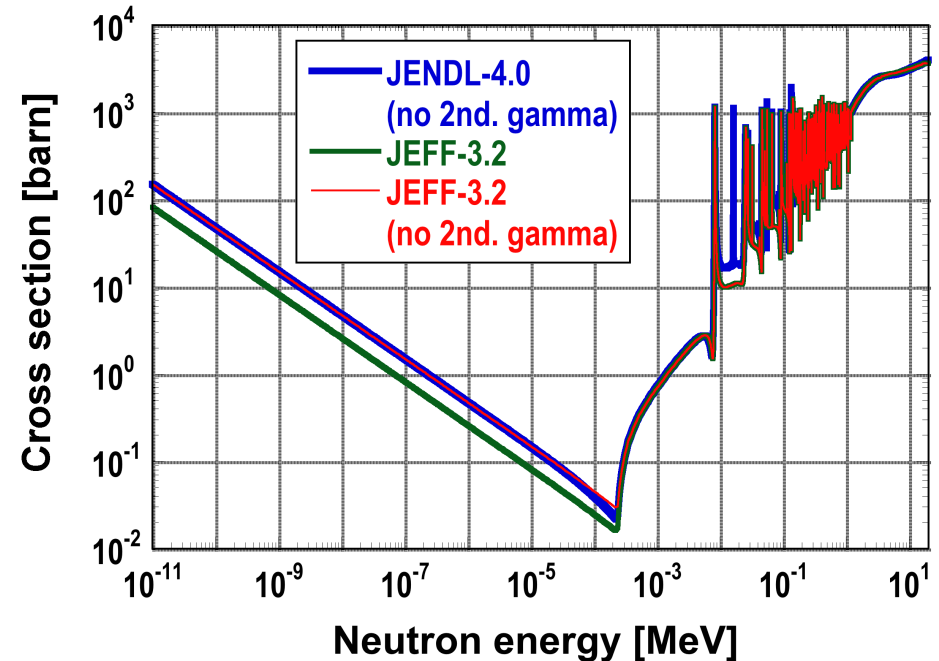
#11



□ This problem also occurs in DPA cross section data.



DPA x-sec. of ^{37}Cl



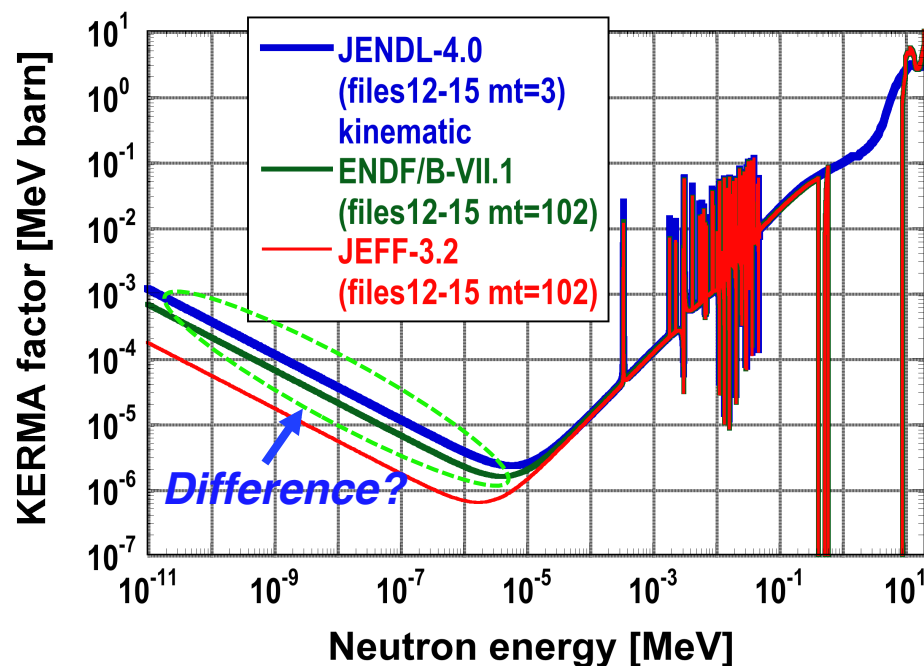
DPA x-sec. of ^{37}Cl

(Secondary gamma data in JEFF-3.2 are deleted.)

