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R-matrix analysis of n+^{nat}Cl reactions relevant to criticality benchmarks and molten-salt reactor designs

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Oak Ridge National Laboratory, Oak Ridge, TN, USA

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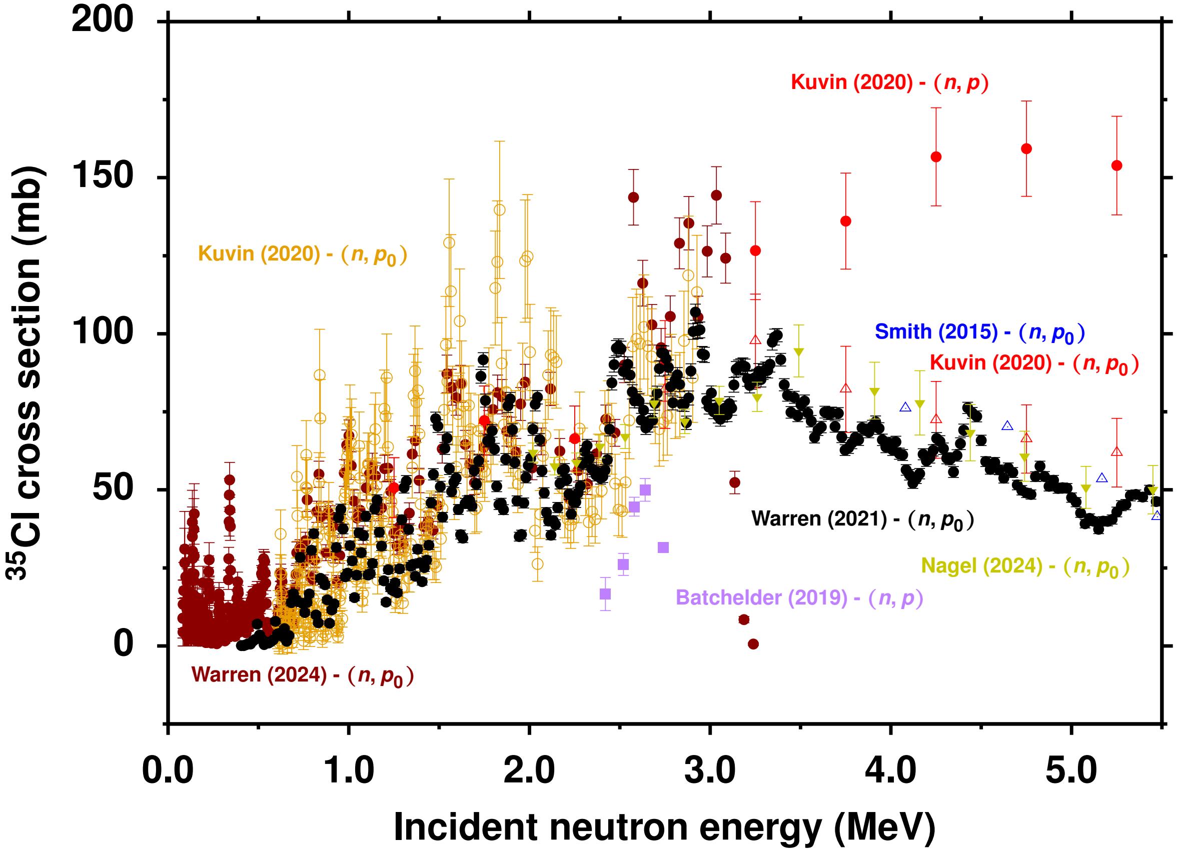
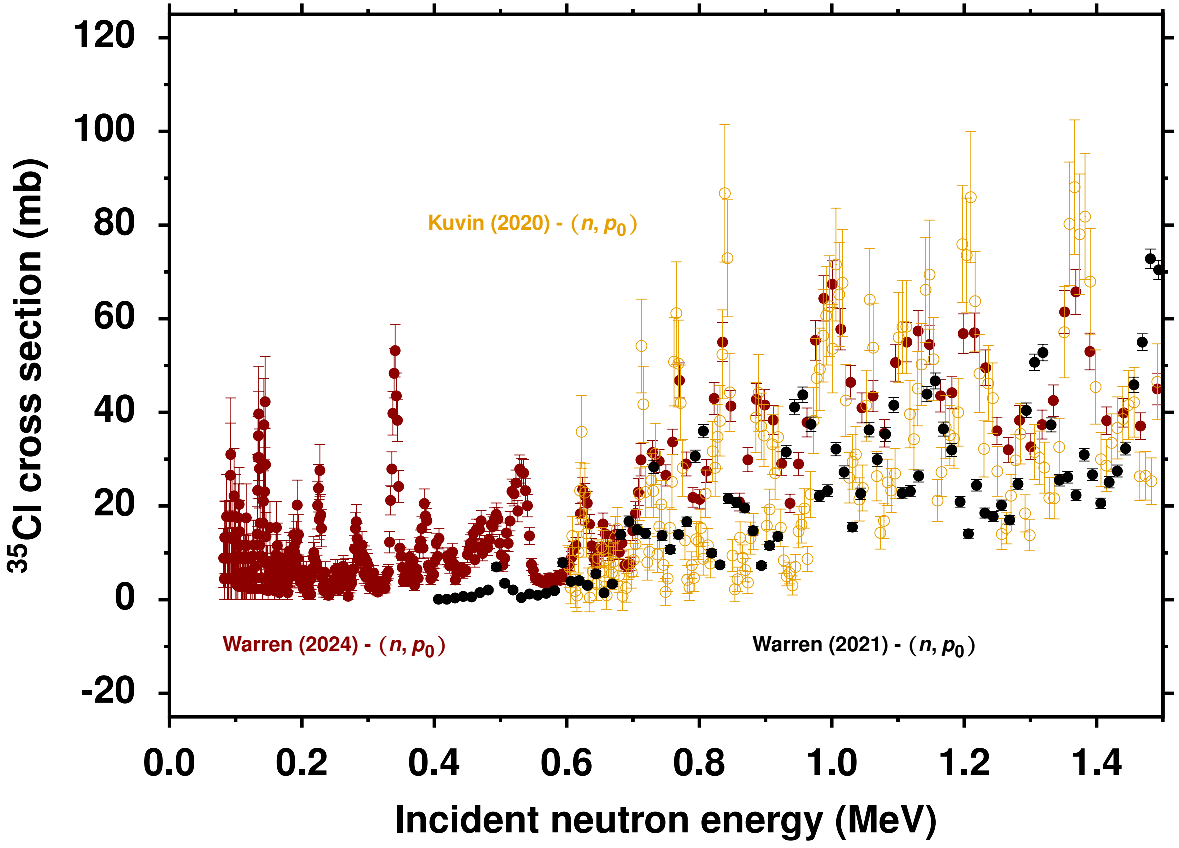
Experimental database



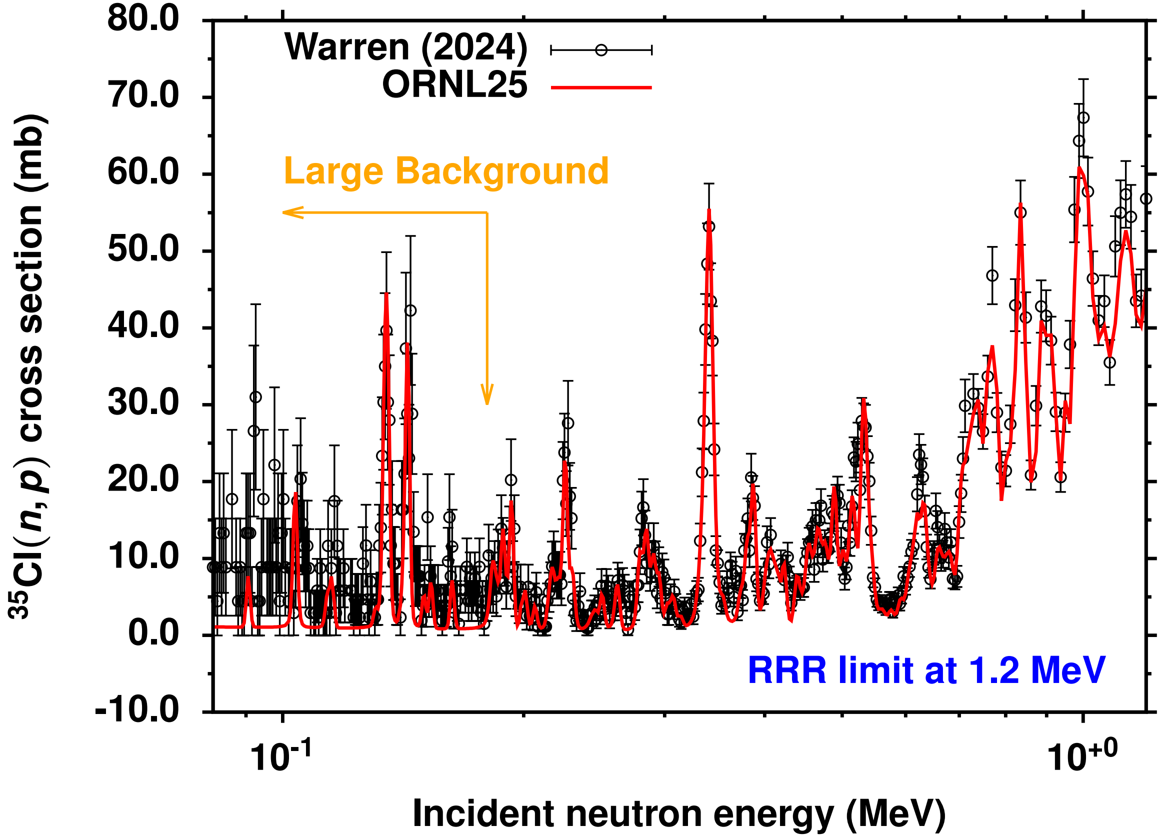
[Complete set of (n,p) measured data]



