Calculation of self-shielding correction for Neutron activation experiments at IREN facility using PHITS and MCNP6

Neutron self-shielding factors?

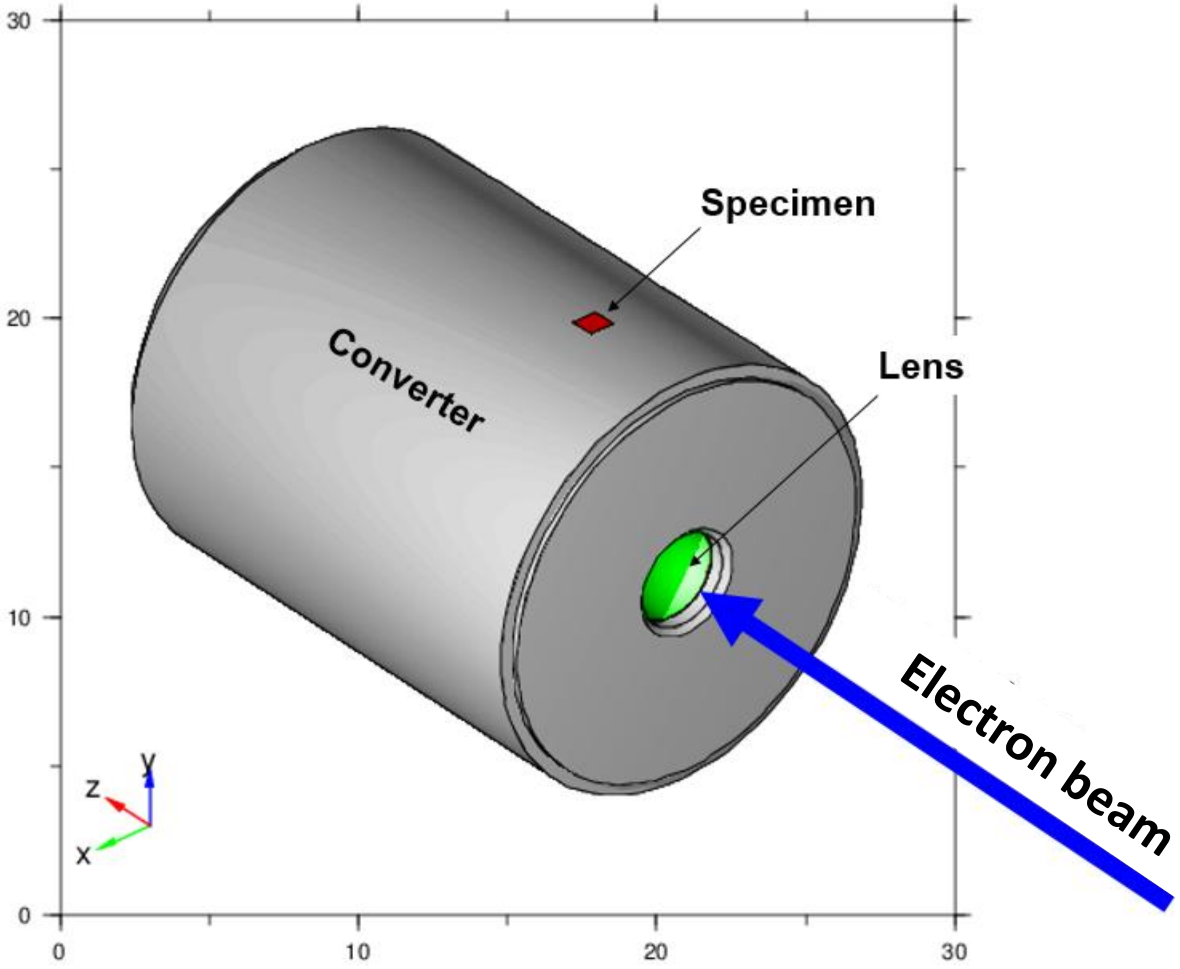
The Neutron self-shielding Factor is a correction factor that accounts for the effect of neutron absorption within the activation sample itself, which causes the neutron flux inside the sample to be non-uniform compared to the external flux.

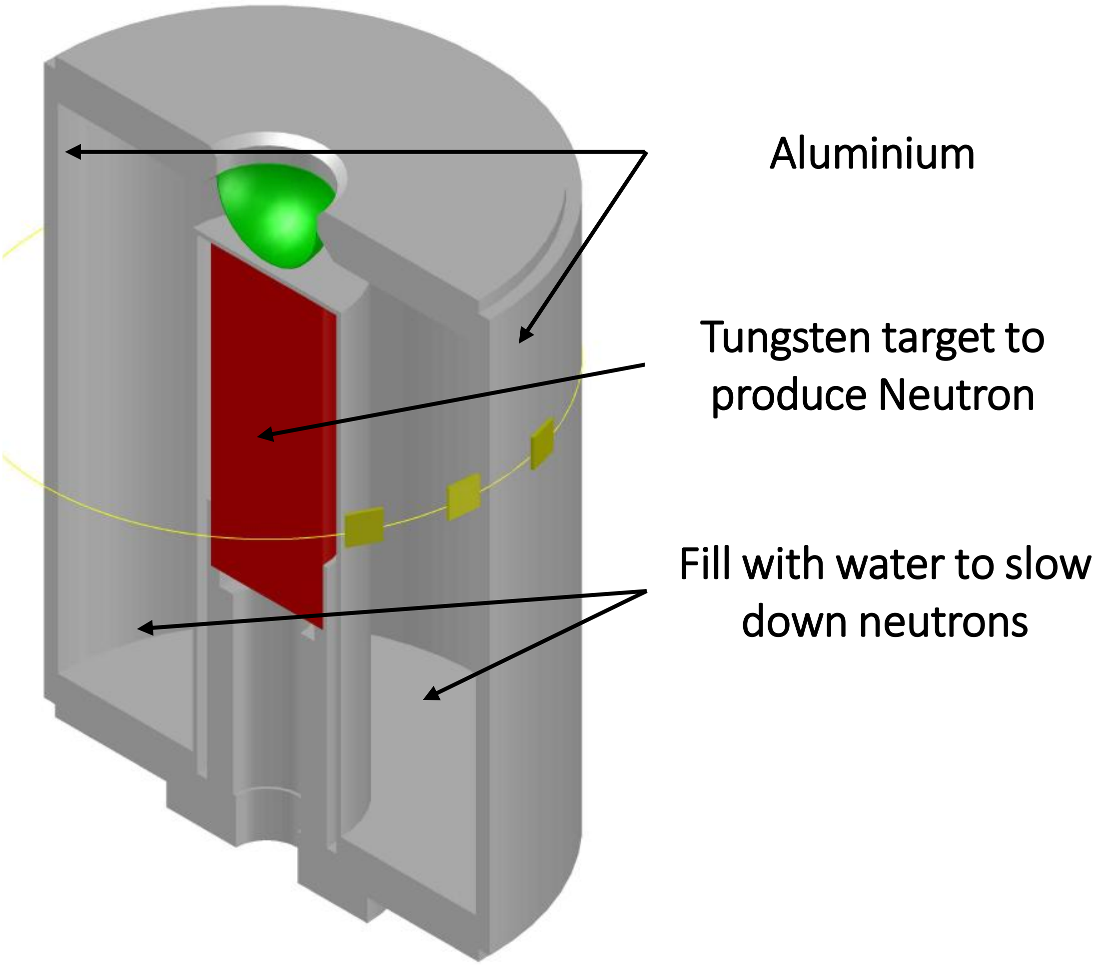
The self-shielding effect depends on several factors:

- neutron absorption cross-section of the element,
- sample's shape,
- elemental composition
- is strongly influenced by the spatial and energy distribution of the neutron field

This effect must be calculated separately for thermal and epithermal neutrons due to their distinct energy distributions.

IREN Converter Structure





Neutron flux distribution in IREN

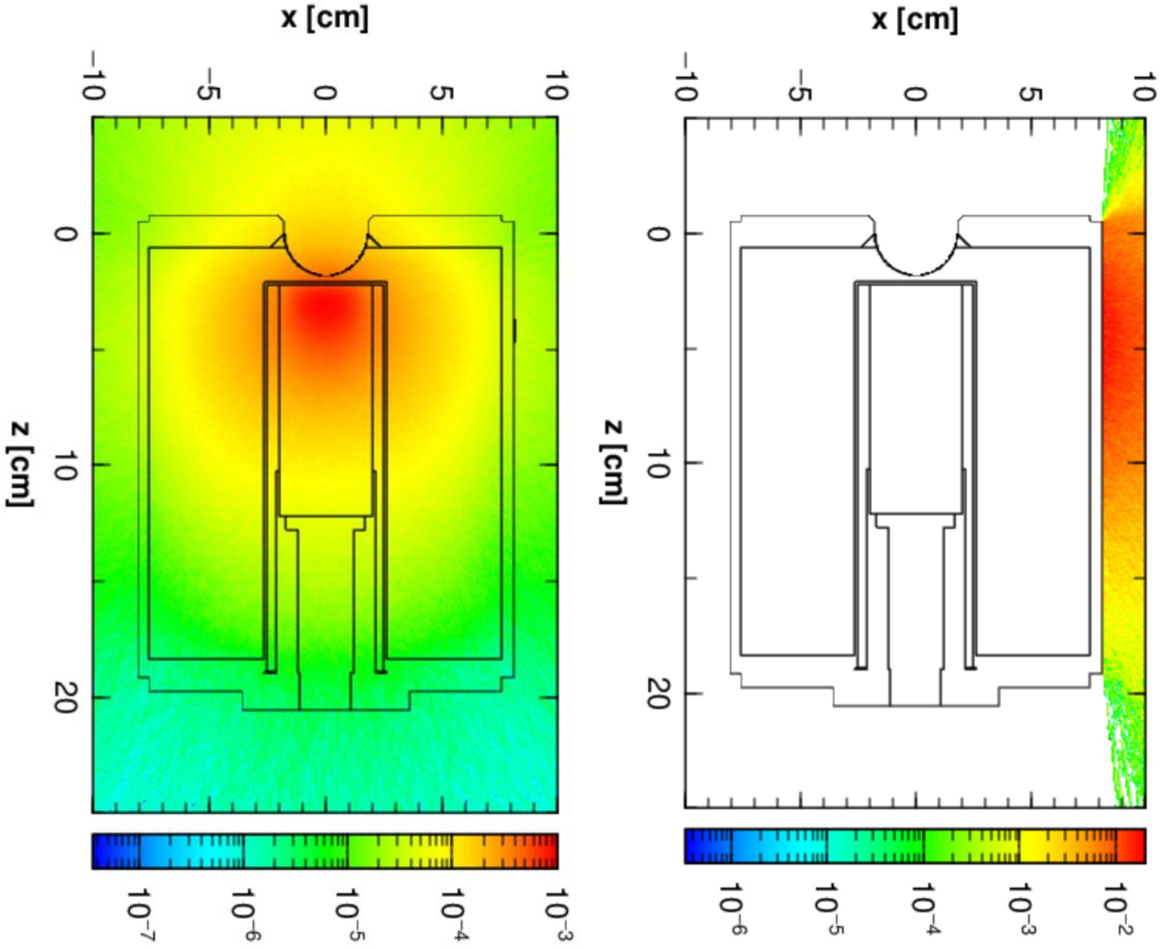


Fig 2b&c: Neutron flux distribution

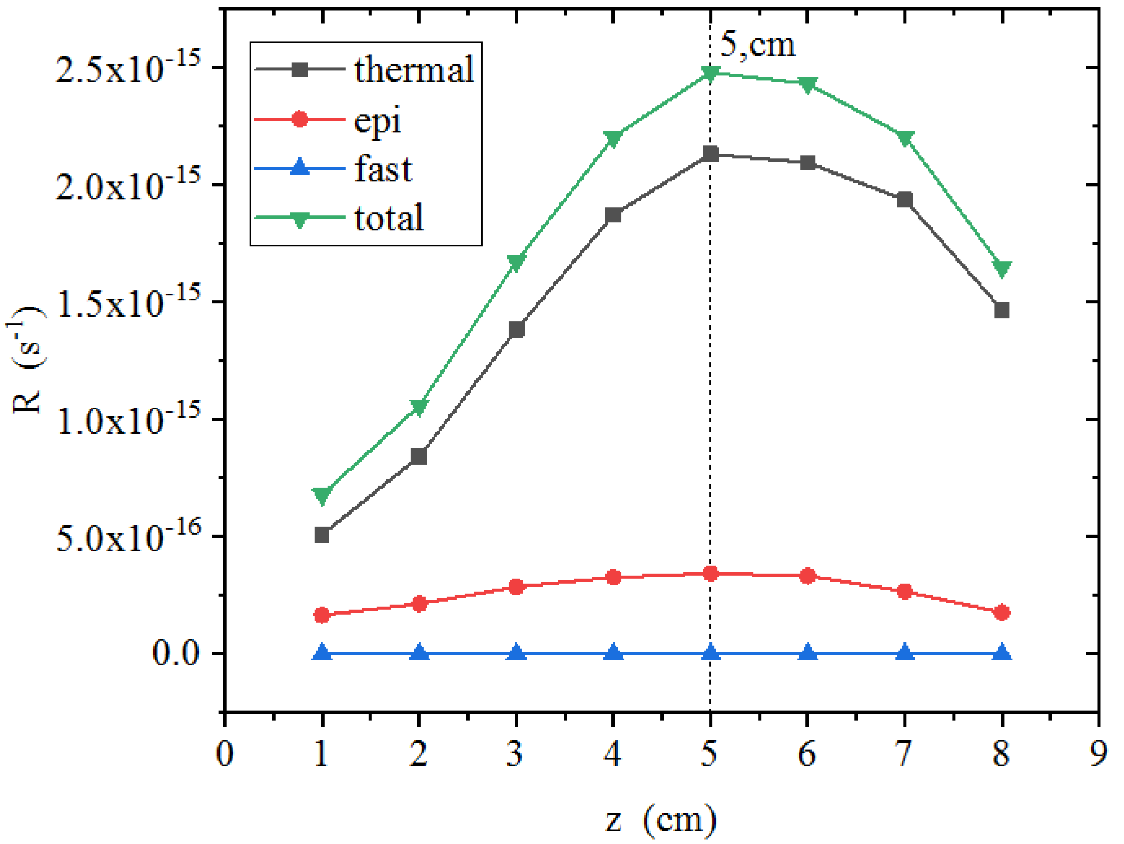


Fig 2a: The reaction rate calculated for ^{63}Cu at 5cm position

Neutron energy spectrum regions