Secondary gamma data in files12-15 mt=3 -(1) #12

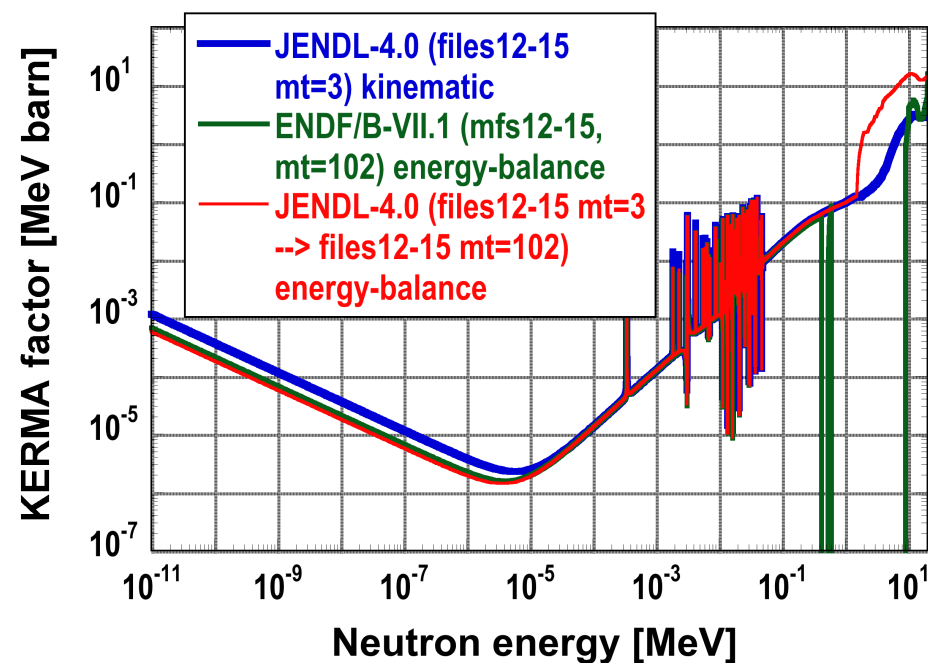


- Most of the nuclear data of nuclei with secondary gamma data in file6 mt=3 **do not keep energy-balance. Kinematic KERMA factors** may be stored in ACE files (e.g., JENDL-4.0 ACE file) as the second best. However the kinematic KERMA factor is also **not correct**.



KERMA factor of ^{92}Mo

Difference between ENDF/B-VII.1 and JEFF-3.2 is due to difference of capture cross section.



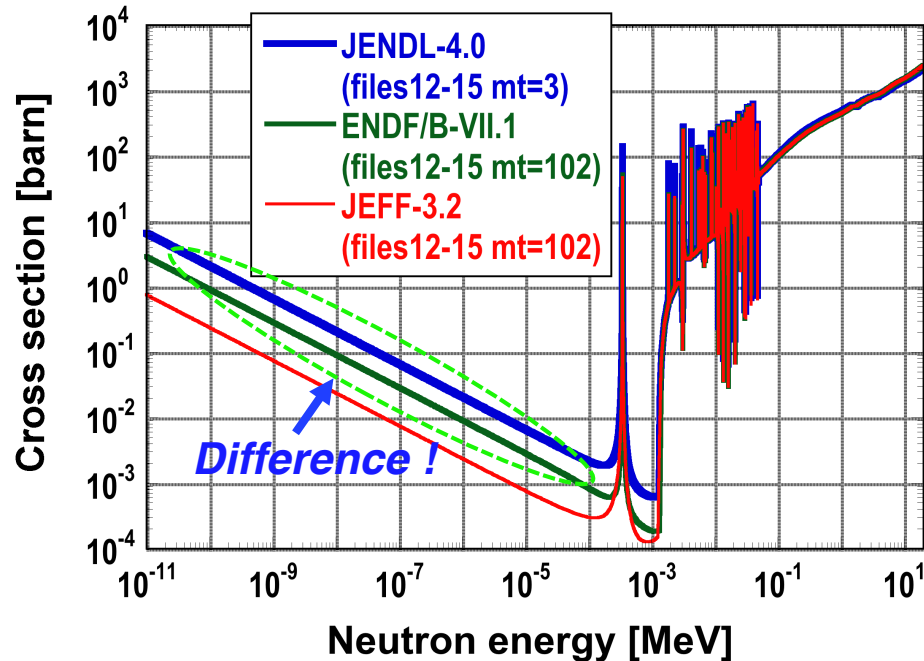
KERMA factor of ^{92}Mo

(Files12-15 mt=3 data in JENDL-4.0 are converted to files12-15 mt=102 data.)