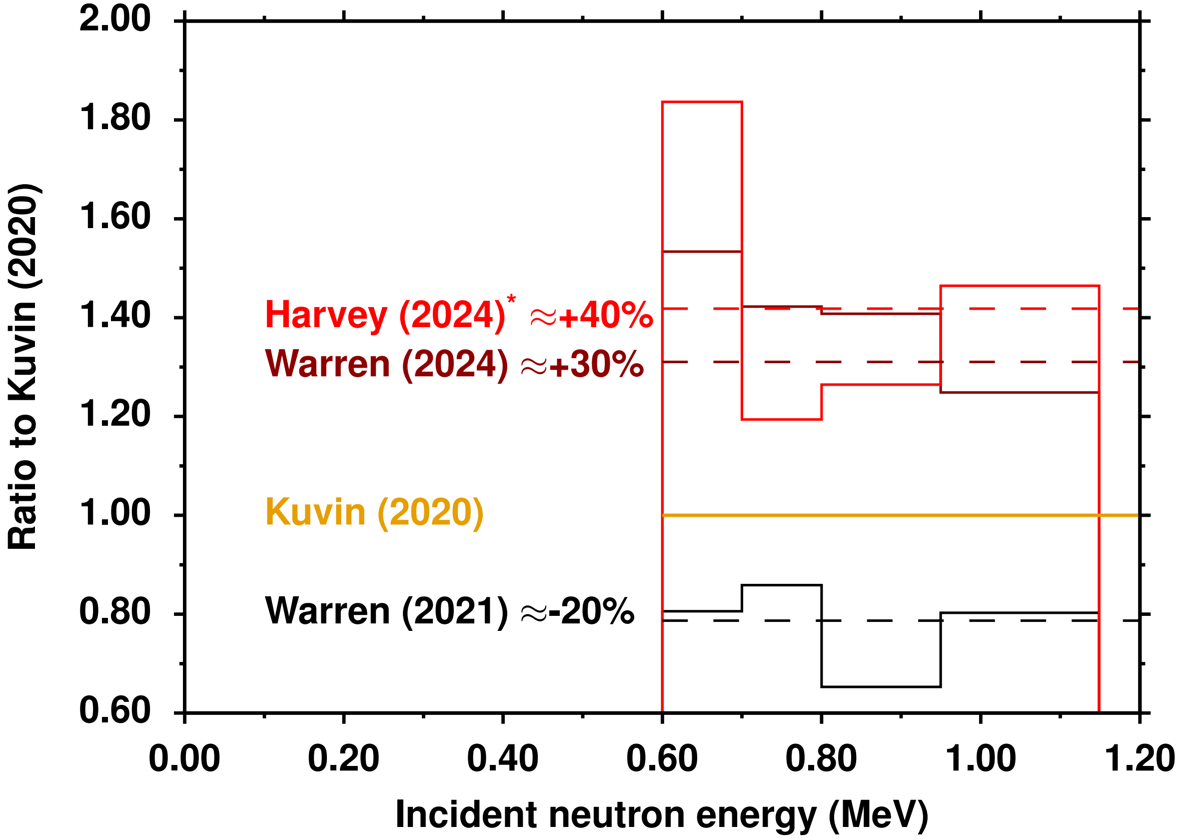
[Relevant to RRR<1.2 MeV*]

*Upper energy bound determined by (n, p_1) threshold.

Evaluation of (n, p) reaction channel

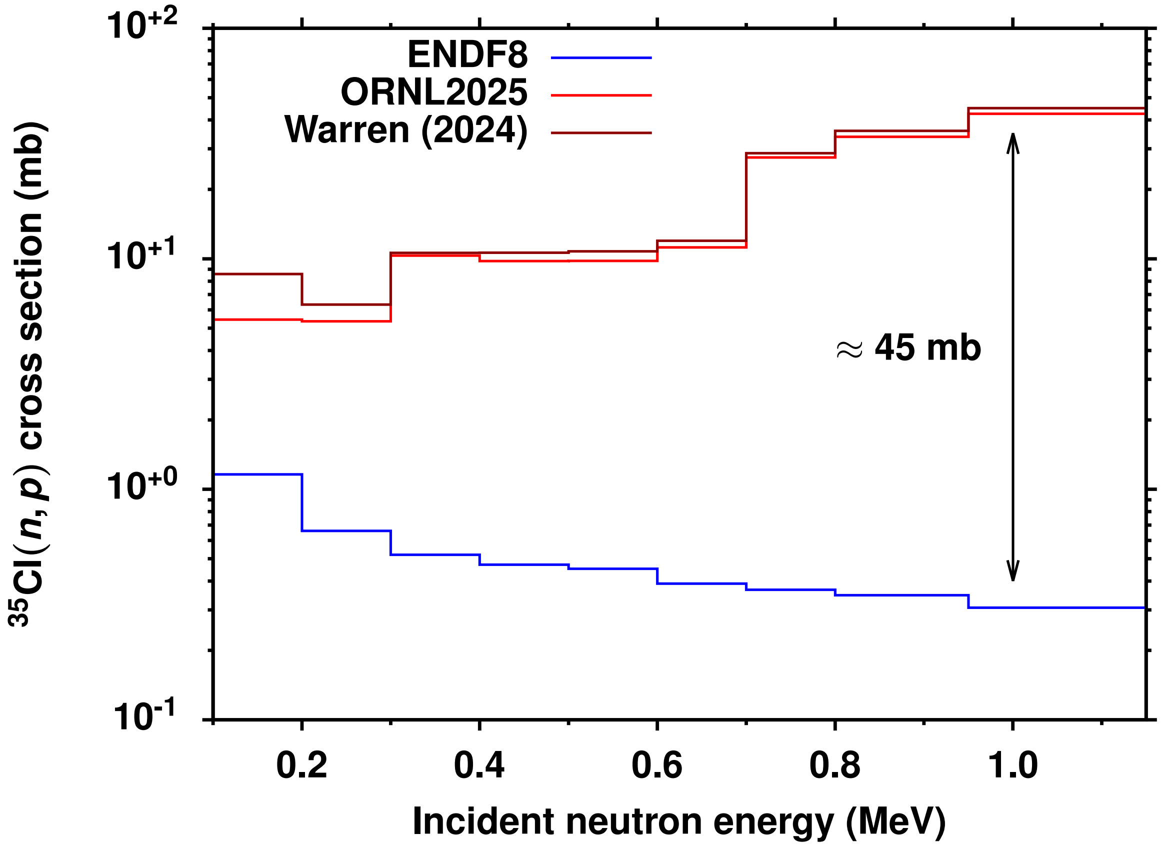


[Pointwise cross section]