$$\varphi_{th}(E_n) = \Phi_1 . \frac{E_n}{(kT)^2} . e^{-E_n/kT} \quad (E_n < E_{Cd} \approx 0.55 \text{ eV})(1)$$

$$\varphi_{epi}(E_n) = \frac{\Phi_2}{{E_n}^{1+\alpha}} \quad (E_{Cd} < E_n \leq 0.2 \text{ MeV})(2)$$

- E_n is neutron energy
- k is the Boltzmann constant
- T is average neutron temperature
- α is the epi-thermal spectrum shape parameter

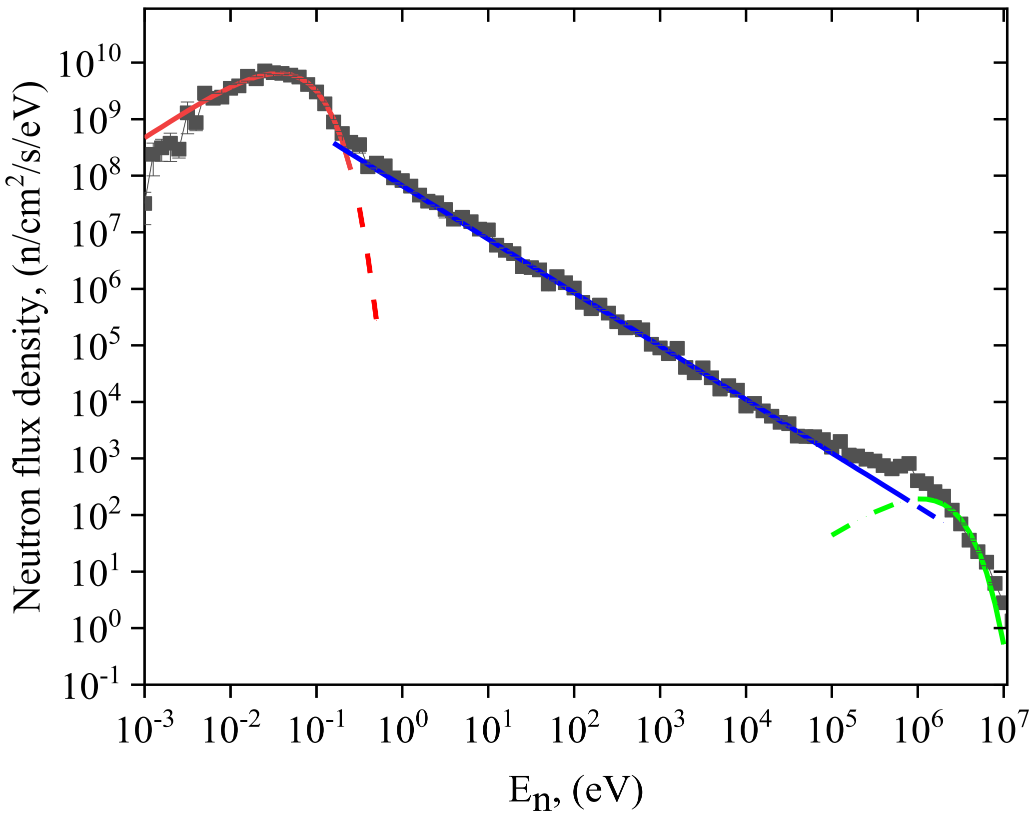


Fig 3: Neutron flux spectrum through surface 1x1cm at 5cm position

Neutron self-shielding factors

Table 1: Comparative reports on calculating G-factors for diverse parametric conditions using MCNP simulations

