Comparative study of PHITS code and NJOY for heating number and recoil spectra under neutron irradiation

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PHITS
Particle and Heavy Ion Transport code System

Contents

- Introduction
- Overview of PHITS code
- Heating number for materials with PHITS and NJOY
- Recoil spectra using PHITS and NJOY-SPKA
- Summary

Introduction

NJOY/HEATR module is widely used processing code to calculate damage data (KERMA, displacement damage energy)

Energy balance method Heating number $= (E + Q_{ij}) - (\bar{E}_{ijn} + \bar{E}_{ij\gamma})$

It is important to validate NJOY with another method such as PHITS code, TRIPOLI, and so on.

PHITS has new independent capabilities such as Event Generator Mode (EGM) for neutron irradiation below 20 MeV.

We report heating number or recoil spectra derived using PHITS-EGM and NJOY with various nuclear data libraries.

What is PHITS?

Particle and Heavy Ion Transport code System

Capability

Transport and collision of nearly all particles over wide energy range using Monte Carlo method

neutron, proton, ions, electron, photon etc

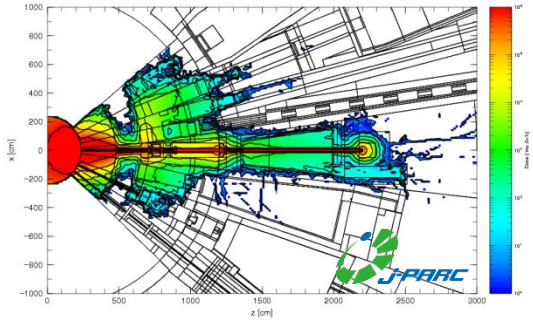
10^{-4} eV to 1 TeV/n

All-in-one-Package

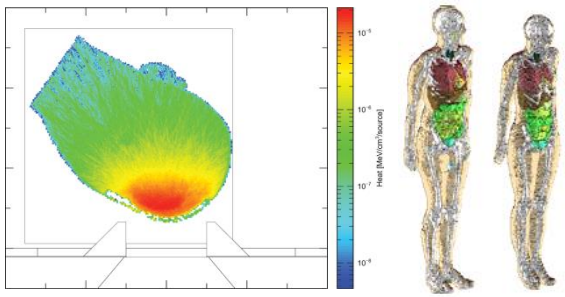
All contents of PHITS (source files, binary, data libraries, graphic utility etc.) are fully integrated in one package

Available in free of charge by submitting application form via PHITS website

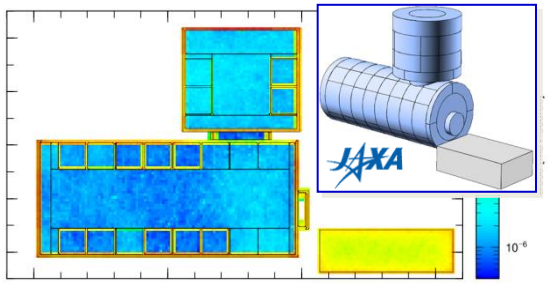
Applications



Accelerator Design



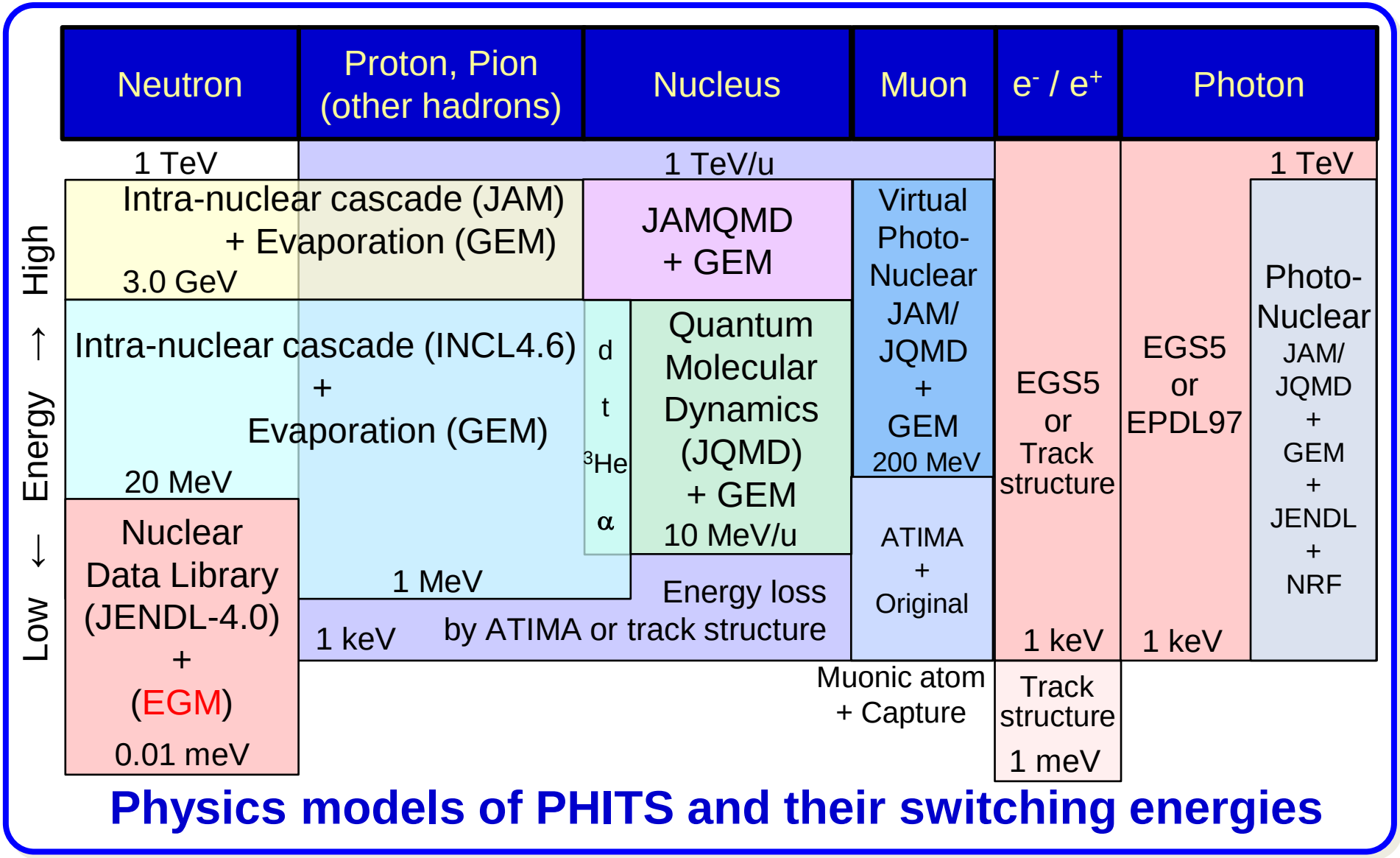
Radiation Therapy & Protection



Space & Geoscience

https://phits.jaea.go.jp/index.html

Map of Models Recommended to Use in PHITS



Physics models of PHITS and their switching energies

Switching energies can be changed by input file of PHITS

Event Generator Mode

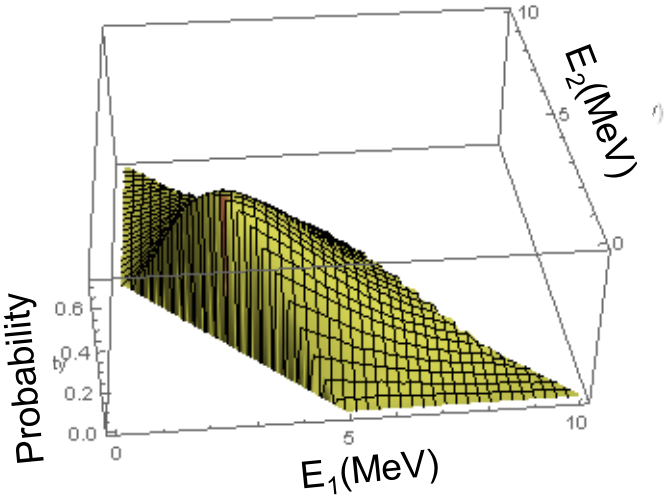
What is event generator mode (EGM)?

Original sampling method of secondary particles using nuclear data library

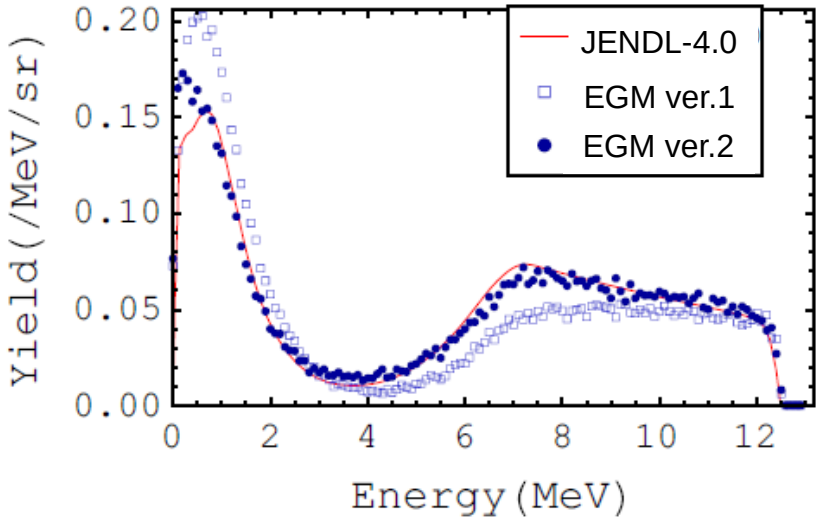
Difference between EGM and conventional method

EGM: Sample all secondary particles from 2D energy sampling space at once, considering energy & momentum conservation in an event

Conventional method: Sample particle by particle from 1D energy distribution



Energy sampling space



Secondary particle yields from ^{150}Nd(n,2n)