Secondary gamma data in files12-15 mt=3 -(1) #13

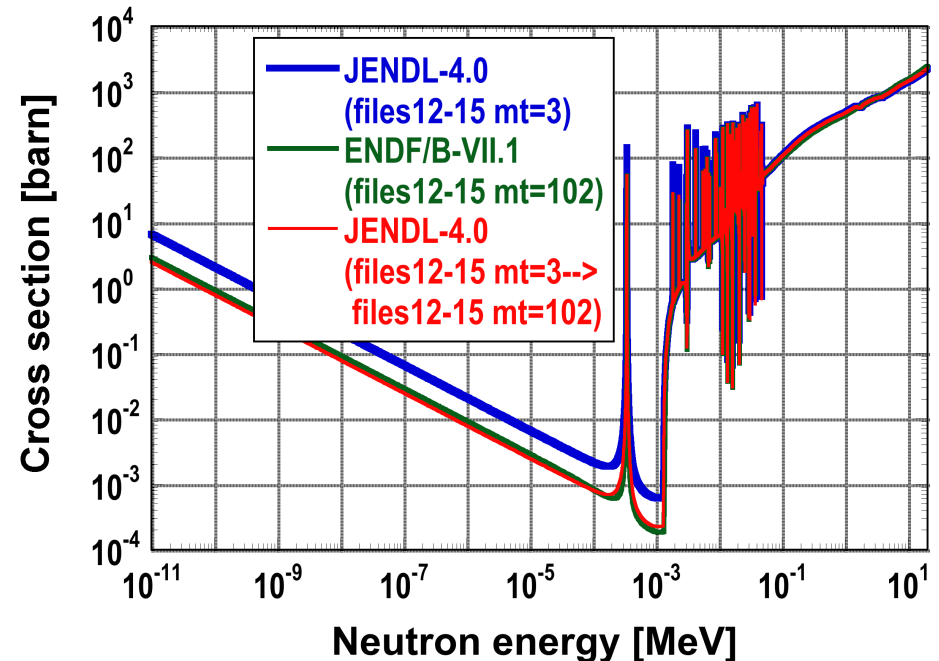


□ This problem also occurs in DPA cross section data.



DPA x-sec. of ^{92}Mo

Difference between ENDF/B-VII.1 and JEFF-3.2 is due to difference of capture cross section.



DPA x-sec. of ^{92}Mo

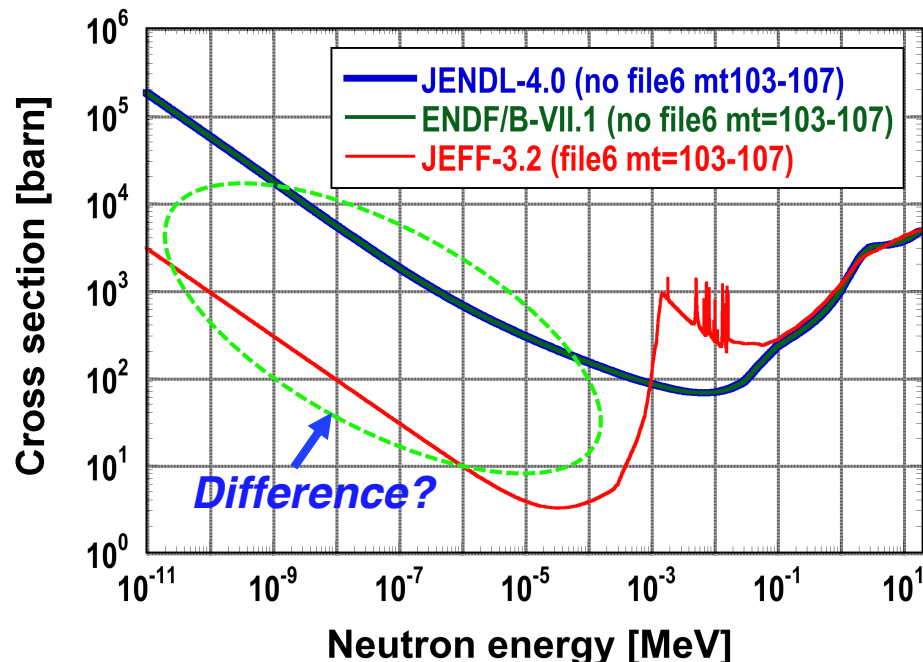
(Files12-15 mt=3 data in JENDL-4.0 are converted to files12-15 mt=102 data.)