Author, year	Neutron source geometry	Neutron energy spectrum	Specimen geometry	Specimen material	Evaluated G-factor
Salgado et al., 2004	// beam, iso. field	Epithermal (monoenergetic, 1/E)	Foil	^{232}Th, ^{197}Au and ^{56}Fe	G_{res}, G_{res*}
Goncalves et al., 2002; Goncalves et al., 2001*	// beam, iso. field	Around resonance region (1/E)	Foil, wire	^{59}Co, ^{63}Cu, ^{197}Au, ^{115}In, ^{55}Mn, ^{185}Re	G_{res}
Goncalves et al., 2001**	// beam, iso. field	Epithermal, around resonance region (1/E)	Foil, wire	Au, Co, Mn	G_{res}
Goncalves et al., 2004	// beam, iso. field	Around resonance region (1/E)	Cylinder	^{59}Co, ^{63}Cu, ^{197}Au, ^{115}In, ^{55}Mn, ^{185}Re	G_{res}
Martinho et al., 2003	iso. field	Around resonance region (1/E)	Foil, wire, sphere	^{59}Co, ^{63}Cu, ^{197}Au, ^{115}In, ^{55}Mn, ^{185}Re	G_{res}
Martinho et al., 2004	iso. field	Thermal (Maxwellian)	Foil, wire, sphere, cylinder	Al, Au, Cd, Co, Cu, Eu, Gd, In, Ir, Mo, Ni, Pb, Pt, Rh, Sc, Sm, Ta	G_{th}
This work	Spatial and spectral fidelity to the electron-beam-driven neutron source		Foil	Au, Cu, W, Zr	G_{th}, G_{epi}

Neutron self-shielding factors

The G-factor is defined as the ratio of the reaction rate in the actual sample to that in an infinitely diluted sample (Goncalves et al., 2002):

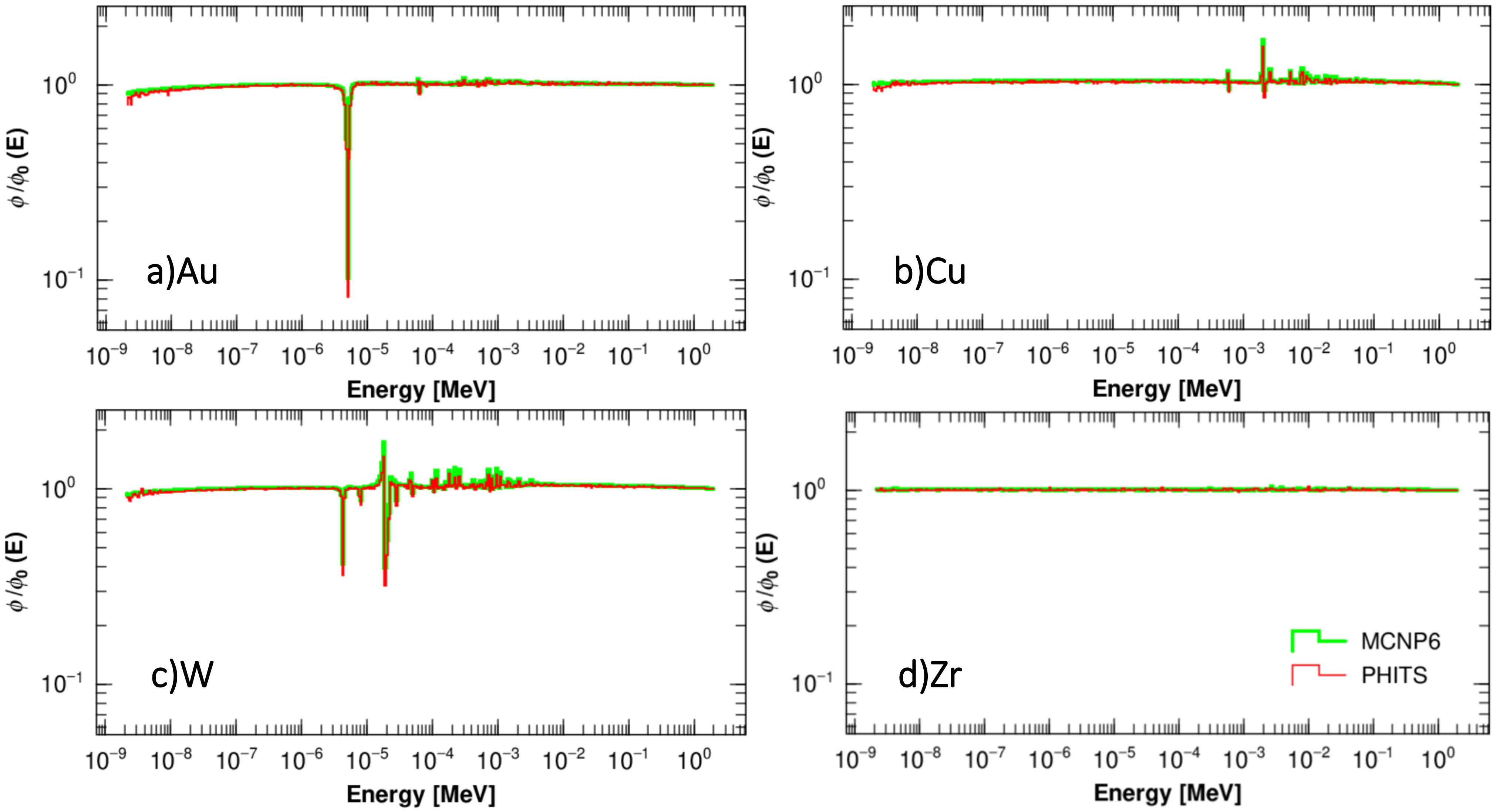
$$G = \frac{\int_{E_1}^{E_2} \phi(E)\sigma(E)dE}{\int_{E_1}^{E_2} \phi_0(E)\sigma(E)dE} \quad (3)$$

- **$\phi(E)$** and **$\phi_0(E)$** are the neutron flux energy distributions in the actual and infinitely diluted sample, respectively;
- **E_1** and **E_2** define the integration bounds (for **G_{th}: $E_1 = 10^{-3}$ eV** and **$E_2 = 0.5$ eV**; for **G_{epi}: $E_1 = 0.5$ eV** and **$E_2 = 0.2$ MeV**);
- **$\sigma(E)$** is the energy-dependent **(n, γ)** reaction cross-section.