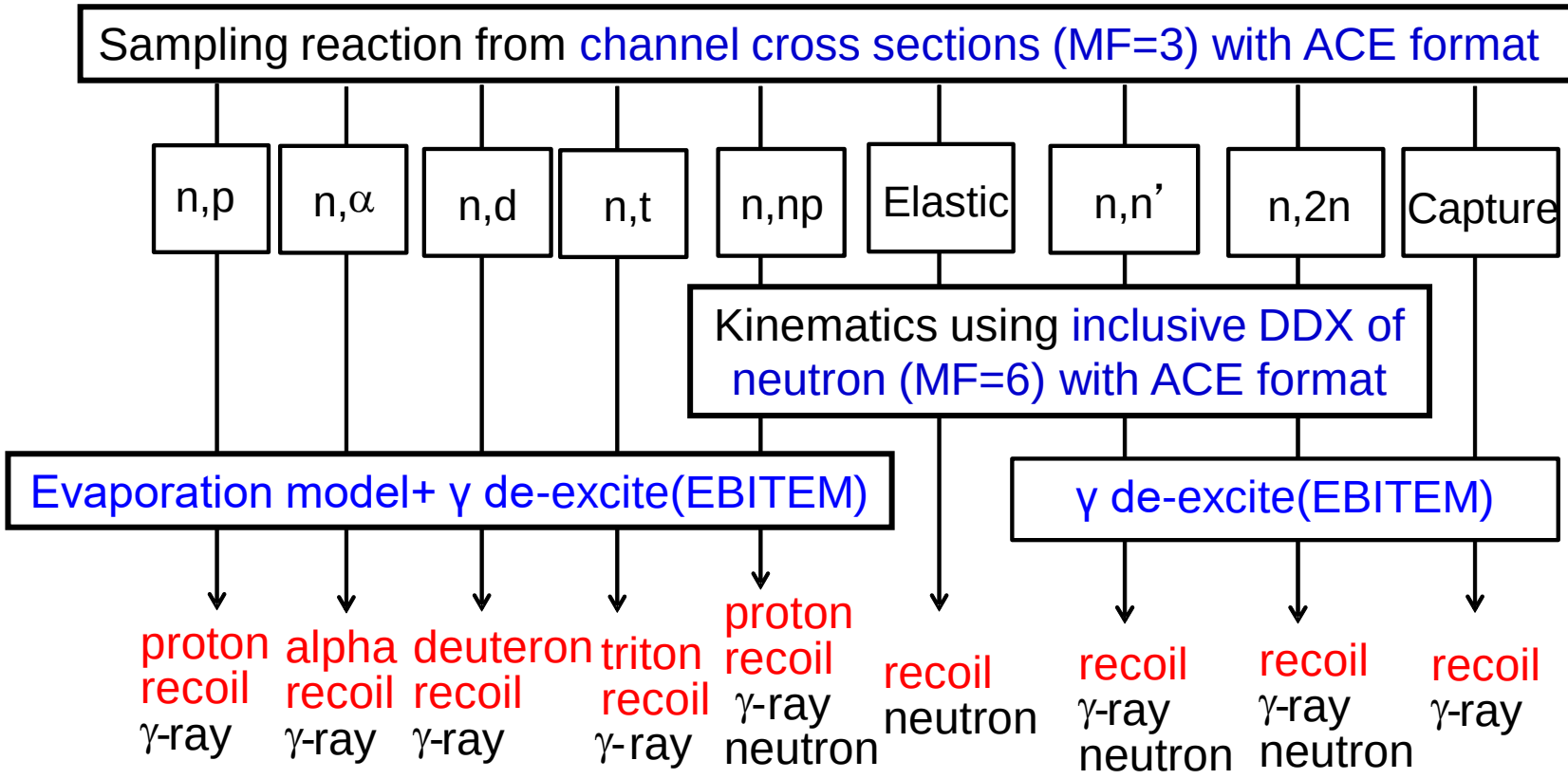
Indispensable in some cases such as detector response simulation

T.Ogawa *et al.*, *NIM A*, **763**, 575-590 (2014)

PHITS-Event Generator Mode (EGM) for low energy neutrons

Monte Carlo simulation of all ejectile with keeping energy and momentum conservation in event-by-event

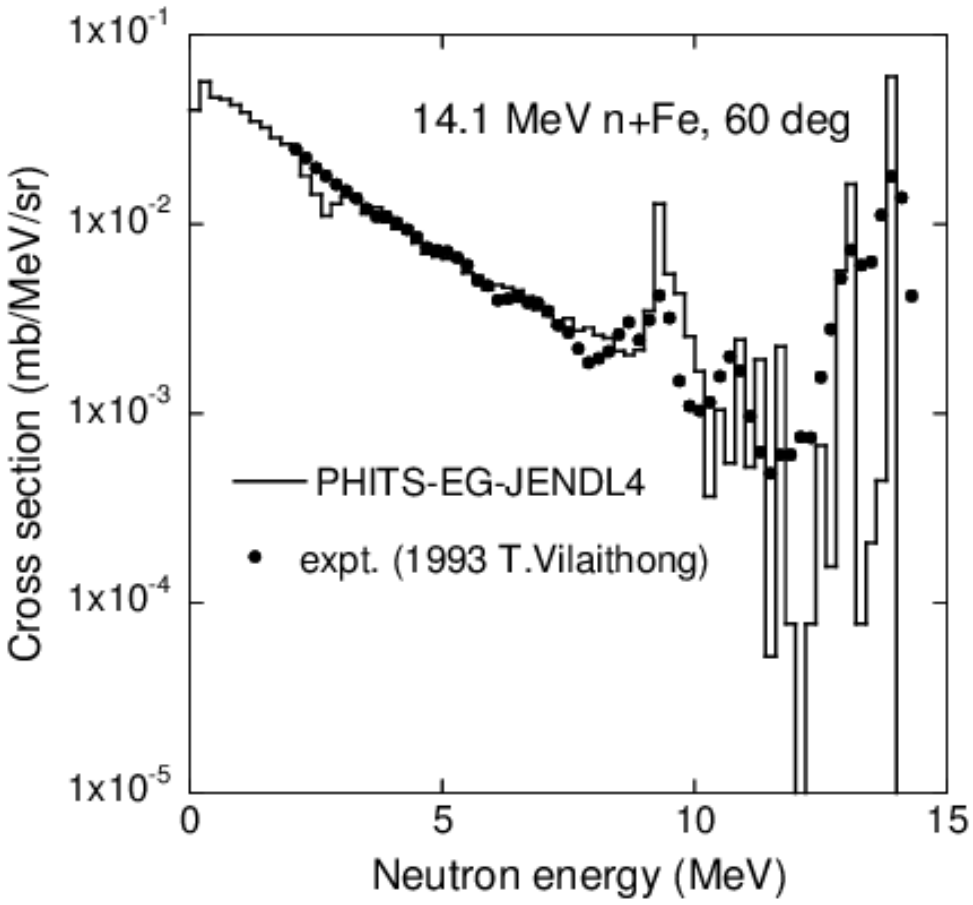
T. Ogawa et al., NIM A 763 (2014) 575-590.

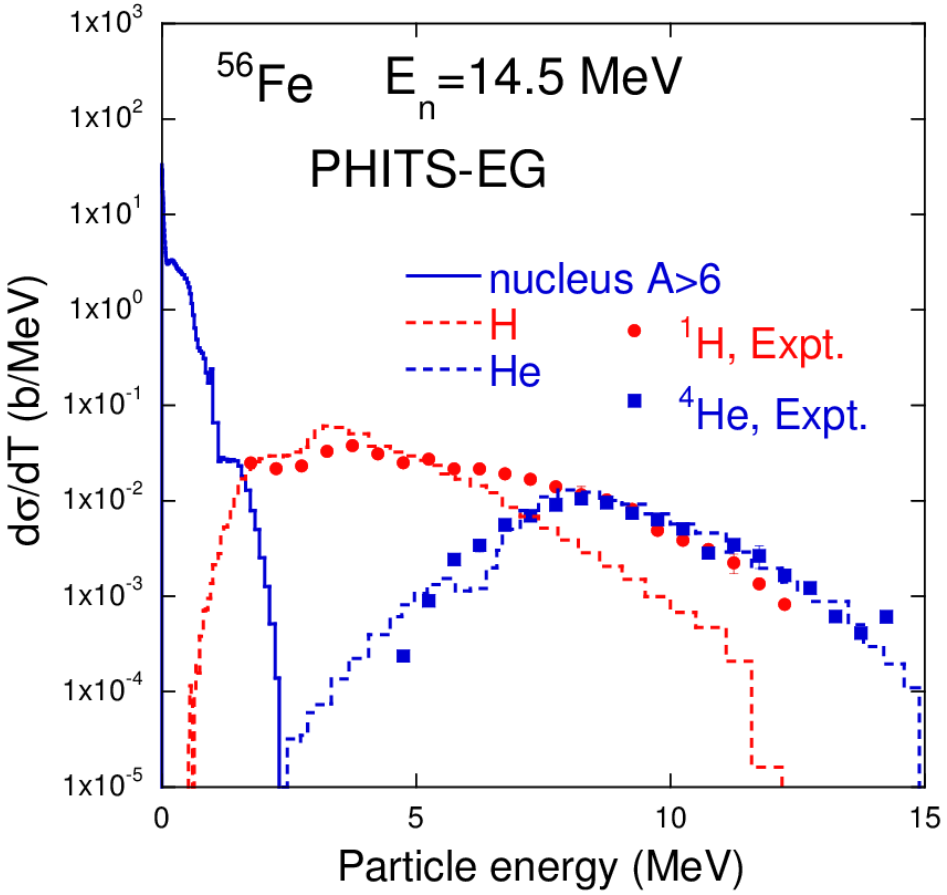


EBITEM is ENDSF-based isomeric transition and isomer production models.
The nuclei were de-excited based on the scheme provided in the ENSDF.

The heating number is determined by the sum of the kinetic energy of the charged particle.