mt=103-107 data without mt=600s-800s data in file6 -(1)

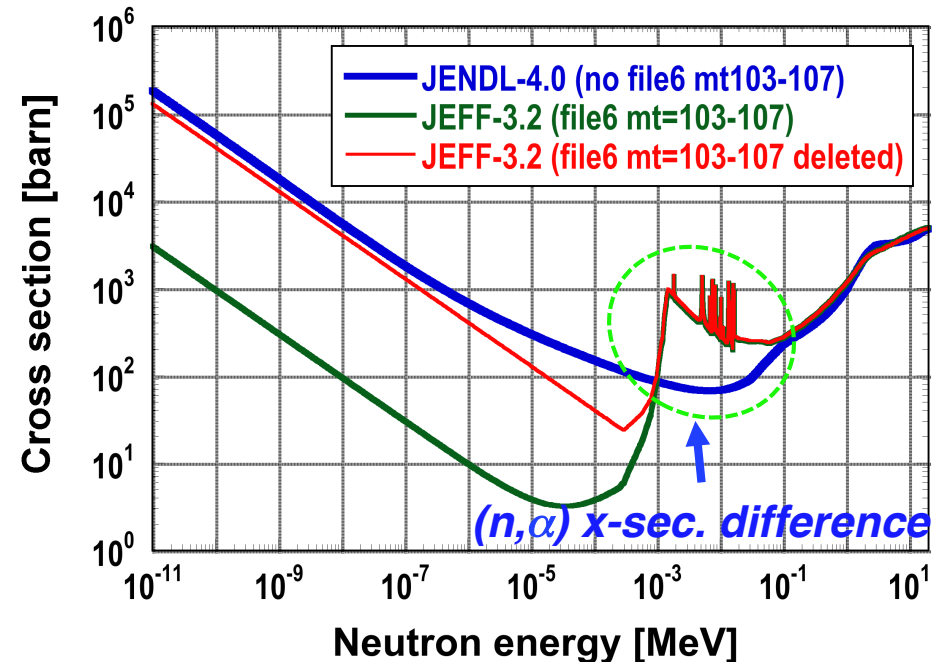
#14



- The DPA cross section data of $^{39-41}\text{K}$ in JEFF-3.2 are much smaller than those in JENDL-4.0 and ENDF/B-VII.1 below 1 keV. However this difference becomes much smaller if file6 mt=103-107 data in JEFF-3.2 are deleted.



DPA x-sec. of ^{40}K



DPA x-sec. of ^{40}K

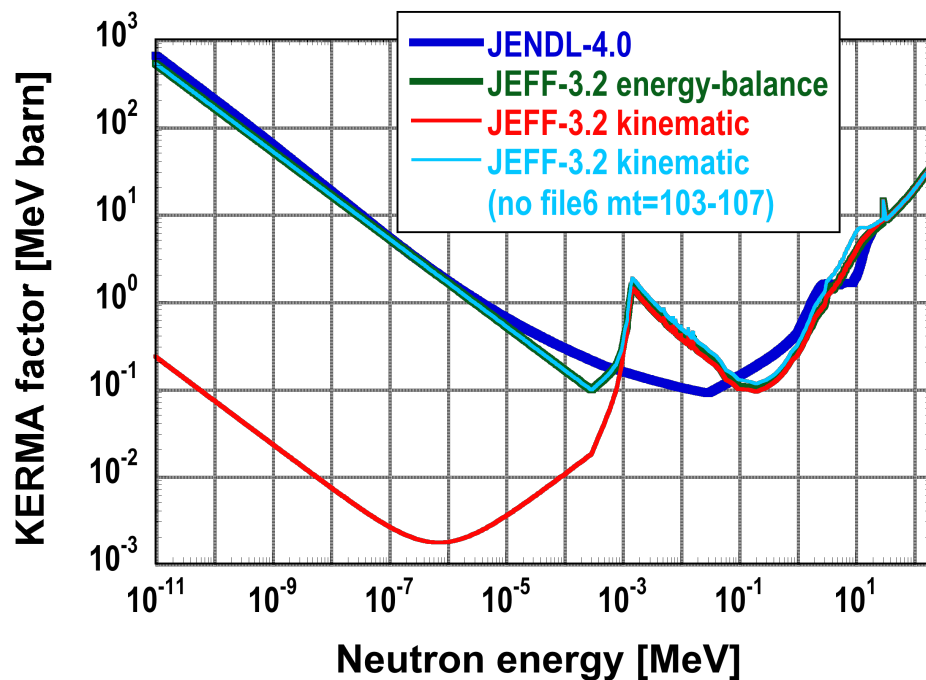
(File6 mt=103-107 data in JEFF-3.2 are deleted.)