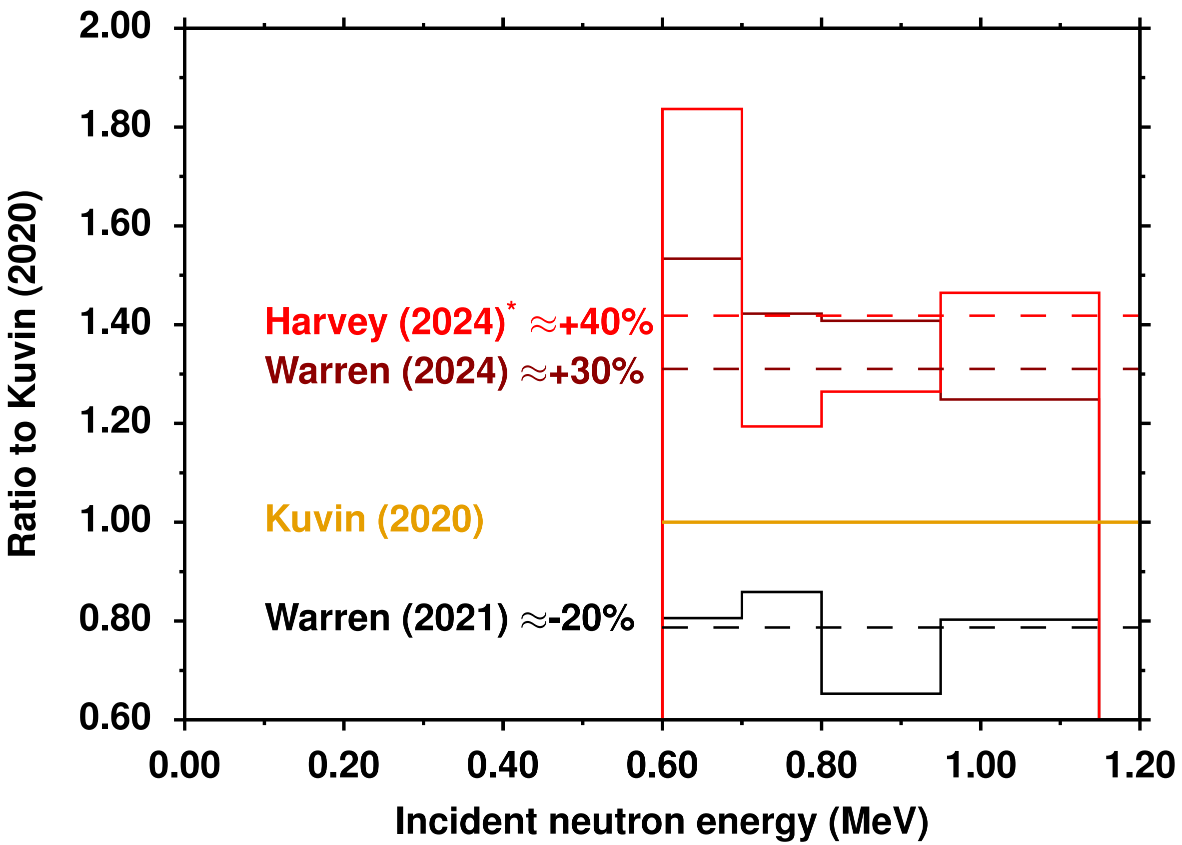


(*) Quantification of the ^{35}Cl(n, p) reaction channel, PNE 157 (2023) 104551

Evaluation of (n,p) reaction channel

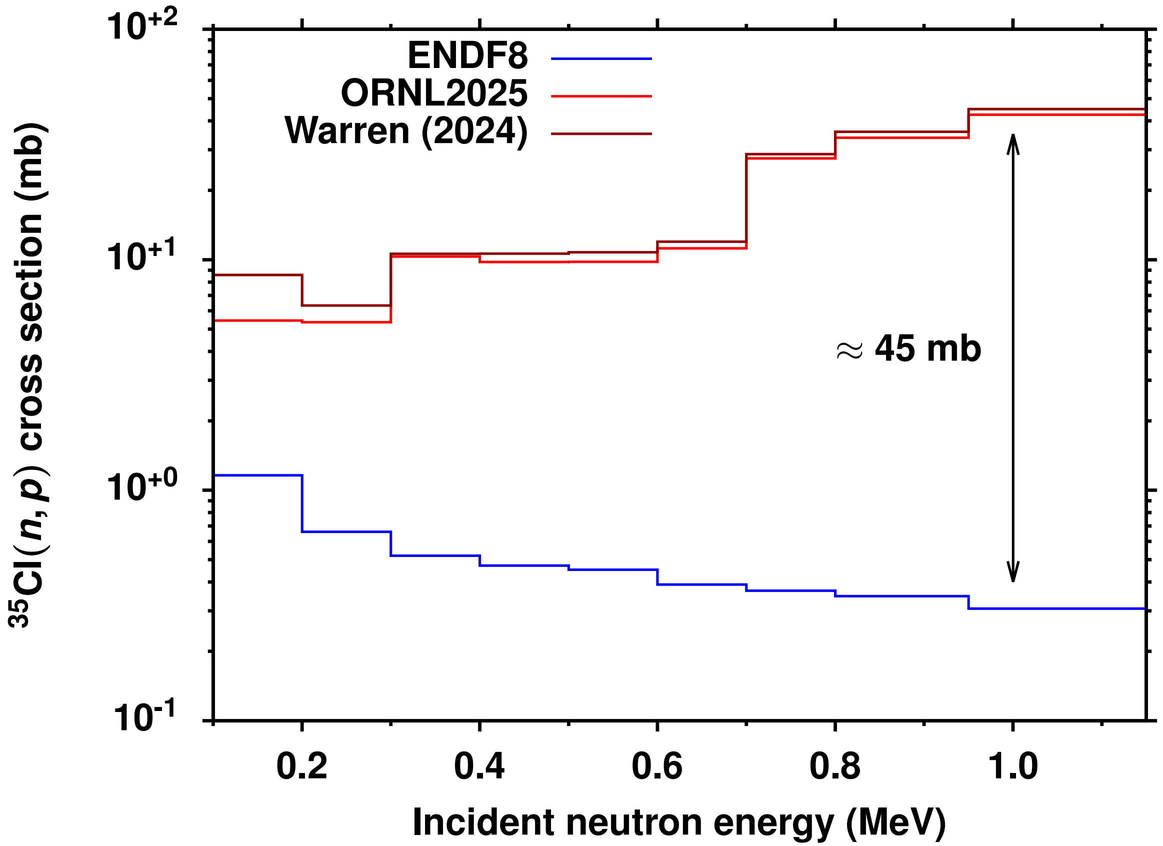


[Group average cross section]

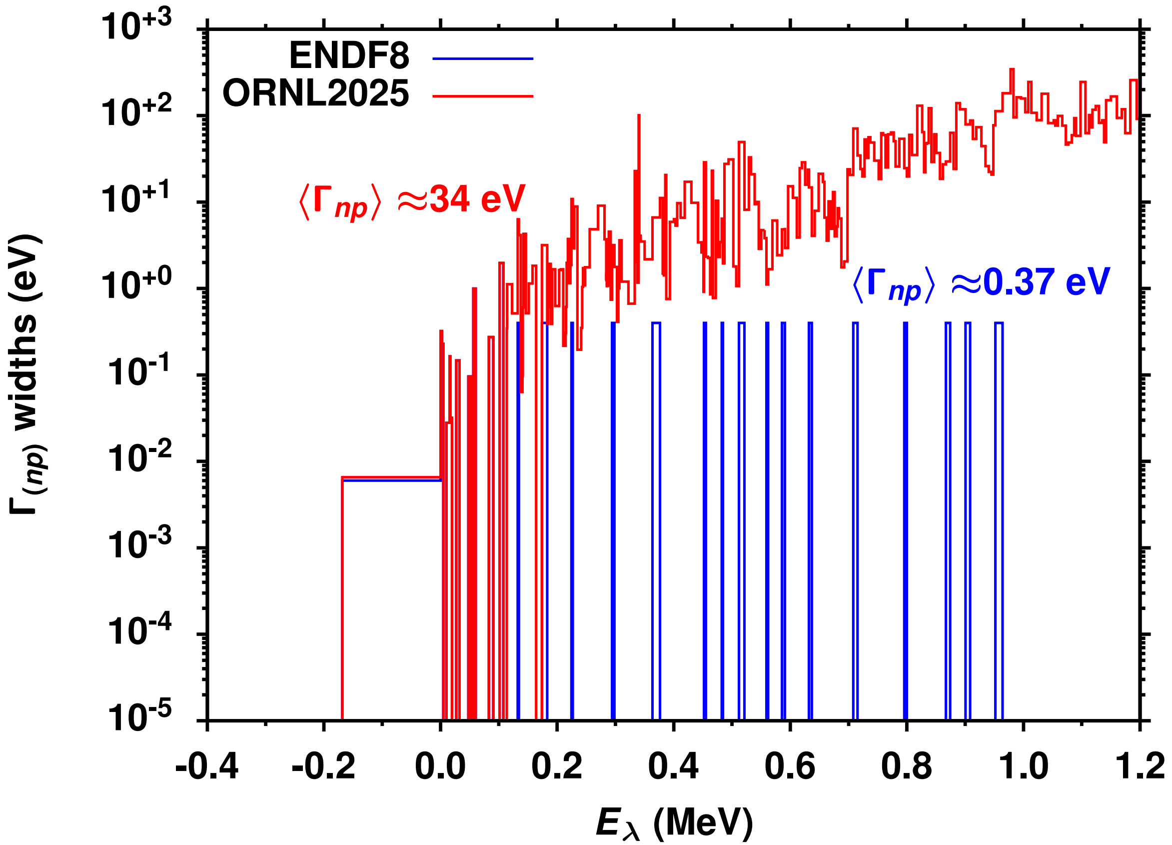


(*) Quantification of the ^{35}Cl(n,p) reaction channel, PNE 157 (2023) 104551

Evaluation of (n, p) reaction channel



[Group average cross section]



[Average proton widths Γ_{np}]