Benchmark calculation for PHITS-EGM





PHITS-EGM can reproduce neutron and α energy spectra,
but it overestimates the experimental data for proton over 5 MeV.

More benchmark calculation for EGM are needed.

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Calculation conditions for heating number

Codes: PHITS2.92/EGM, NJOY2012.50/HEATR

Materials: ^{56}Fe, ^{58}Ni, ^{63}Cu, ^{47}Ti, ^{52}Cr, ^{184}W

Neutron energy range: 10^{-11} MeV - 20 MeV

Output: Heating number (MeV)

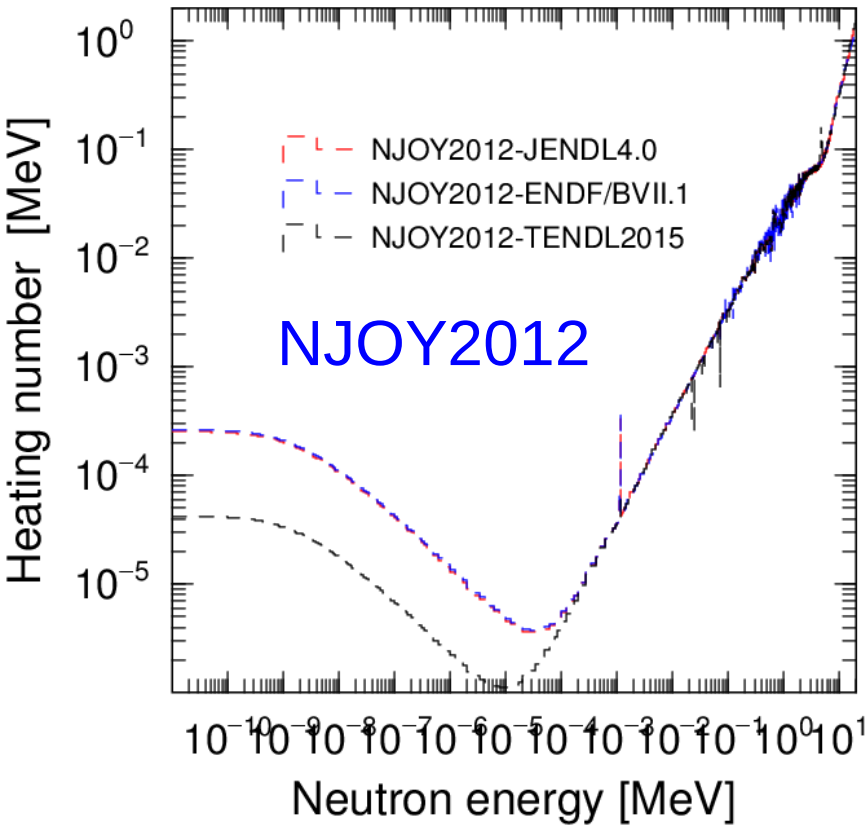
Example (in13) in package of NJOY2012 was used for data processing.

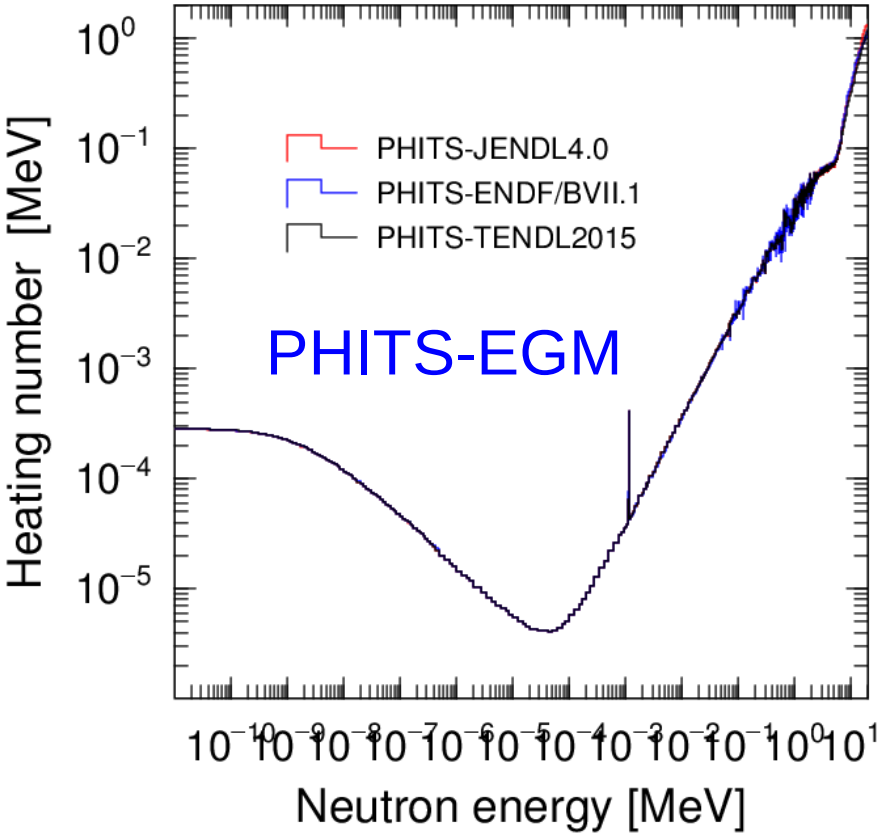
```
heatr
-21 -23 -24/
$MAT1 6 0 1 0 2/
302 303 304 402 443 444
```

Nuclear data libraries: ENDF-BVII.1, JENDL-4.0, TENDL-2015

PHITS-EGM: Only channel cross sections (MF=3) and neutron DDX (MF=6) in the ACE format library are used.

Heating number for ^{56}Fe



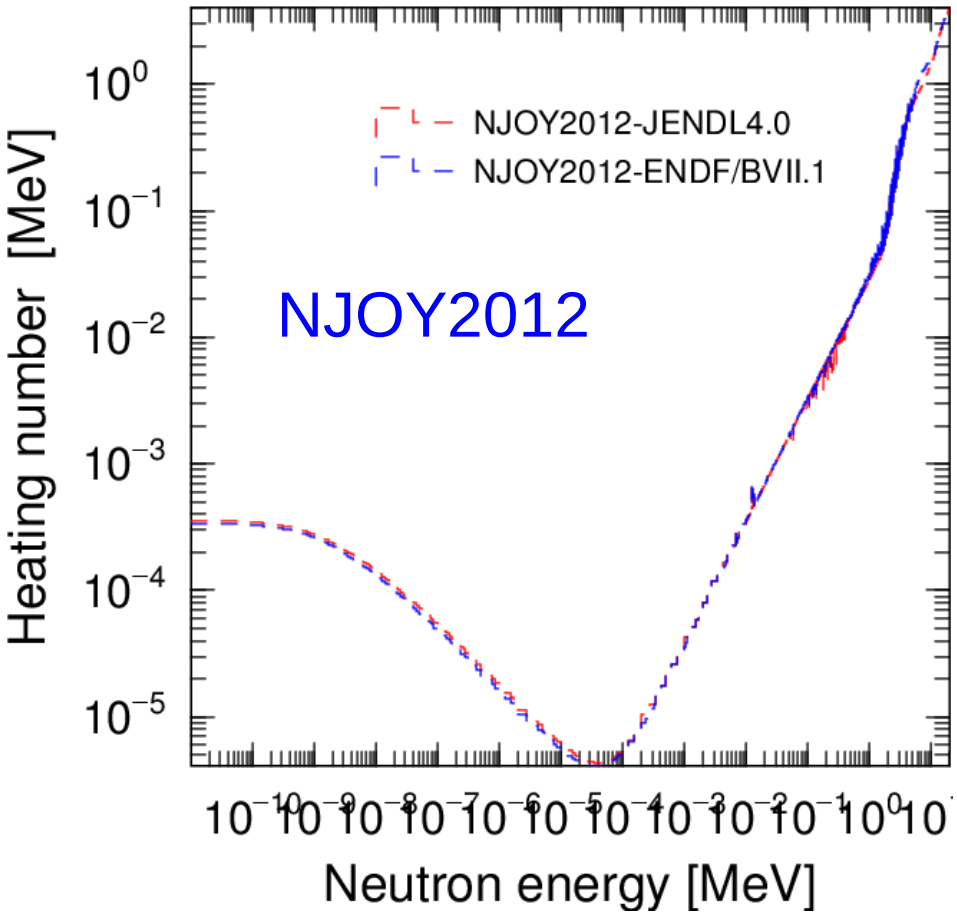


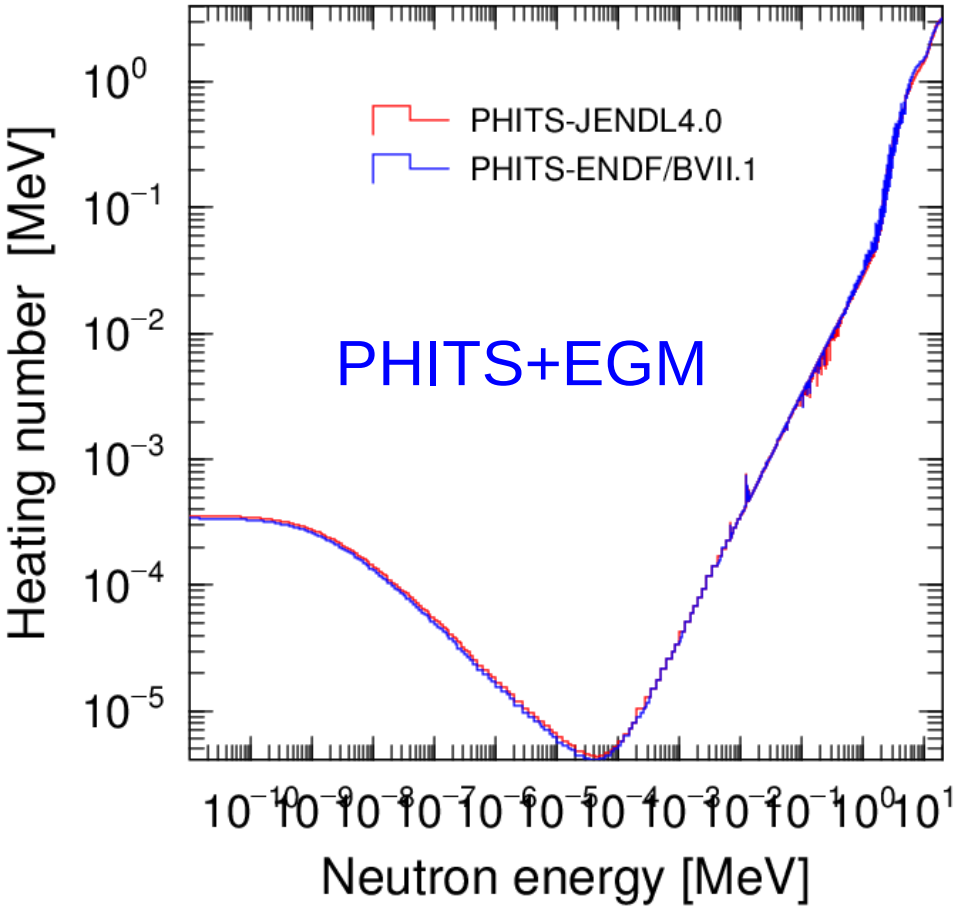
NJOY2012-TENDL2015 is smaller than the others in the neutron capture region. There may be a problem with the secondary γ-ray data for TENDL2015.