mt=103-107 data without mt=600s-800s data in file6 -(2)

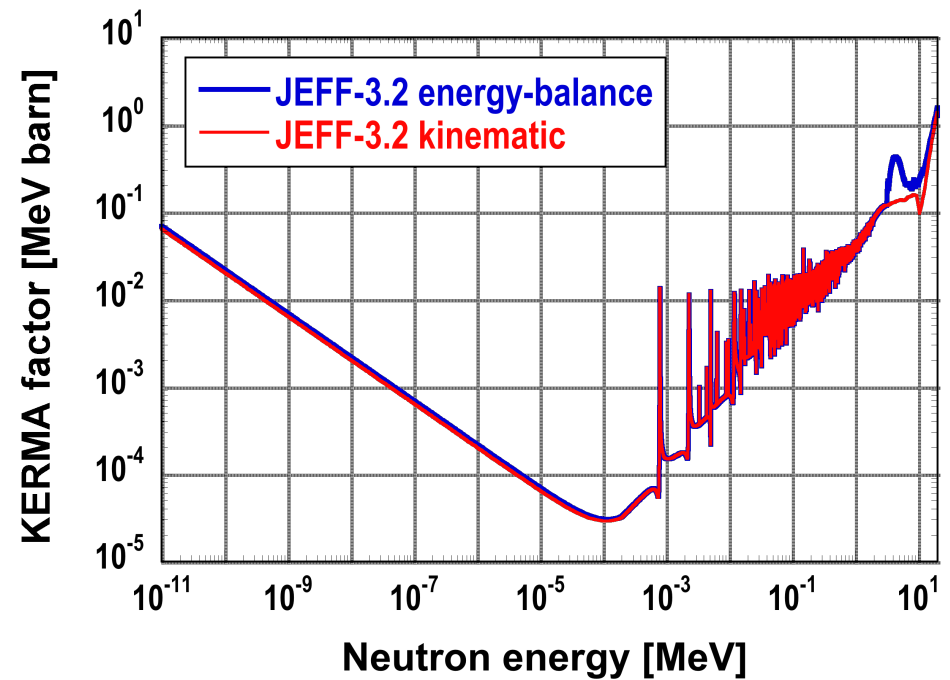
#15



- ❑ The energy-balance KERMA factors of $^{39-41}\text{K}$ in JEFF-3.2 have no problem, while the **kinematic KERMA factors** have the same problem as the DPA cross sections.
- ❑ It seems that **NJOY processes not mt=103-107 data in file6** but mt=600s-800s data in file6 (e.g., JEFF-3.2 ^{209}Bi).



KERMA factor of ^{40}K



KERMA factor of ^{209}Bi

Concluding Remarks

#16



- ❑ We examined **KERMA factors** and **DPA cross section data** in the official ACE files of **JENDL-4.0**, **ENDF/B-VII.1** and **JEFF-3.2** in more detail.
- ❑ It is newly found out that KERMA and DPA data of **a lot of nuclei** are **different** among JENDL-4.0, ENDF/B-VII.1 and JEFF-3.2.
- ❑ Reasons for most of the differences of KERMA and DPA data among the nuclear data libraries are successfully **categorized** as the followings.
 - 1) Huge secondary particle production yield
 - 2) No secondary gamma
 - 3) Secondary gamma data in files 12-15 mt=3
 - 4) mt=103-107 data without mt=600s-800s data in file 6
- ❑ **Incorrect nuclear data and/or NJOY should be revised and the ACE files also should be revised.**



Thank you for your attention!