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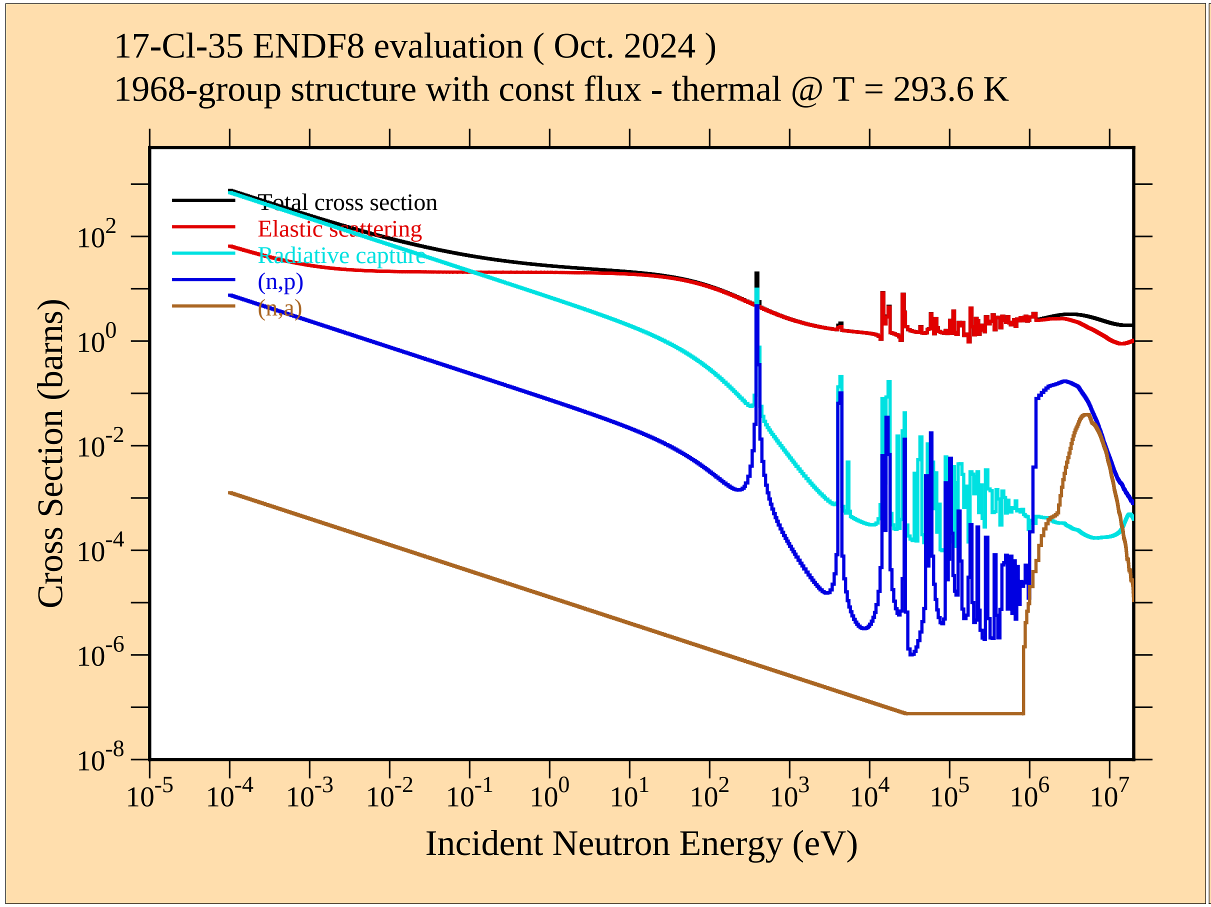
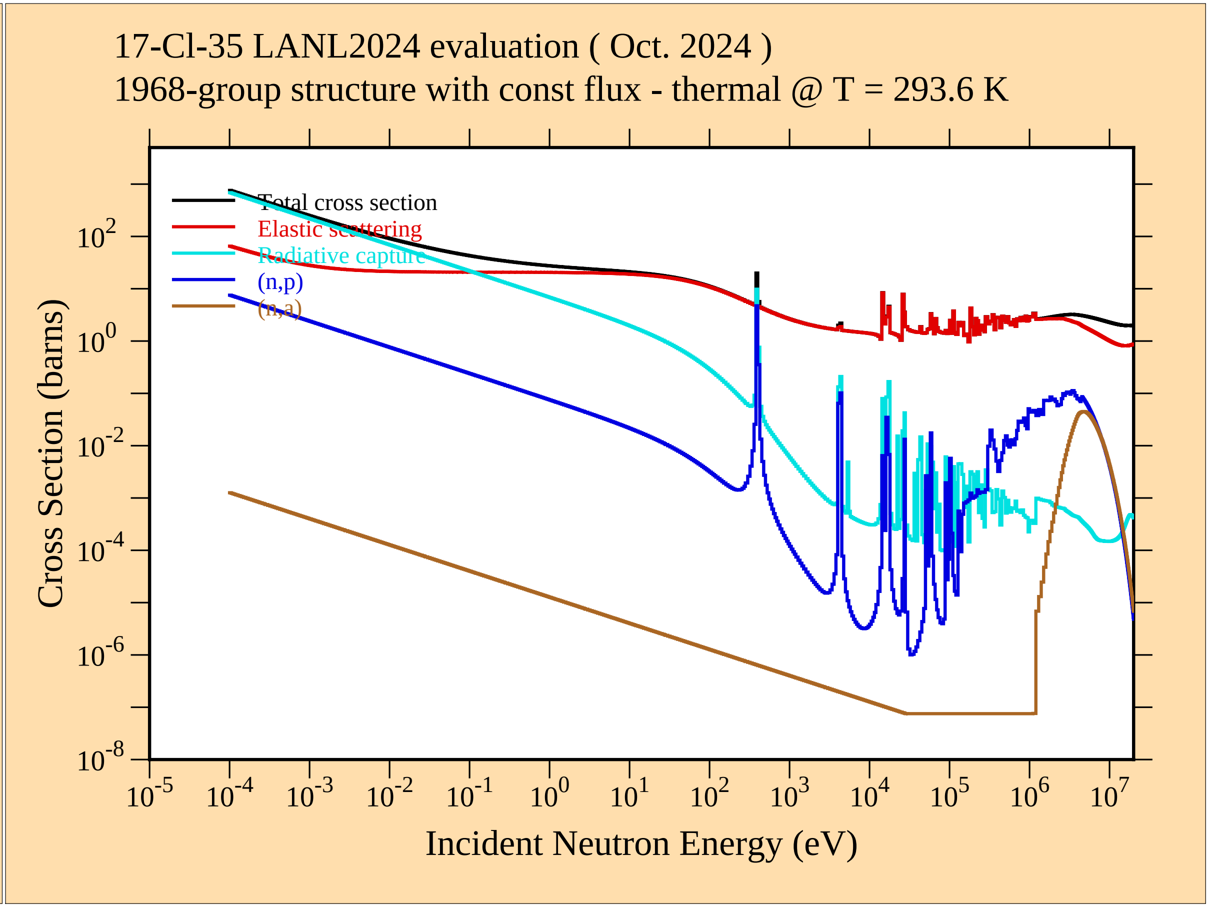
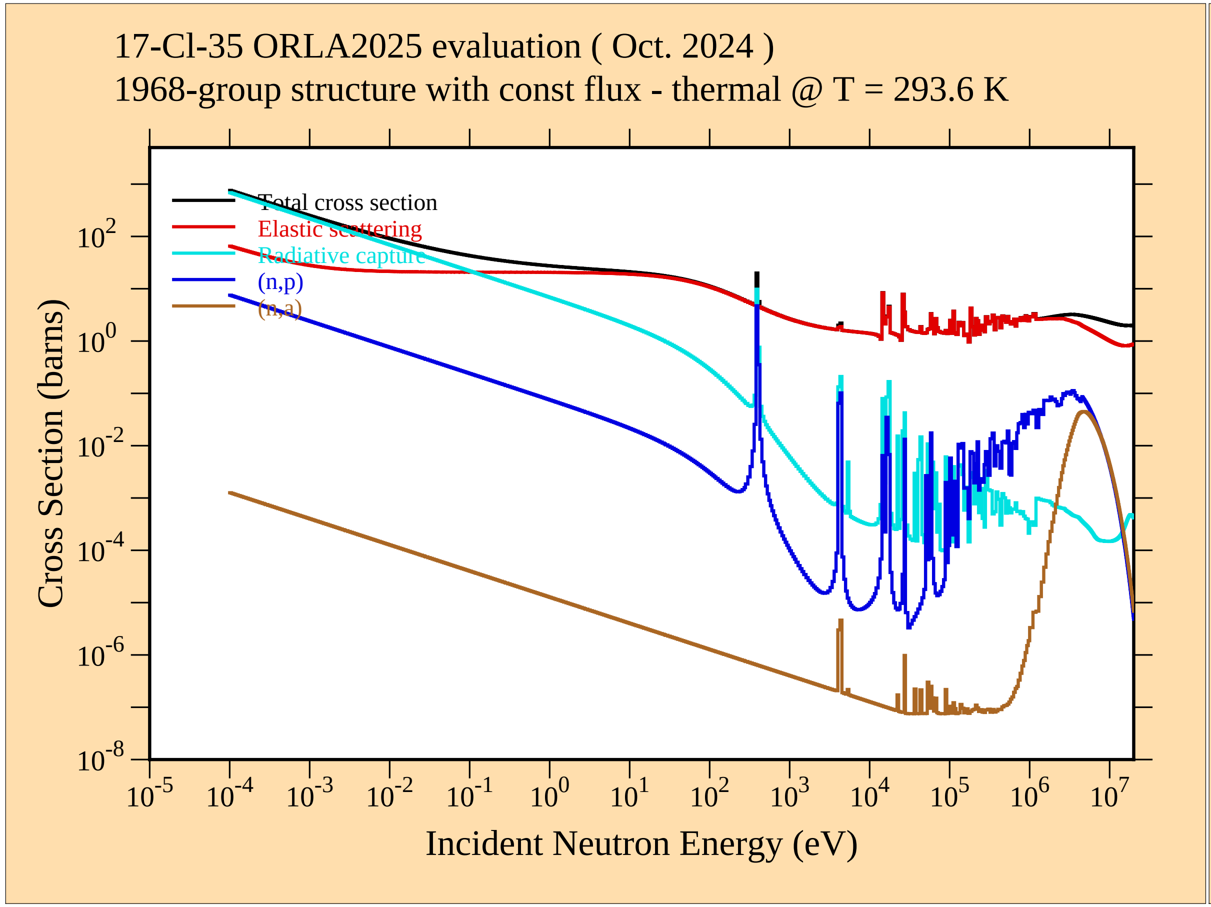
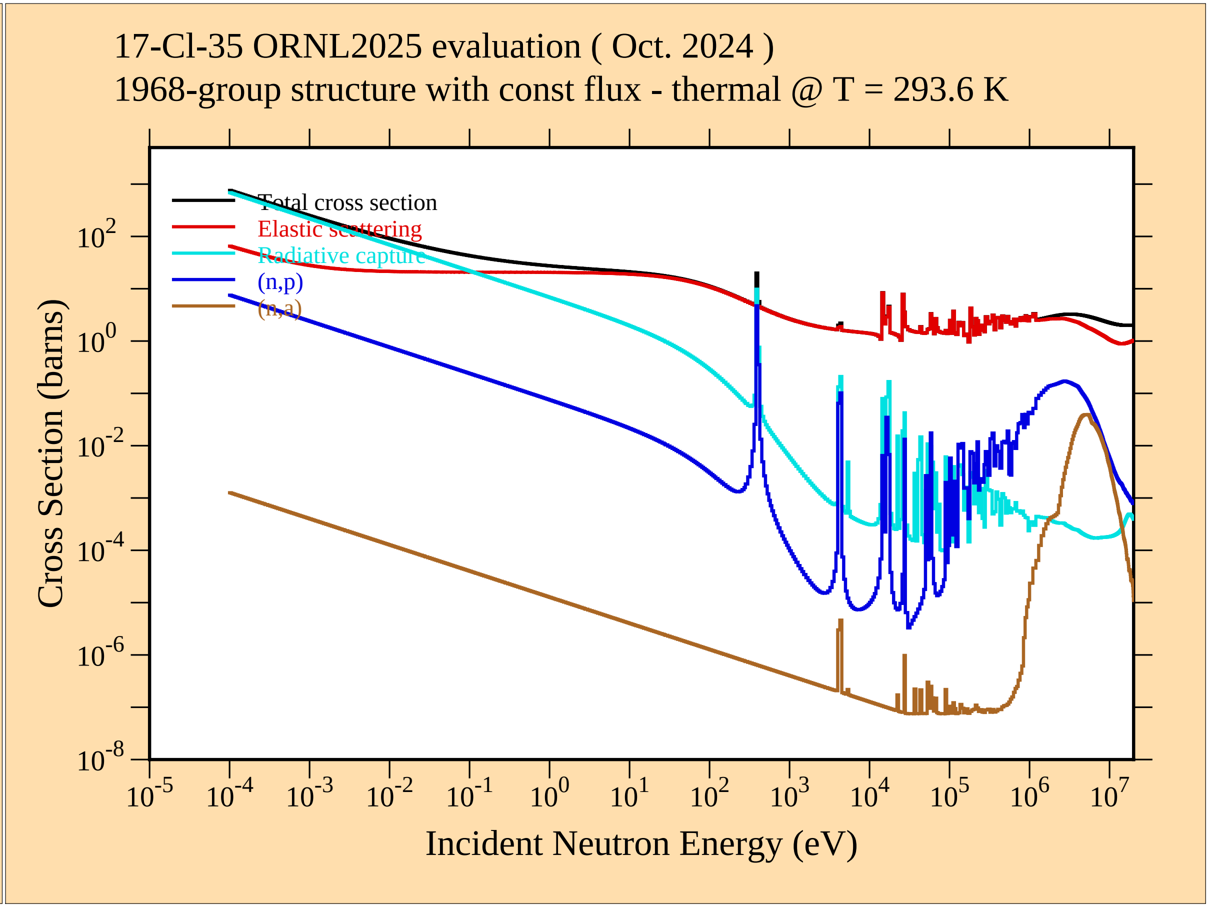
Averaged group cross sections