For PHITS-EGM, the heating number using EBITEM model and data libraries (MF=3) are the same in the neutron capture region.

➡ The recoil energy generated by the capture reaction is the same regardless of the data library.

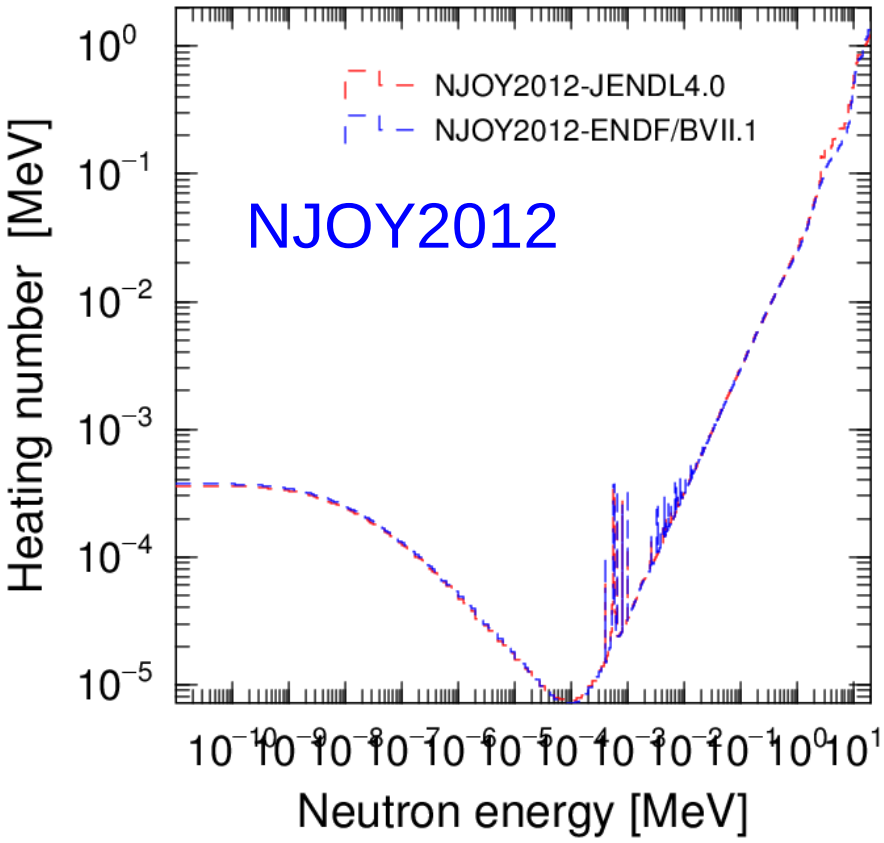
Heating number for ^{58}Ni

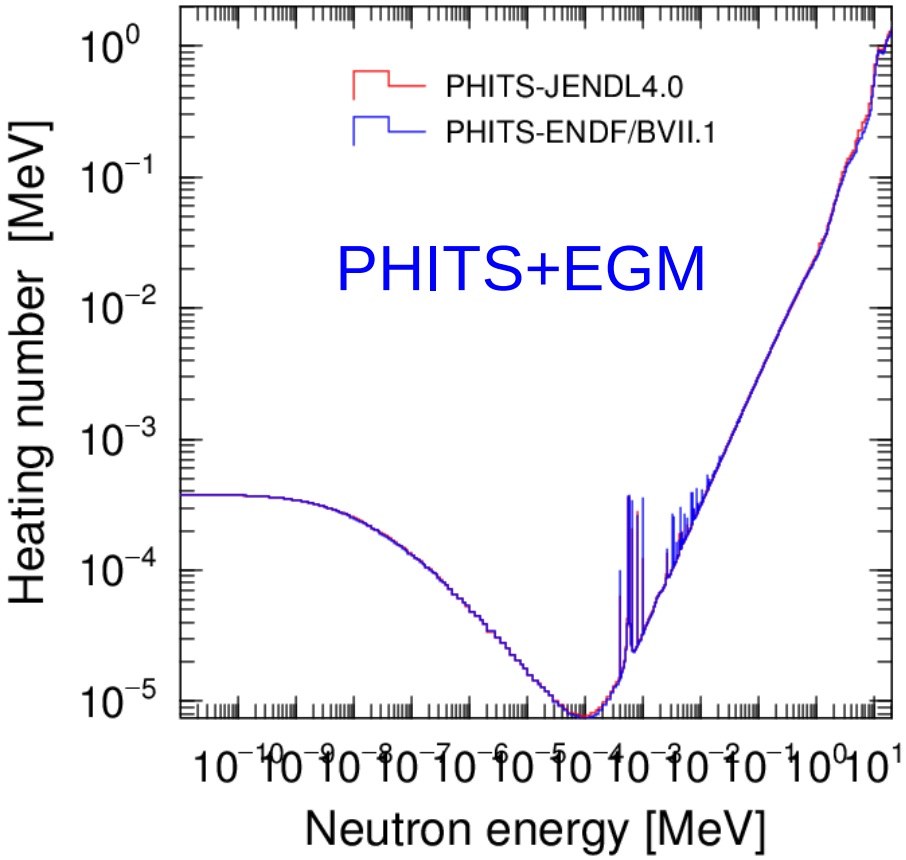




Agreements between NJOY2012 and PHITS are good.
Agreements among data libraries are also good.