Table 2: Samples used in experiments and simulations

Foil	Density (g/cm^3)	Dimension (mm)	Isotopes
Au	19.32	10x10x0.1	^{197}Au (100%)
Cu	8.96	10x10x0.5	^{63}Cu (69.15%), ^{65}Cu (30.85%)
W	19.3	10x9x0.35	^{180}W (0.12%), ^{182}W (26.5%), ^{183}W (14.31%), ^{184}W (30.64%), ^{186}W (28.43%)
Zr	6.51	10x9x0.1	^{90}Zr (51.45%), ^{91}Zr (11.22%), ^{92}Zr(17.15%), ^{94}Zr (17.38%), ^{96}Zr (2.8%)

Transmission function (ϕ/ ϕ$_0$(E))



Results & Discussion

Table 3: Comparison of Neutron self-shielding factor results from 2 simulations

Isotopes	Gth			Gepi		
	PHITS	MCNP	Diff_Gth	PHITS	MCNP	Diff_Gepi
197Au	0.962±0.006	0.974±0.004	1.2%	0.337±0.009	0.360±0.001	6.3%
63Cu	1.018±0.016	1.026±0.014	0.8%	0.979±0.030	0.988±0.009	1.0%
94Zr	1.003±0.014	1.006±0.007	0.2%	1.004±0.043	1.007±0.006	0.4%
96Zr	1.003±0.007	1.006±0.005	0.2%	1.001±0.076	1.009±0.004	0.7%
186W	0.982±0.007	0.989±0.004	0.7%	0.496±0.016	0.541±0.002	8.4%

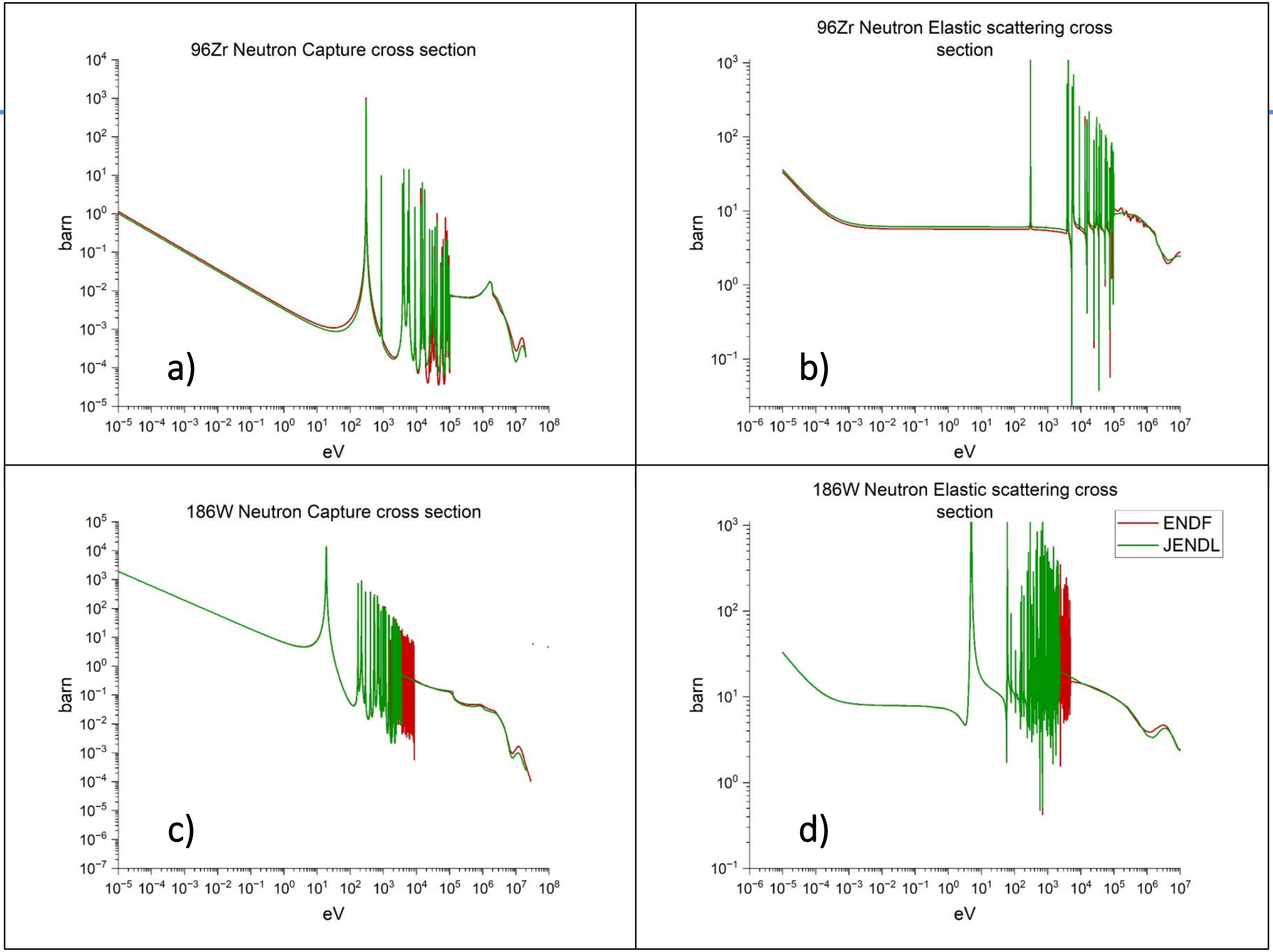


Fig: Comparison of neutron section between ENDF and JENDL

Thermal neutron cross-section

Formula to determine Thermal neutron cross-section σ_0 as follows:

$$\sigma_{0,x} = \sigma_{0,Au} \times \frac{R_x - F_{Cd}\, R_{x,Cd}}{R_{Au} - F_{Cd}\, R_{Au,Cd}} \times \frac{G_{th,Au} \cdot g_{Au}}{G_{th,x} \cdot g_x} \quad (6)$$

- $\sigma_{0,Au}$ = 98.65 ± 0.09 barn
- R_x and $R_{x,Cd}$ are reaction rates per atom for isotope in bare and Cd-covered
- F_{cd} is cadmium correction factor
- g_x is Westcott factor correction
- G_{th} is thermal neutron self-shielding factor

Resonance integral

Formula to determine Resonance integral $I_0(\alpha)$:

$$I_{0,x}(\alpha) = I_{0,Au}(\alpha) \times \frac{\sigma_{0,x}.g_x}{\sigma_{0,Au}.g_{Au}} \times \frac{(CR-F_{Cd})_{Au}}{(CR-F_{Cd})_x} \times \frac{G_{e,Au}.G_{th,x}}{G_{th,Au}.G_{e,x}} \quad (7)$$

- $\mathbf{I_{0,Au}}$ = 1550 ± 28 barn
- $CR = \frac{R_x}{R_{x,Cd}}$
- R_x and $R_{x,Cd}$ are reaction rates per atom for isotope in bare and Cd-covered
- F_{cd} is cadmium correction factor
- g_x is Westcott factor correction
- G_{th} is thermal neutron self-shielding factor
- G_e is epi-thermal neutron self-shielding factor