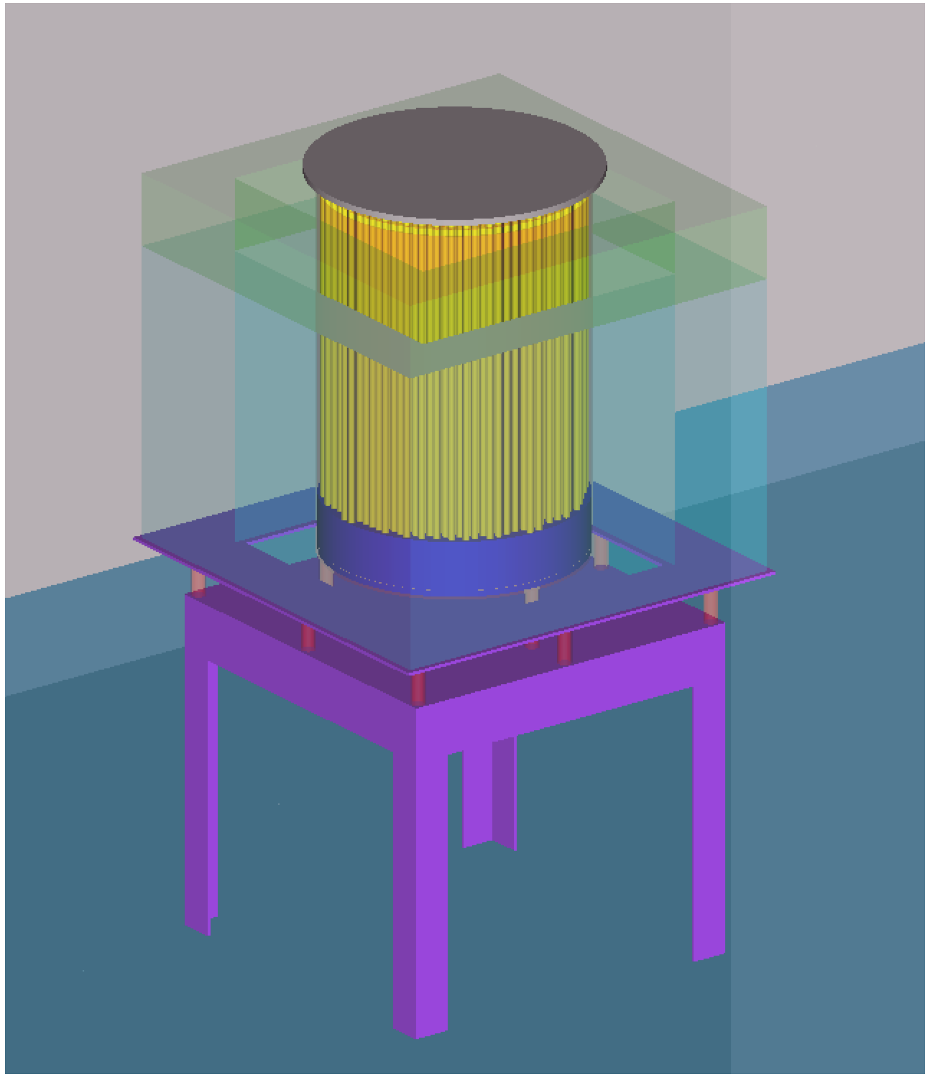


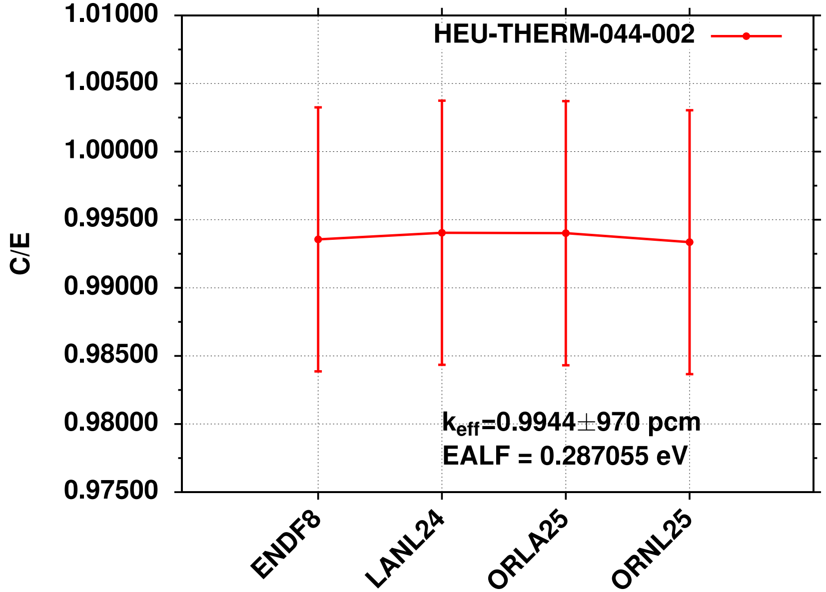
Averaged group cross sections

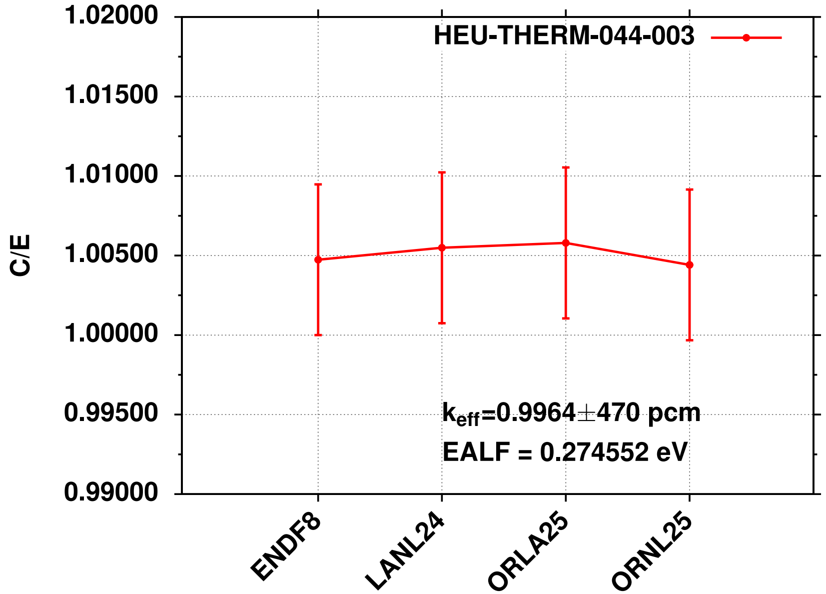




Benchmarking to HEU criticality safety designs

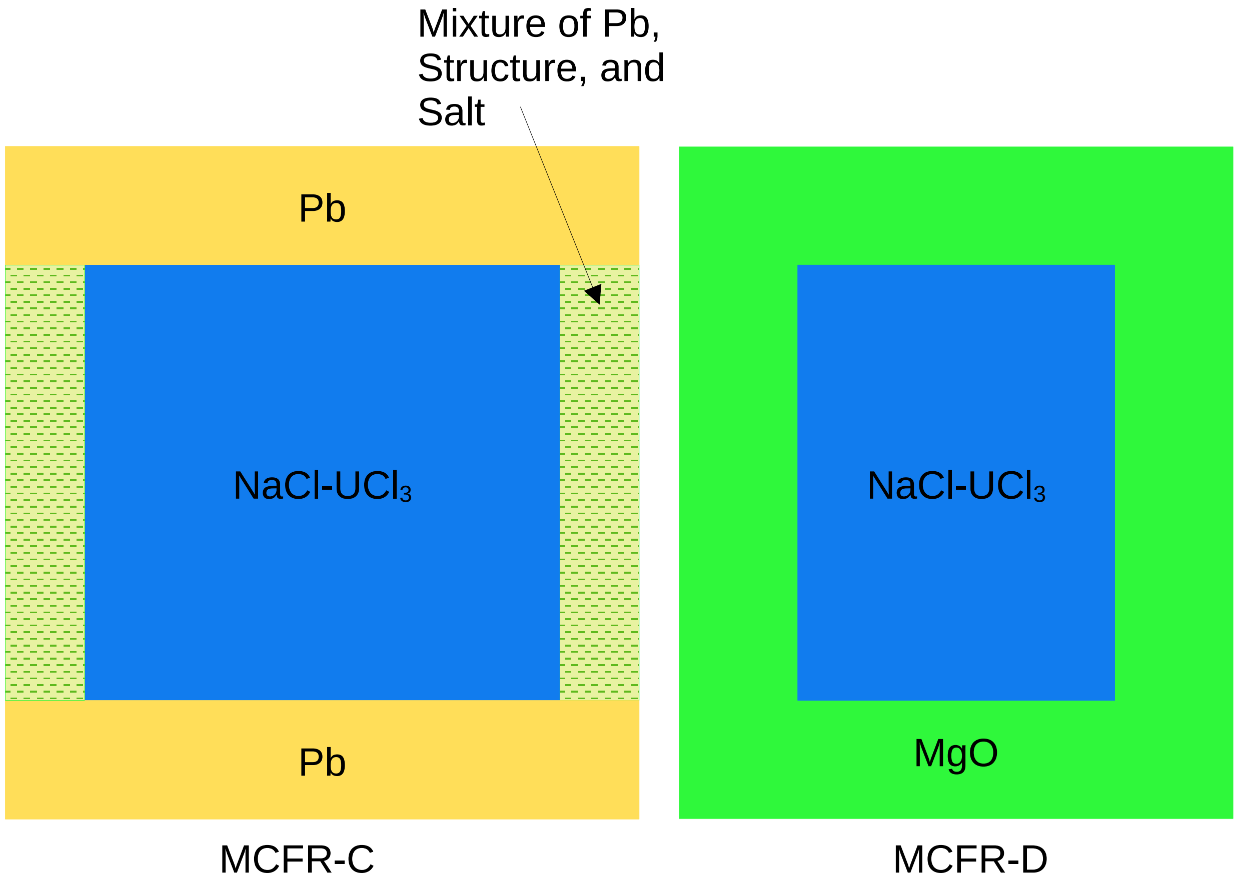






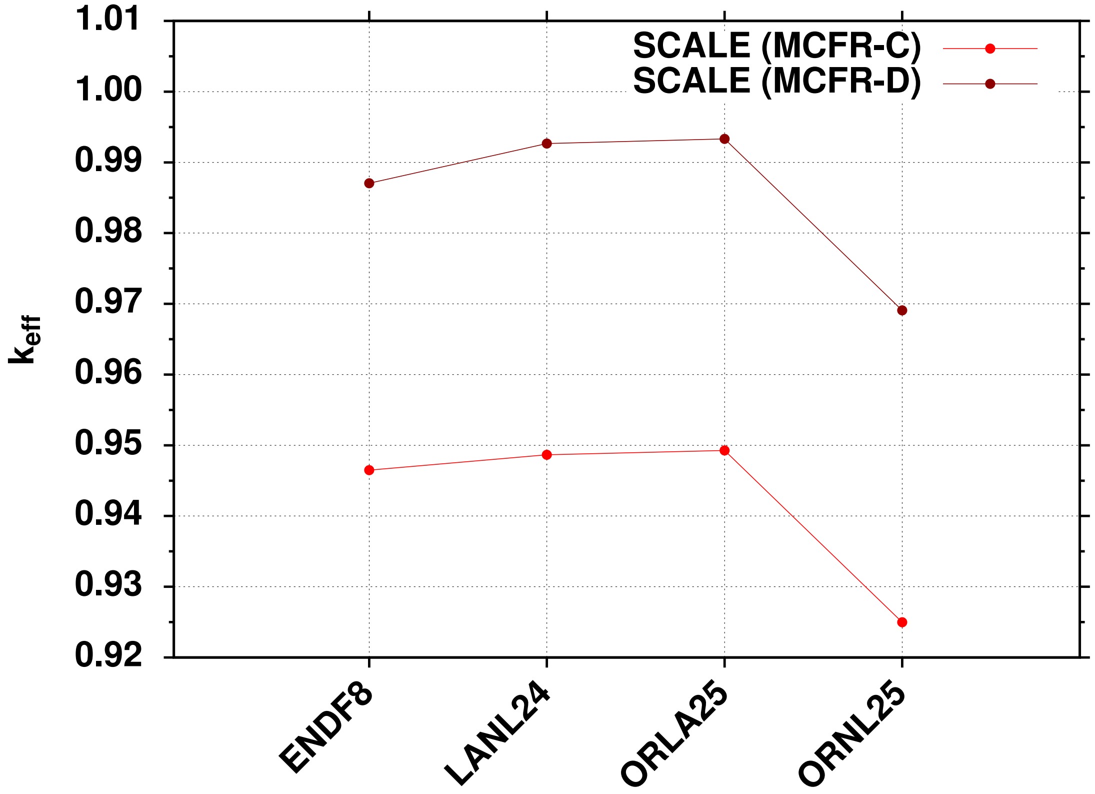
MCFR designs[†] (updated to use naturally enriched Cl)

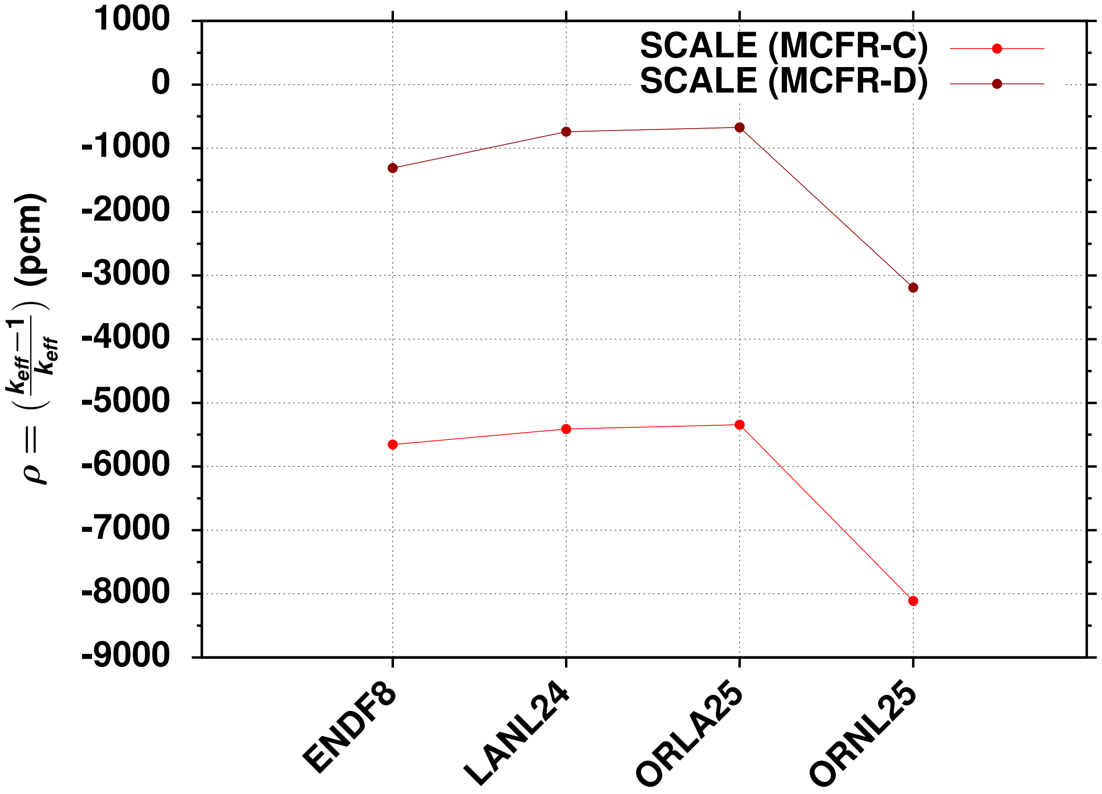
	MCFR-C	MCFR-D
Power (MWTh)	1200	180
^{235}U Wt%	12.5%	19.75%
Active core diameter (cm)	420	190
Active core heigth (cm)	500	350
Salt	NaCl-UCl_3	
Fuel salt temp. (K)	973.15	968.15
Reflector	Pb	MgO
Reflector thick. (cm)	100	90
Reflector clad	Inconel	
Reflector clad thick. (cm)	1	
^{35}Cl at%	75.76%	



[†]M. Wargon, J. Latkowski, T. Cisneros, Representative neutronics models of MCFR reactors (2023). DOI 10.13140/RG.2.2.15127.55208.