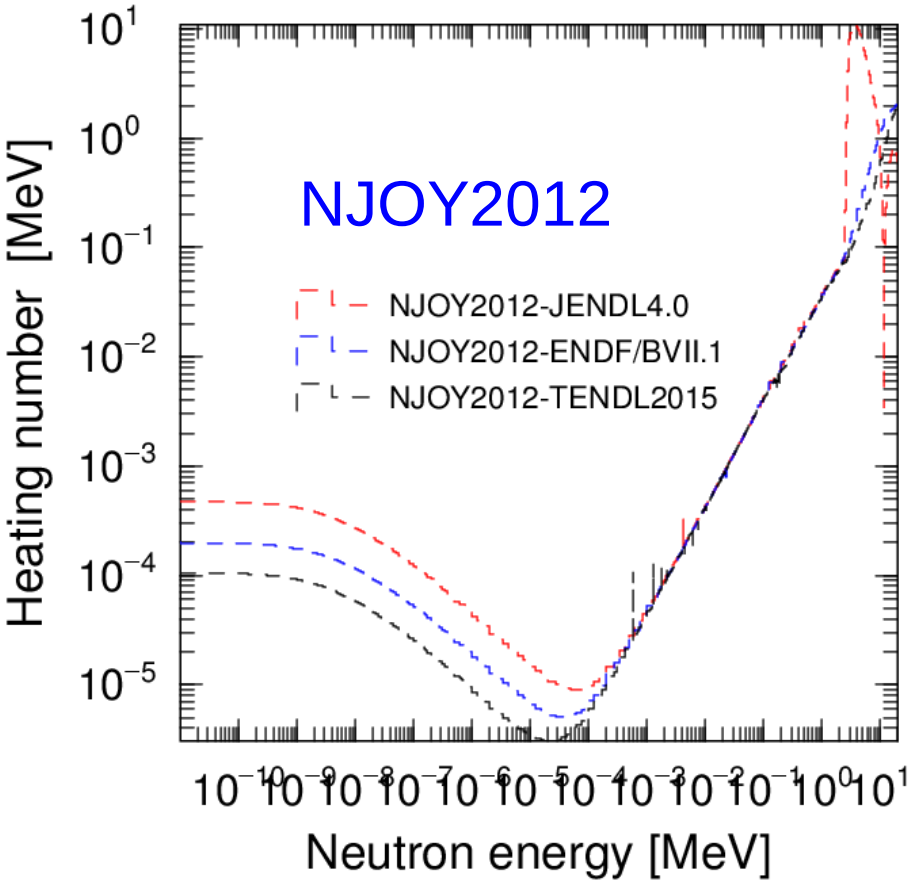
Heating number for ^{63}Cu

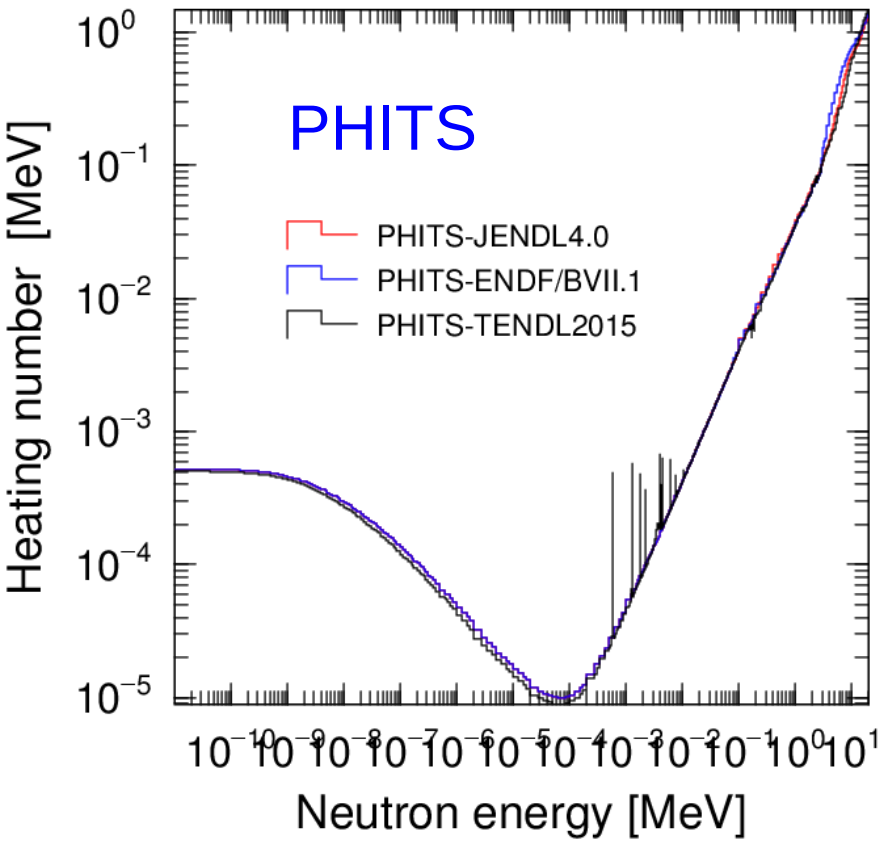




Agreements between NJOY2012 and PHITS are good.
Agreements among data libraries are also good.

Heating number for ^{47}Ti

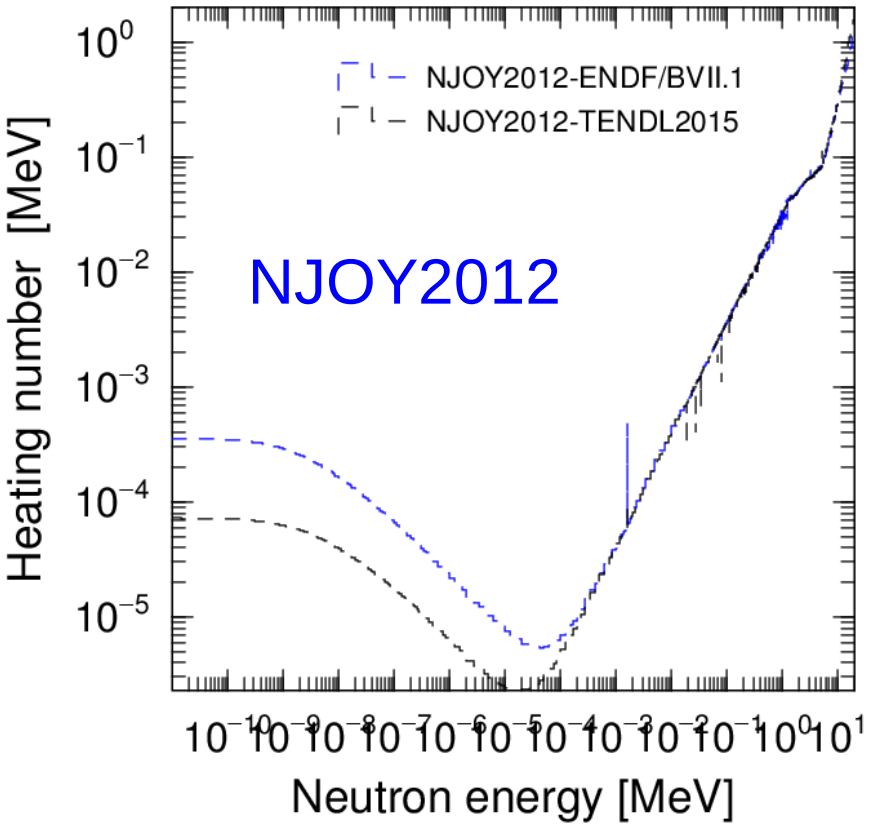


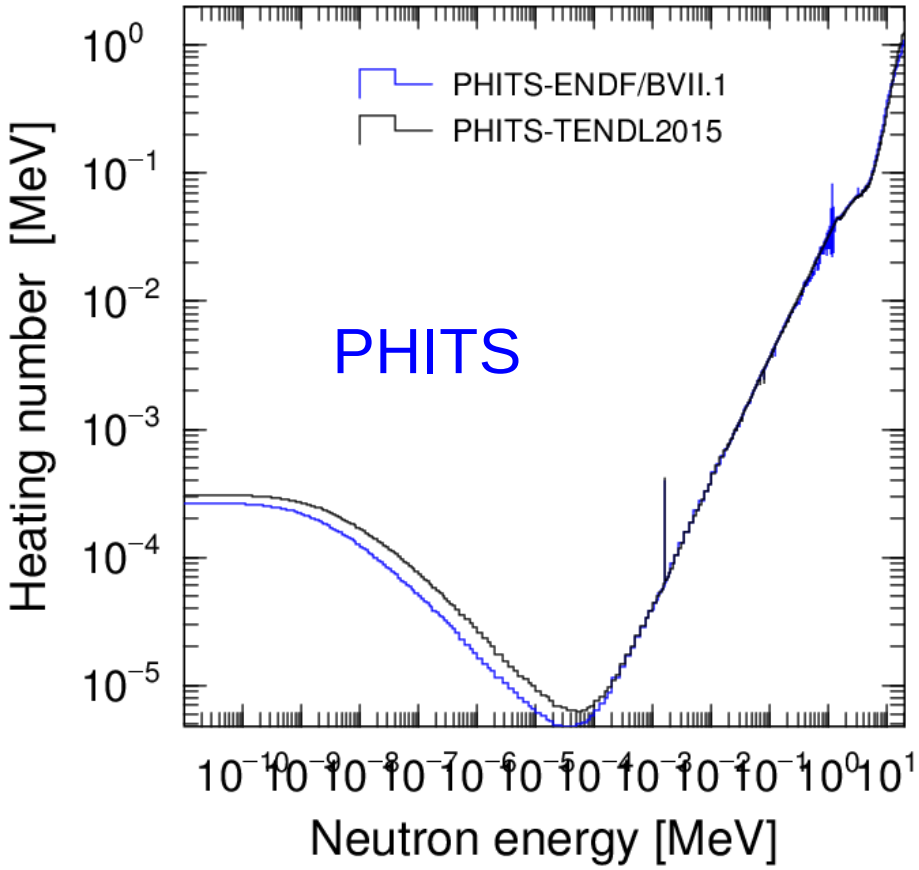


For NJOY2012, there are discrepancy in the neutron capture region. There may be a problem with the secondary γ-ray data.

PHITS-EGM results in the neutron capture region are similar to NJOY2012-JENDL4.0.

Heating number for ^{52}Cr



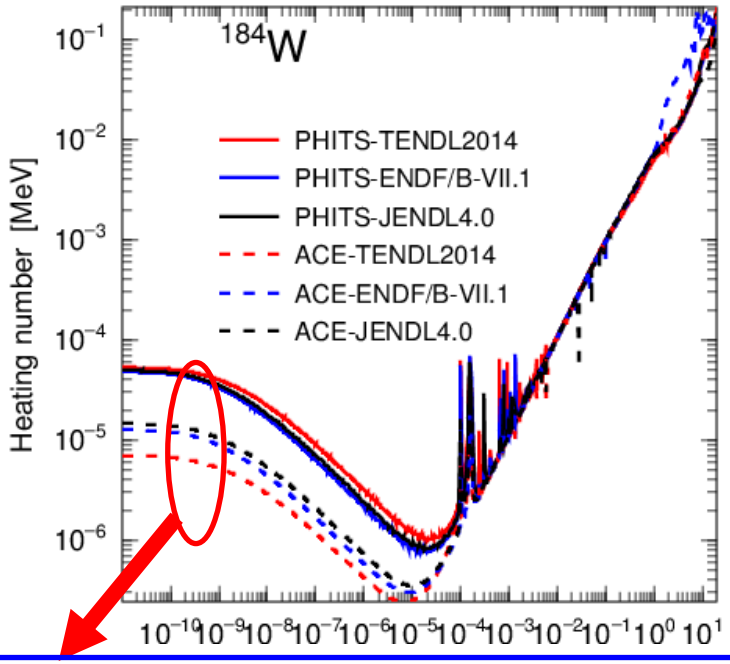


Agreements between NJOY2012+ENDF/BVII.1 and PHITS are good.

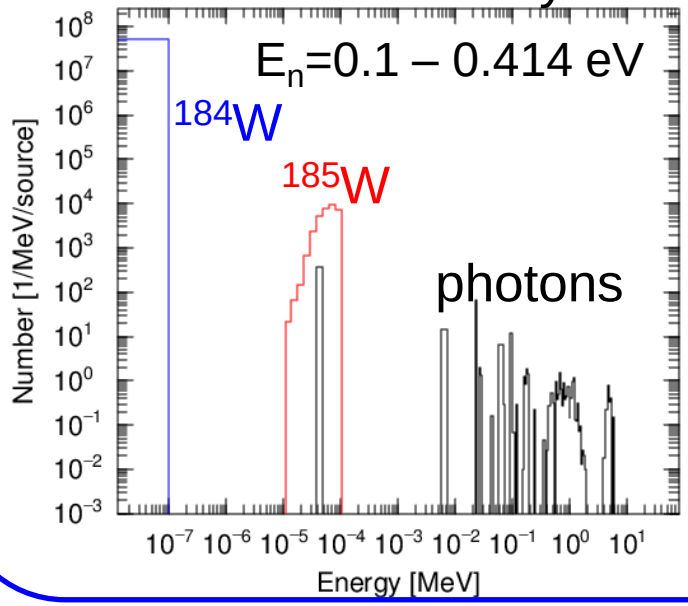
For PHITS, there are difference In neutron capture region,

Neutron capture cross sections are different between ENDF/BVII.1 and TEND2015.