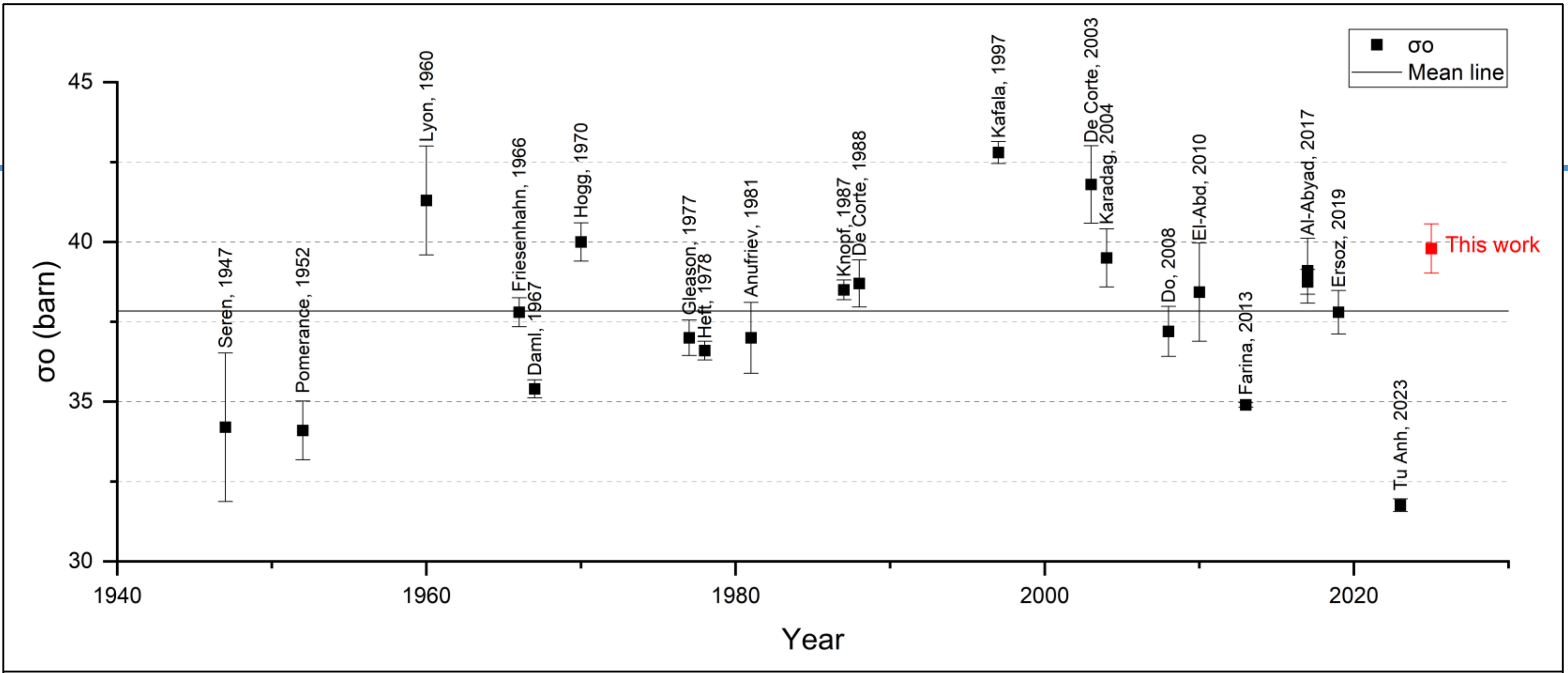


Fig a: Comparison of neutron cross-section σ_o of $^{186}W(\gamma,n)^{187}W$ reaction

This work: $\sigma_o = 40.659 \pm 1.936$ (barn)

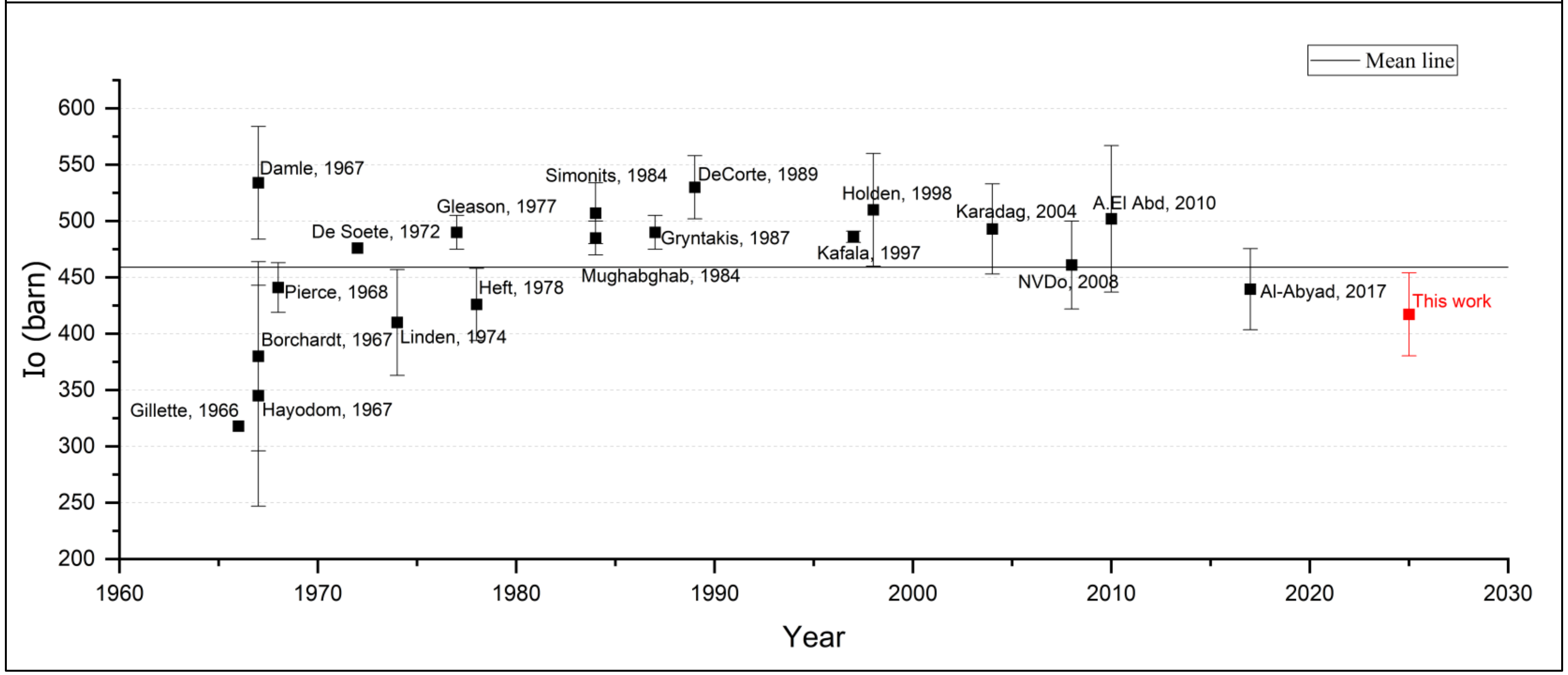


Fig b: Comparison of resonance integral I_o of $^{186}W(\gamma,n)^{187}W$ reaction