Benchmarking to MCFR designs

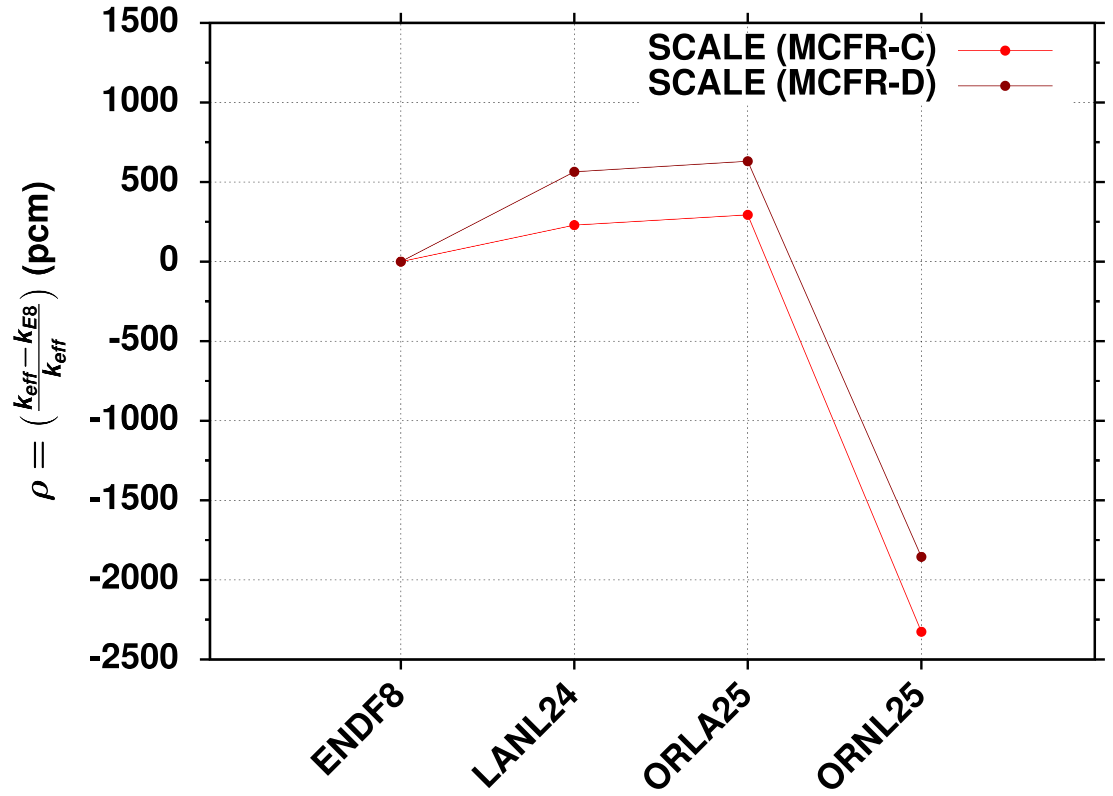


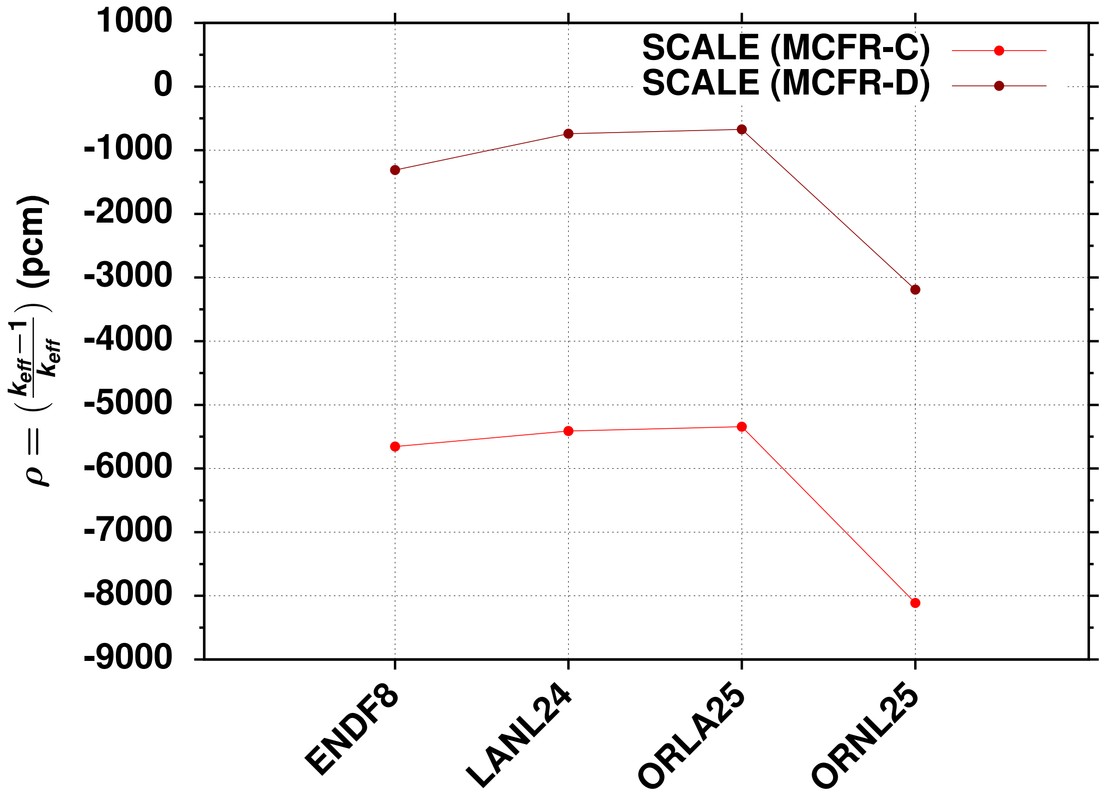


LANL24 and ORLA25 have similar (n,p) reactions, therefore similar k_{eff}

The increased reactivity of LANL24 and ORLA25 is mainly due to the decreased (n,p) above 1.2 MeV

Benchmarking to MCFR designs





ORNL25 shows a strong reduction of reactivity by having increased (n, p)

With respect to ENDF8, there is a compansation effect by having increased (n, p) below 1.2 MeV and decreased it above

REACTION RATES

Table 1: SCALE MCFR-C calculations of reaction rates in salt (10^{-9} n/cm^3-s)

Isotope	MT	ENDF8	LANL2024	ORLA2025	ORNL2025
^{35}Cl	102	0.210264	0.213186	0.209766	0.201281
	103	0.883108	0.848046	0.845636	1.211560
	104	0.000276	0.000345	0.000345	0.000275
	107	0.097952	0.117260	0.117321	0.097942
	101*	1.19229	1.17957	1.17390	1.51178

Table 2: SCALE MCFR-D calculations of reaction rates in salt (10^{-8} n/cm^3-s)

Isotope	MT	ENDF8	LANL2024	ORLA2025	ORNL2025
^{35}Cl	102	0.484937	0.485655	0.484530	0.474971
	103	0.559959	0.512053	0.507108	0.739074
	104	0.000179	0.000225	0.000225	0.000179
	107	0.063603	0.076266	0.076248	0.063590
	101*	1.10905	1.07460	1.06855	1.27819

(*) Neutron disappearance.

REACTION MODELING AND PROPOSED UPDATES

- The URR reaction modeling implemented in the SAMMY tool system is based on the Hauser-Feshbach (HF) theory with width fluctuation corrections
- The essential parameters are the channel pole strengths s_c closely related to the particle-channel (neutron) transmission coefficients[‡]