Heating number for ^{184}W



Analysis of recoil spectra using PHITS-EGM



^{185}W produced by the neutron capture reaction and ^{184}W produced by the neutron elastic reactions

Heating number is obtained by the sum of kinetic energies of ^{185}W and ^{184}W.

If PHITS-EGM is correct, there may be a problem with the secondary γ-ray data.

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Calculation conditions for recoil spectra

Codes: PHITS2.92/EGM, NJOY2012.50/HEATR + SPKA*

*Recoil spectra can be extracted from NJOY output at one neutron Energy or fold with n-Spectrum by code SPKA-6C. Details are in https://www-nds.iaea.org/CRPdpa/

Materials: Si, Fe, Mn, Zr, W, Be, C

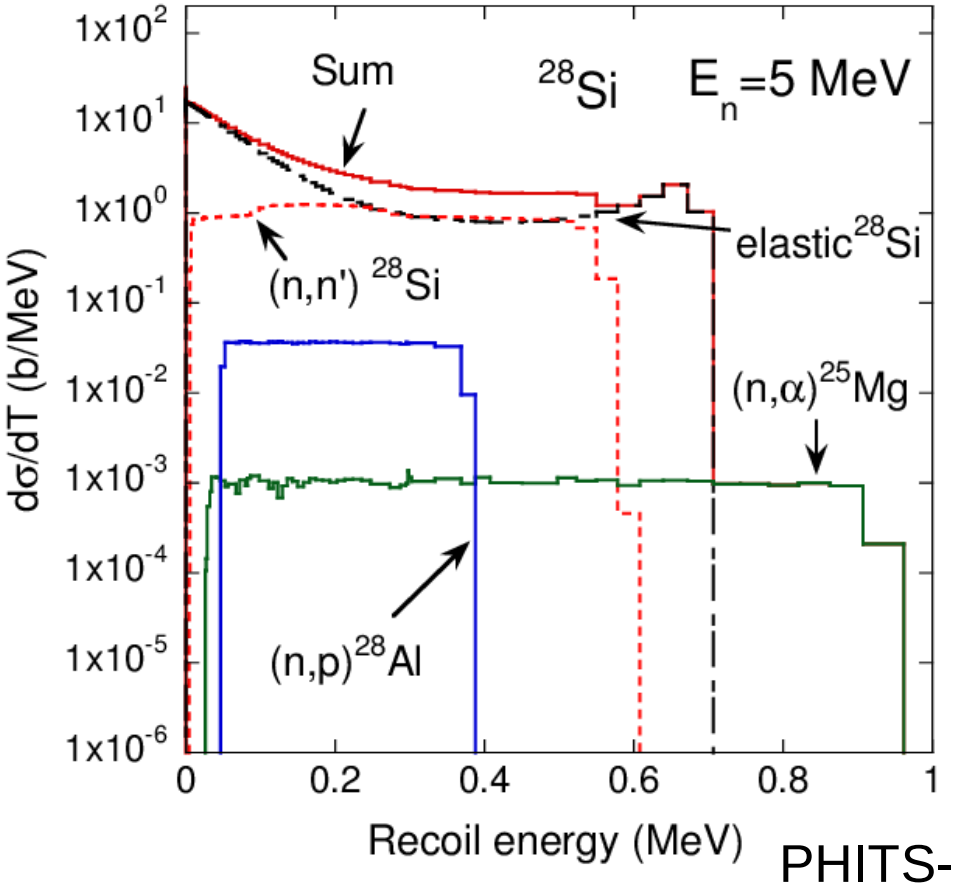
Neutron energy: 5 MeV and 14.5 MeV

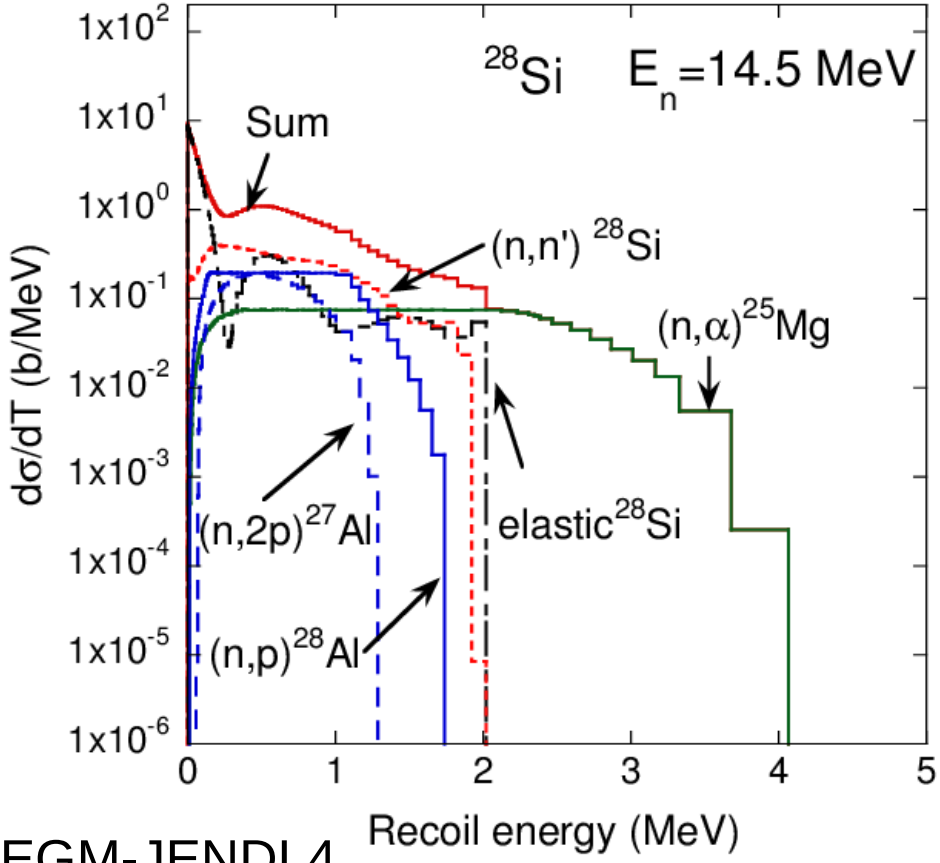
Output: differential cross section (b/MeV)

Nuclear data libraries: ENDF-BVII.1, JENDL-4.0, TENDL-2014, JEFF-3.2

Recoil spectra for n+Si using PHITS-EGM

PHITS-EGM can calculate contribution reaction channel.
It is useful for comparison and verification with recoil spectra using NJOY.