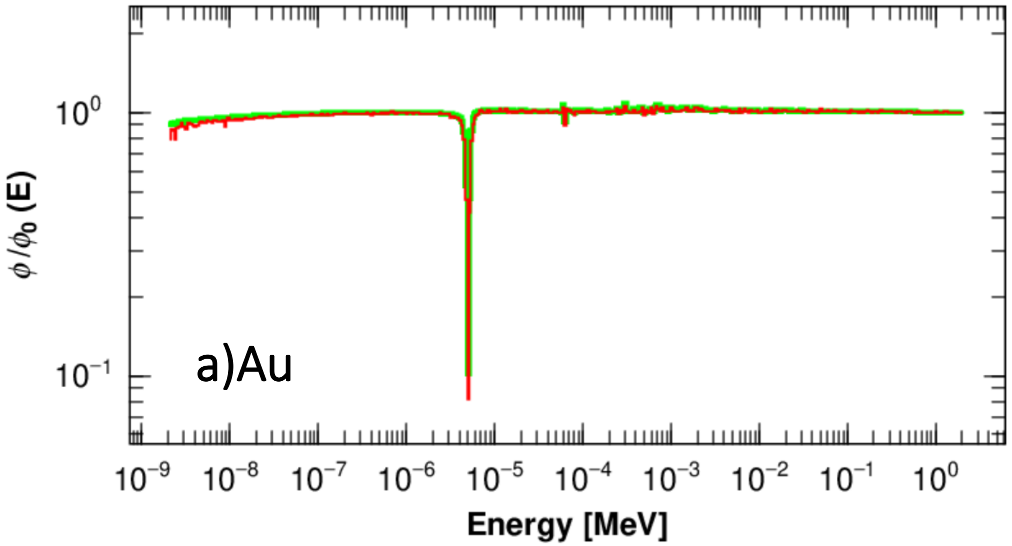
MCNP: $I_o = 417.50 \pm 36.796$ (barn)
PHITS : $I_o = 406.75 \pm 36.796$ (barn)
Difference: 2.6%

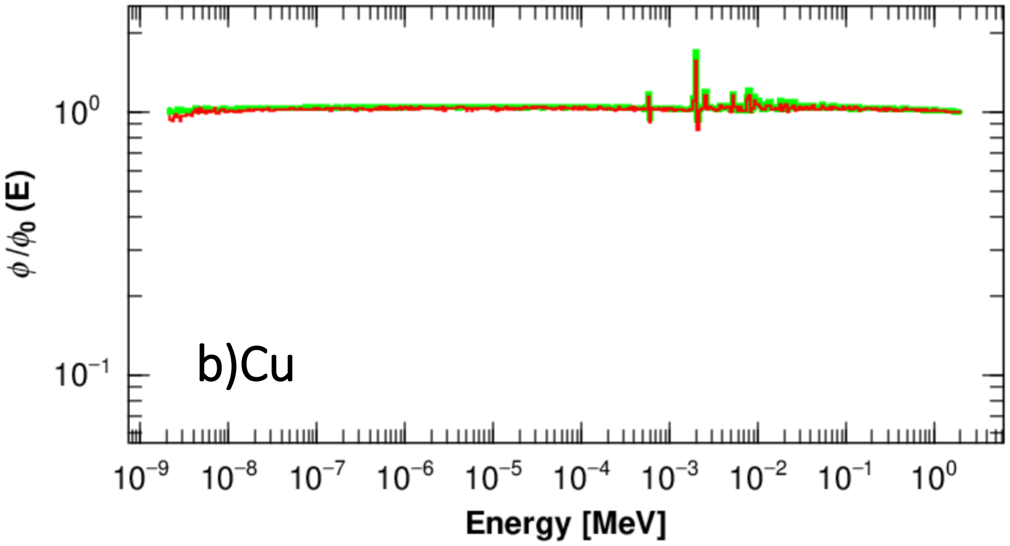
Conclusion

- PHITS v3.21 uses JENDL-4.0 nuclear data library (Shibata et al., 2011).
- MCNP6.1 uses ENDF/B-VII.1 (Kulesza et al., 2022).
- The Gth values obtained from the two computational codes show a discrepancy of less than 1.2%, indicating good agreement and reliability of the results.
- The observed differences in neutron self-shielding factors in the epithermal region, particularly for ^{197}Au (6.3%) and ^{186}W (8.4%), are primarily caused by significant difference in the neutron cross sections between the nuclear data libraries employed.
- Results and calculations are still being updated.

THANKS FOR YOUR ATTENTION

Transmission function ($\phi/\phi_0(E)$)