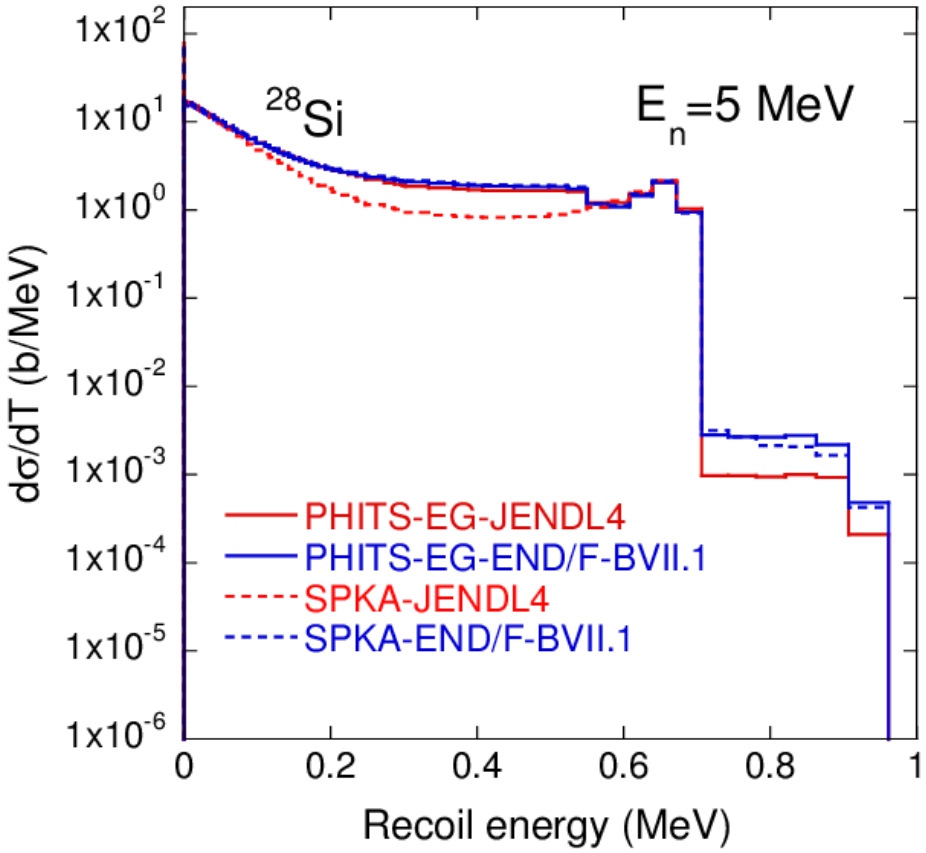


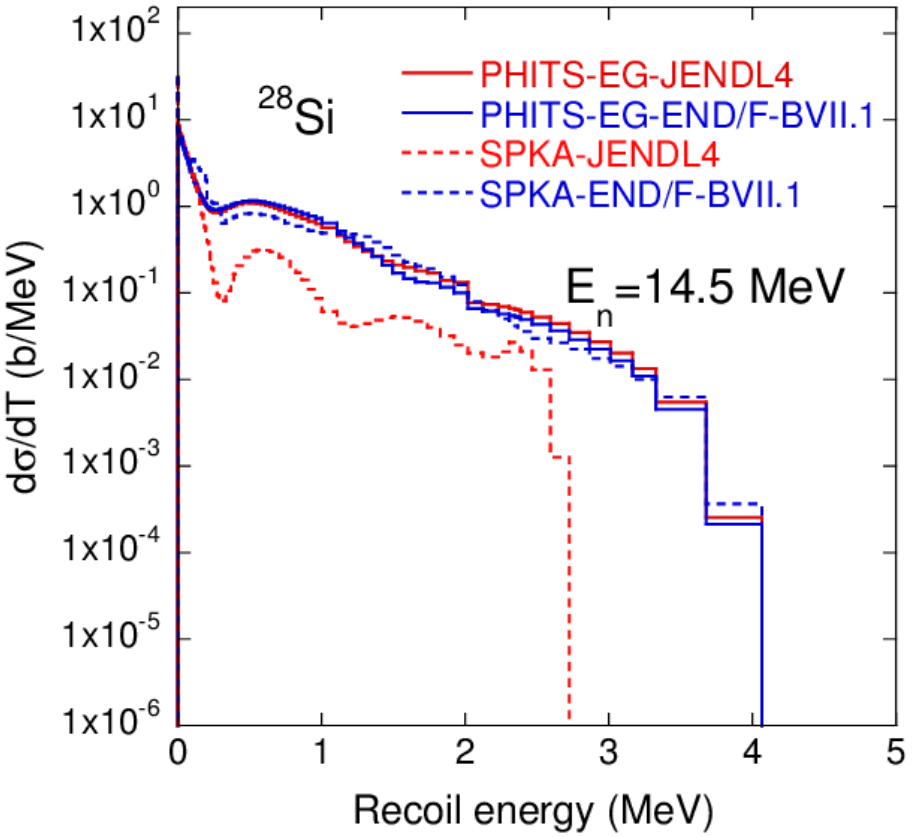


PHITS-EGM-JENDL4

5 MeV: Elastic and (n,n') contributions are large in the recoil spectra.
14 MeV: (n,α) is dominant for higher energy.

Recoil spectra for n+Si using PHITS-EGM and NJOY-SPKA

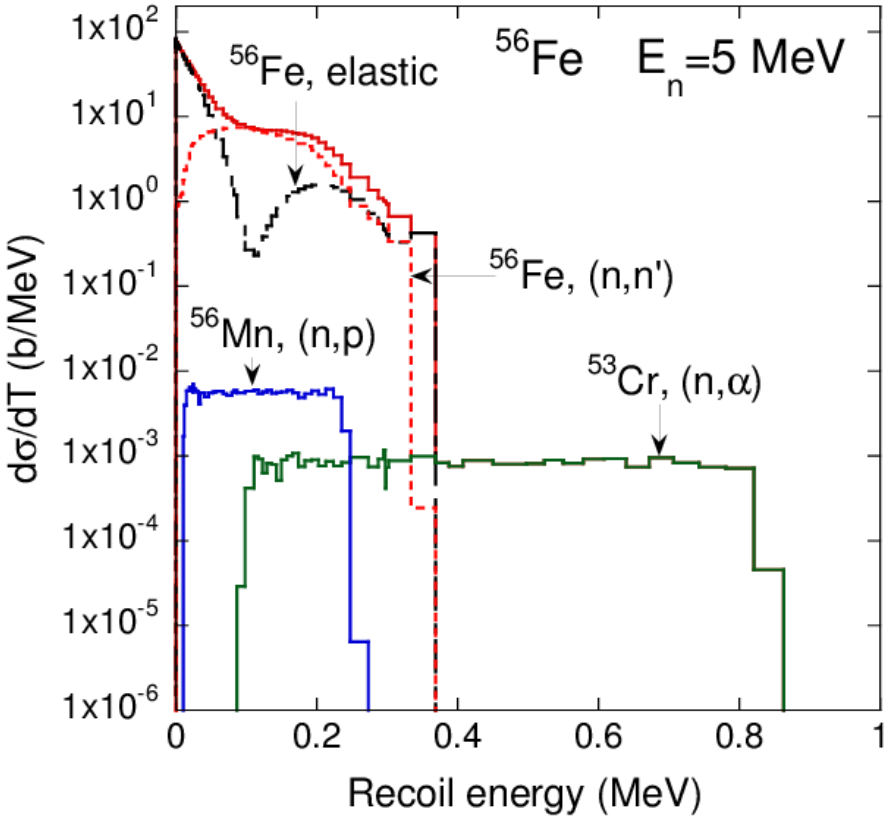


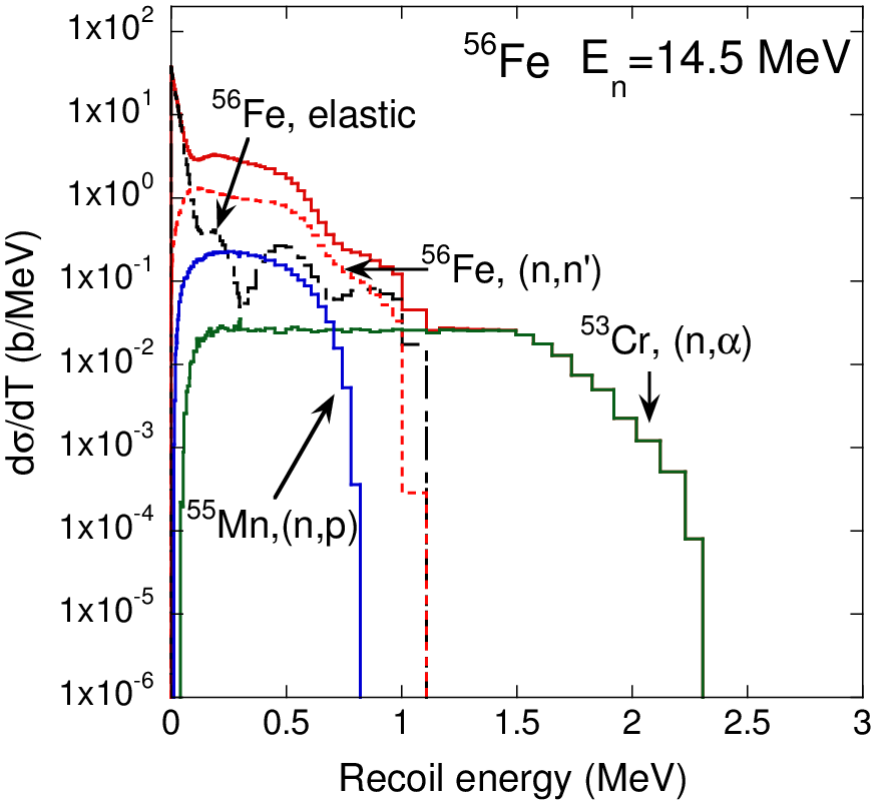


PHITS and NJOY-SPKA are in good agreement without SPKA-JENDL4.
JENDL4 is considered to contain only the elastic component.

Recoil spectra for n+Fe with PHITS-EGM

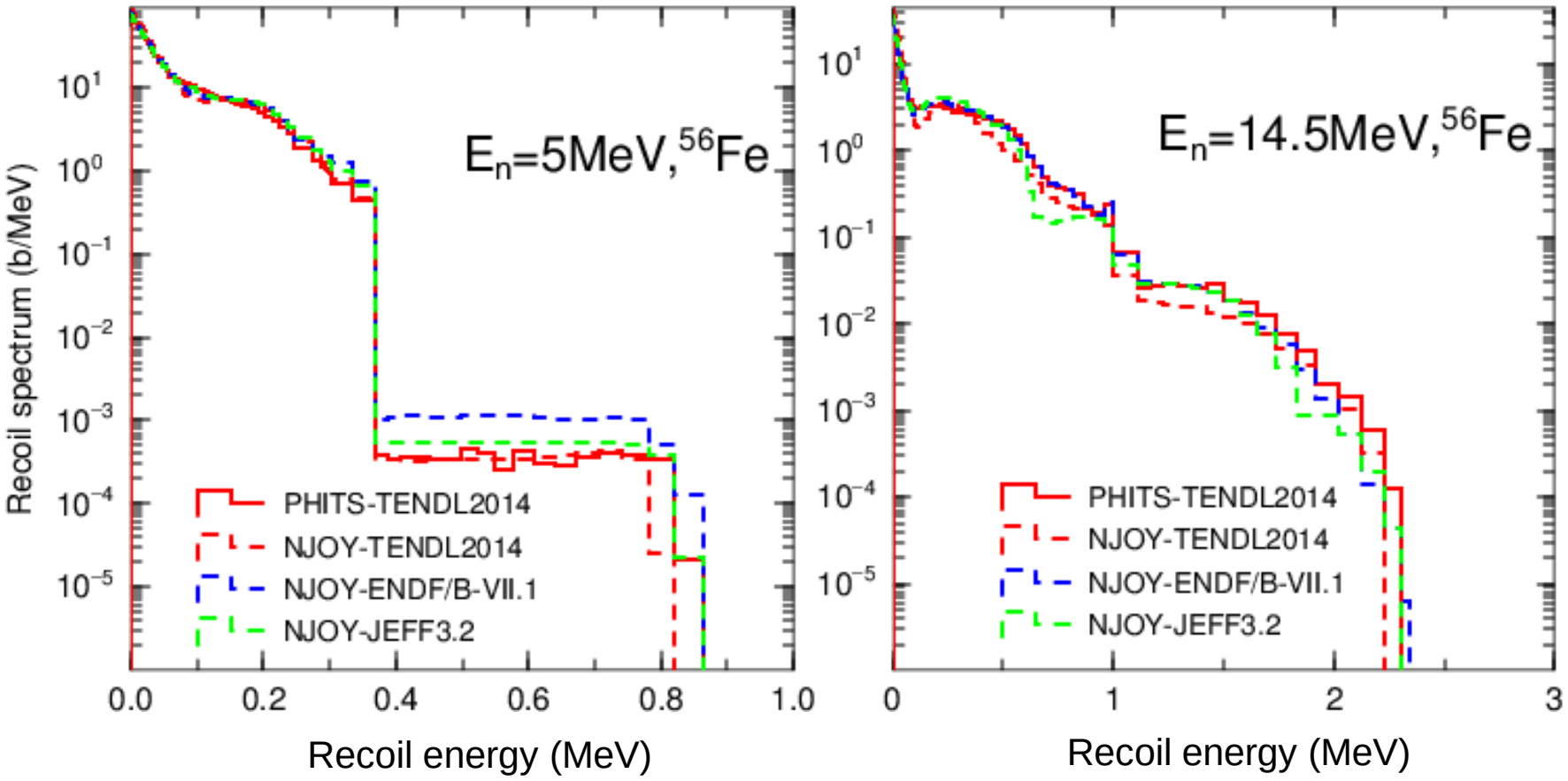
PHITS-EGM can calculate contribution reaction channel on PKA spectra.