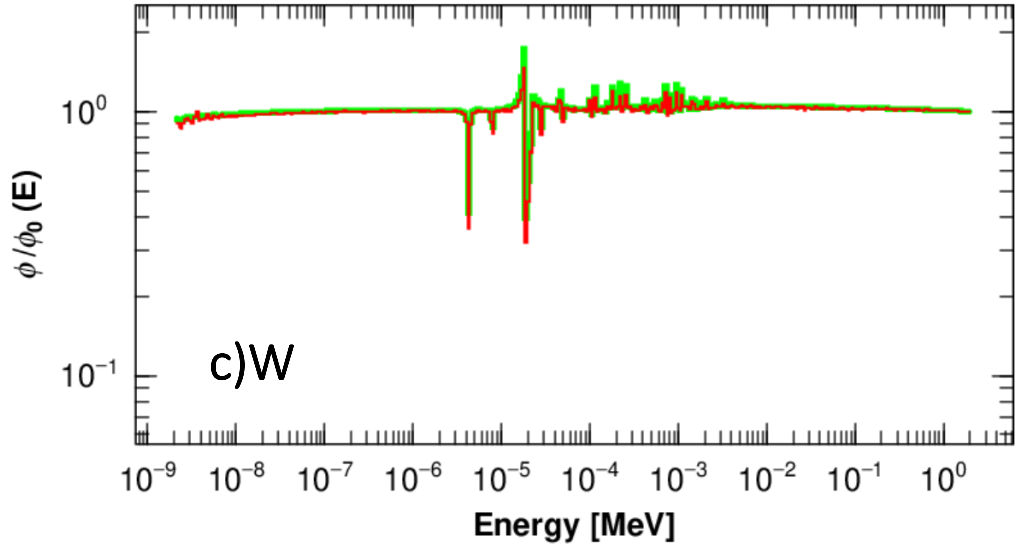


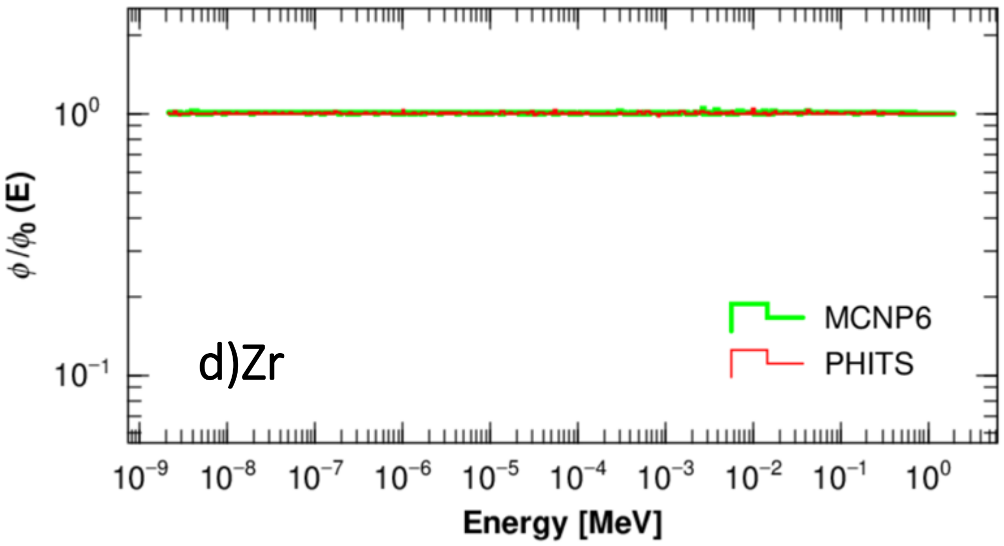


In the $\phi/\phi_0(E)$ spectrum of gold – a high neutron absorber (**Fig.a**), a pronounced dip ($\phi/\phi_0 = 0.08$) occurs at the energy groups of 4.75–5.0 eV, corresponding to the strong resonance absorption of ^{197}Au (27×10^3 barns at 4.9 eV) (Shibata et al., 2011). Depression in the thermal energy region reflects the dominance of absorption cross-section over that of scattering ($\sigma_\gamma > \sigma_s$) herein.

In the $\phi/\phi_0(E)$ spectrum of copper (**Fig.b**), minimal spectral variation is observed except near 1.9–2.1 keV, where ϕ/ϕ_0 peaks at 1.42 (1.9–2.0 keV) before declining to 0.85 (2.0–2.1 keV). As a neutron scatterer ($\sigma_s > \sigma_\gamma$) (Shibata et al., 2011), this behavior arises from resonance self-shielding, whereas neutrons near resonance energies undergo multiple scattering, delaying absorption until energy loss shifts them below resonance thresholds (Goncalves et al., 2002).

Transmission function ($\phi/\phi_0(E)$)





The transmission spectrum $\phi/\phi_0(E)$ for tungsten (**Fig.c**) exhibits complex energy-dependent behavior due to contributions from its isotopic composition (^{180}W, ^{182}W, ^{183}W, ^{184}W, and ^{186}W). Pronounced dips in ϕ/ϕ_0, attributed to resonance absorption, occur at the energy groups of 4.0–4.25 eV (ϕ/ϕ_0 = 0.33), 18–19 eV (ϕ/ϕ_0 = 0.36), 19–20 eV (ϕ/ϕ_0 = 0.38), 20–21 eV (ϕ/ϕ_0 = 0.59), and 21–22 eV (ϕ/ϕ_0 = 0.54). Localized increases in ϕ/ϕ_0, similarly to copper's behavior, arise from neutron scattering moderation effects prior to absorption below resonance energies.

For zirconium (**Fig.d**), $\phi/\phi_0 \sim 1$ across all energy groups, indicating negligible self-shielding. This neutrality stems from zirconium's low absorption and scattering cross-sections. A 0.1 mm zirconium foil thus introduces minimal perturbation to the neutron field, validating its use as a reference material in irradiation geometries where self-shielding corrections are unnecessary.

Neutron self-shielding factor in isotropic neutron field

Table 2: Comparison of Neutron self-shielding factor in isotropic neutron field

Isotopes	Gth			Gepi		
	MATSSF Code (Trkov et al. 2009)	MCNP	Diff_Gth	MATSSF Code (Trkov et al. 2009)	MCNP	Diff_Gepi
197Au	0.8837±0.0084	0.8648±0.0242	2.1%	0.2142±0.009	0.2777±0.0123	22.8%
94Zr	0.9997±0.0015	0.9975±0.0032	0.2%	0.9812±0.0018	1.0062±0.0223	2.5%
96Zr	0.9997±0.0015	0.9975±0.0032	0.2%	0.9773±0.0018	0.9972±0.0715	2.0%
186W	0.9168±0.0017	0.9120±0.0192	0.5%	0.2524±0.0023	0.3588±0.0215	29.7%

Reaction rate

$$R_{th,x} = \Phi_{th}.\sigma_{0,x}.G_{th,x}.g_x \tag{4}$$

$$R_{e,x} = \Phi_e.I_{0,x}(\alpha).G_{e,x} = F_{Cd}\,R_{x,Cd} \tag{5}$$

- $R_{th,x}$ and $R_{e,x}$ are reaction rates per atom for isotope in the thermal and epi-thermal energy regions of neutrons