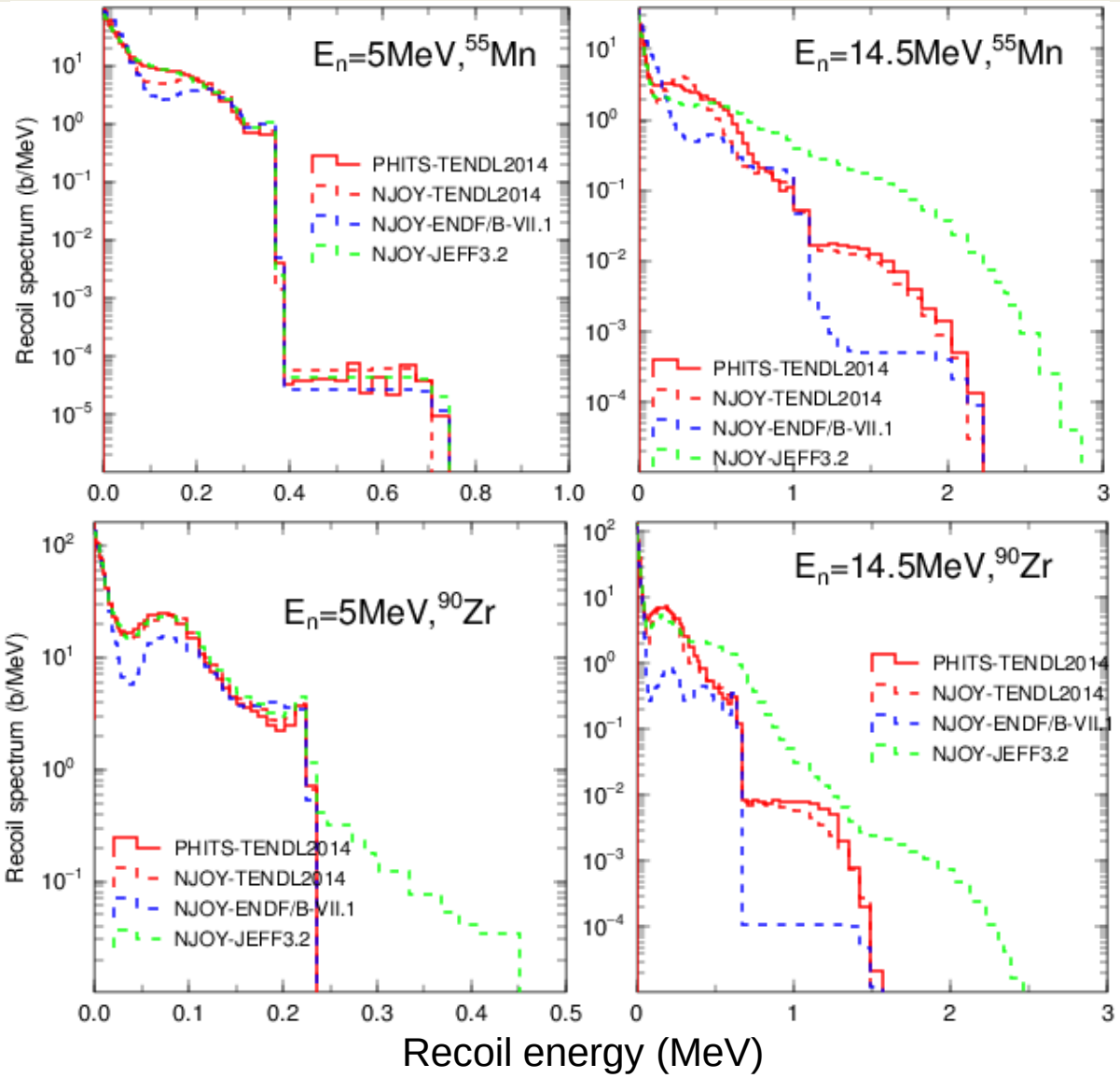
5 MeV: Contribution of elastic and (n,n') are large in recoil spectra.
14 MeV: (n,α) is dominant for higher energy.

Recoil spectra for n+Fe using PHITS-EGM and NJOY-SPKA



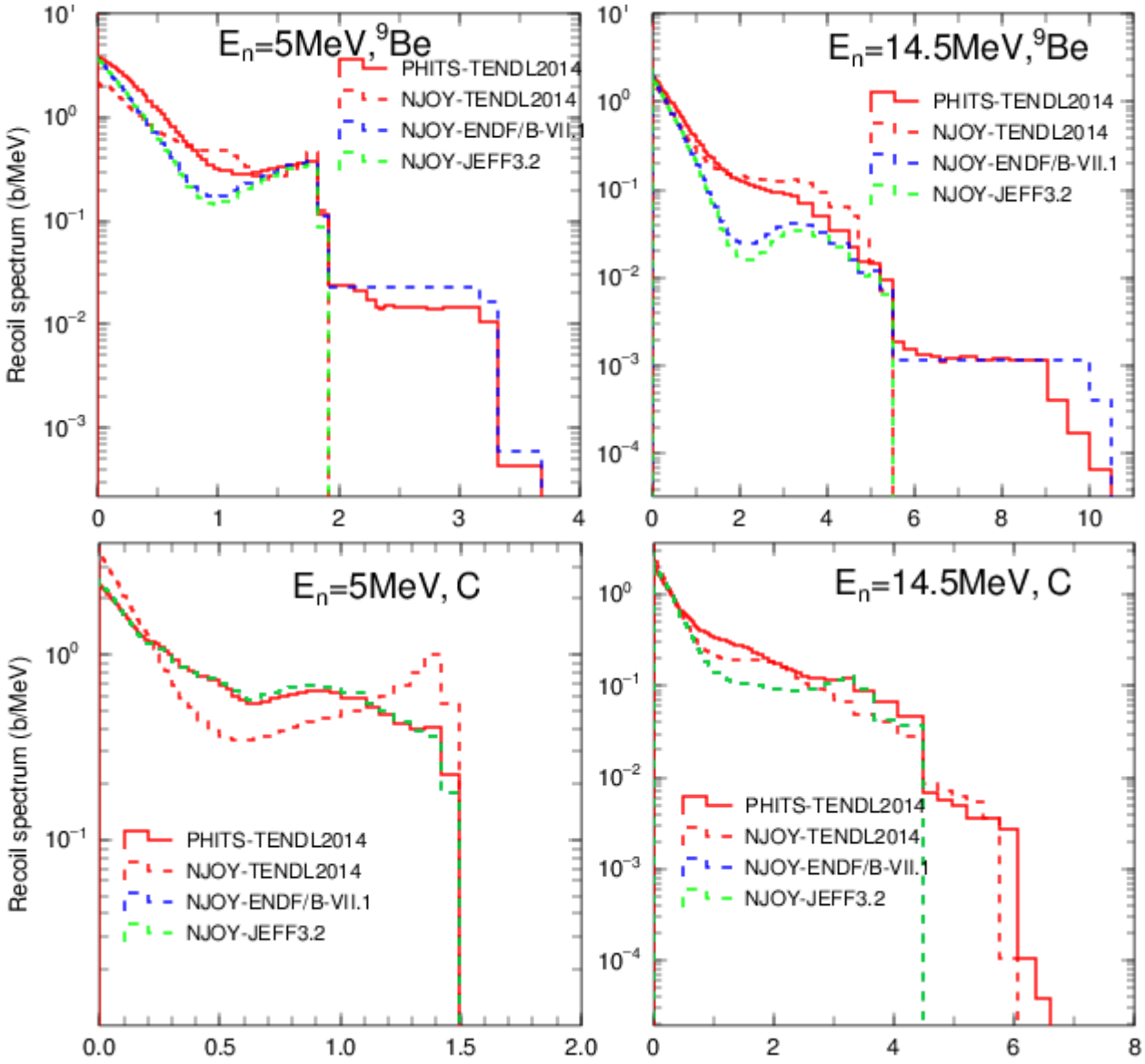
Overall, PHITS and NJOY-SPKA are in good agreement.

Recoil spectra for ^{55}Mn and ^{90}Zr using PHITS-EGM and NJOY-SPKA



- ✓ PHITS and NJOY-SPKA with TENDL2014 are in good agreement.
- ✓ ENDF/BVII.1 may lacks Information of some reaction.
- ✓ JEFF3.2 may have strange energy-angle distributions.

Recoil spectra for ^{9}Be and ^{nat}C using PHITS-EGM and NJOY-SPKA



*JEFF3.2 is same with ENDF/BVII.1 for C.

✓ TENDL2014, ENDF/BVII.1 and JEFF3.2 may lack Information of energy-angle distributions for PKA.

Summary

- PHITS-EGM can calculate heating number and recoil energy spectra using a different method than NJOY.
- Overall, PHITS-EGM results with different ACE format libraries (MF3 and MF6) are almost same.
- Overall, NJOY2012 results are good agreements with PHITS-EGM results except for neutron capture region.
- PHITS-EGM is useful for validating the latest version of NJOY results and various nuclear data libraries.