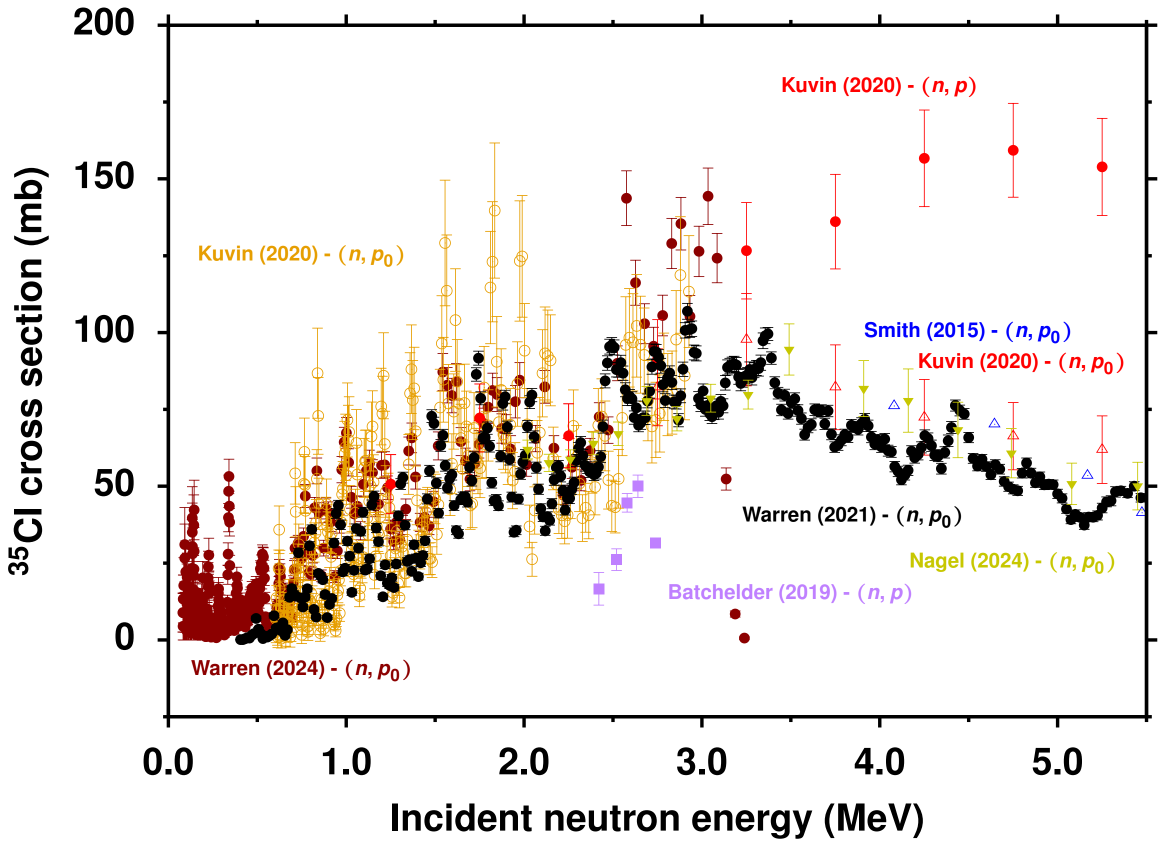
$$T_c = 1 - |\bar{U}_{cc}|^2 = \frac{4\pi s_c P_c}{|1 - \bar{R}_{cc} L_c^0|^2},$$

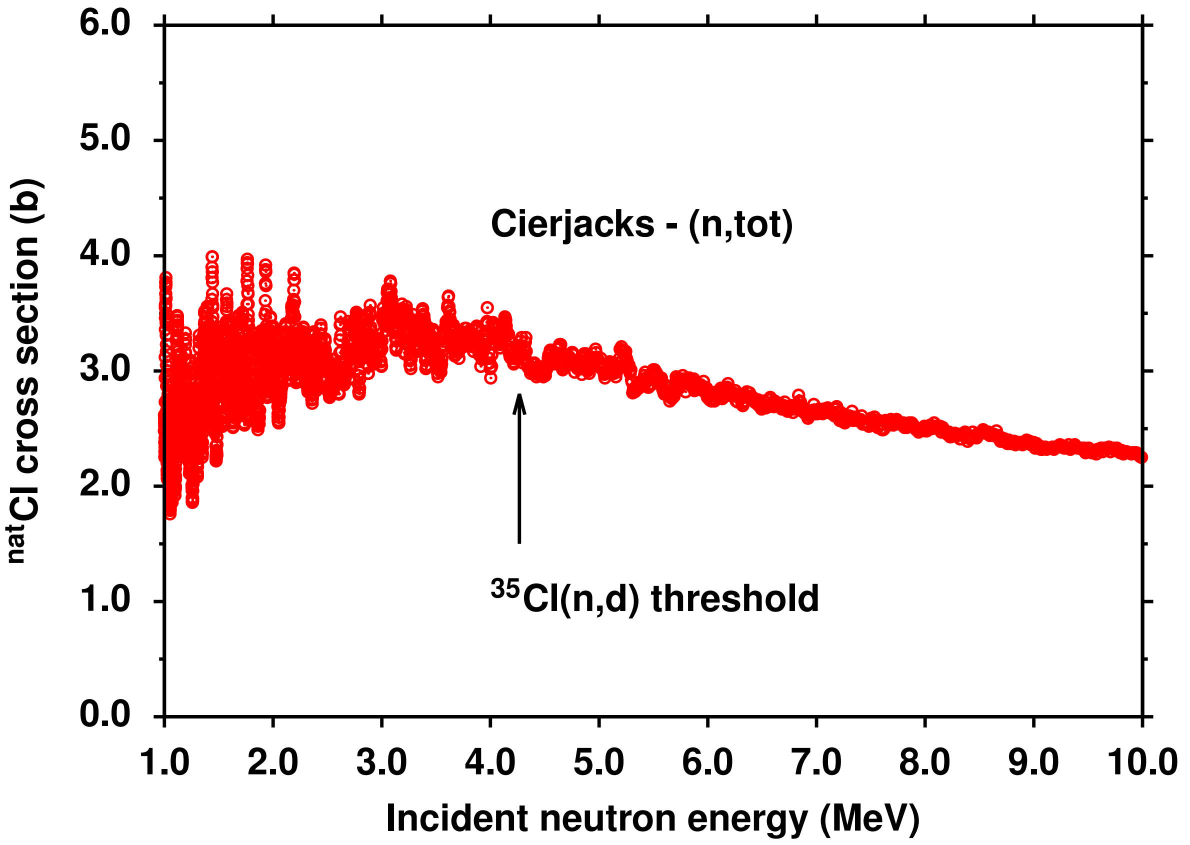
with $\bar{R}_{cc} = R_c^\infty + \imath\pi s_c$ and $L_c^0 = S_c + \imath P_c - B_c$.

- <u>Expanding SAMMY capabilities</u>
  - Inclusion of particle-channel T_c for charged particles such as proton and α-particle
  - Inclusion of strength functions for inelastic channels
  - Consistent format to translate SAMMY URR parameters to ENDF and/or GNDS

[‡]Photon and fission transmission coefficients are defined as $T_\gamma = 2\pi\bar{\Gamma}_\gamma/D_c$ and $T_\mathrm{f} = 2\pi\bar{\Gamma}_\mathrm{f}/D_c$ for an average level spacing D_c.

URR Upper energy range





Fluctuating measured data available for (n,tot) and (n,p) channels. E=4.266 MeV, coinciding with the ^{35}Cl(n,d) threshold, looks like a good energy for the transition from URR to fast neutron range

APPENDIX: Notes on Boundary conditions[§]

Scattering matrix (omitting indeces)

$$\begin{aligned}\mathbf{W} &= P^{\frac{1}{2}}(1-\mathbf{R}L)^{-1}(1-\mathbf{R}L^*)P^{-\frac{1}{2}} \\ &= 1+2\imath P^{\frac{1}{2}}(1-\mathbf{R}L)^{-1}\mathbf{R}P^{\frac{1}{2}} \\ &= 1+2\imath P^{\frac{1}{2}}[1-\mathbf{R}(S-B)-\imath\mathbf{R}P]^{-1}\mathbf{R}P^{\frac{1}{2}} \\ &= 1+2\imath\mathbf{X}\end{aligned}$$

with $L=S-B+\imath P$ and $|L|^2=(S-B)^2+P^2$

$$\mathbf{X}=P^{\frac{1}{2}}[1-\mathbf{R}(S-B)-\imath\mathbf{R}P]^{-1}\mathbf{R}P^{\frac{1}{2}}$$

Numerically, the matrix $\mathbf{X}$ for $P\neq 0$ is found by

$$\begin{aligned}[1-\mathbf{R}(S-B)-\imath\mathbf{R}P]P^{-\frac{1}{2}}\mathbf{X} &= \mathbf{R}P^{\frac{1}{2}} \\ P^{\frac{1}{2}}[P^{-\frac{1}{2}}-\mathbf{R}(S-B)P^{-\frac{1}{2}}-\imath\mathbf{R}P^{\frac{1}{2}}]\mathbf{X} &= P^{\frac{1}{2}}\mathbf{R}P^{\frac{1}{2}} \\ [1-P^{\frac{1}{2}}\mathbf{R}(S-B)P^{-\frac{1}{2}}-\imath P^{\frac{1}{2}}\mathbf{R}P^{\frac{1}{2}}]\mathbf{X} &= P^{\frac{1}{2}}\mathbf{R}P^{\frac{1}{2}} \\ [1-\mathbf{Y}(S-B)P^{-1}-\imath\mathbf{Y}]\mathbf{X} &= \mathbf{Y}\end{aligned}$$

For $B=S$, one has $(1-\imath\mathbf{Y})\mathbf{X}=\mathbf{Y}$

$$L^{-1}=\begin{cases}\frac{S-B}{(S-B)^2+P^2}-\imath\frac{P}{(S-B)^2+P^2} & B\neq S \\ -\frac{\imath}{P} & B=S\end{cases}$$

Two big conditions in NJOY, PREPRO[a], SAMRML, ...

`If( )` $[P>10^{-8}$ `.and.` $B\neq S$ `.and.` ...] `then`

⋮

matrix elements of $(L^{-1}-\mathbf{R})_{ij}$

⋮

`else` $[P<<1$ but $P\neq 0]$ `then`

⋮

$(1-\imath\mathbf{Y})\mathbf{X}=\mathbf{Y}$ or similar is used

⋮

`endif`

[a]PREPRO defines the module as $|L|^2=(2S-B)^2+P^2$ (?!). Also $S=0$ for s-wave penetrability of outgoing charged-particle, and, for $B=S$ and $P=0$, $L^{-1}=0$.

[§]Reference: SAMMY manual and Ian J. Thompson, private communications.

ACKNOWLEDGMENTS

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NCSP
NUCLEAR CRITICALITY SAFETY PROGRAM

OAK RIDGE National Laboratory

ORNL Nuclear data team

Thank you!

ACRONYMS AND LABELS

ENDF	Evaluated Nuclear Data File
LANL	Los Alamos National Laboratory
MCFR-X	Molten Chloride Fast Reactor - X=C≡Commercial and X=D≡Design
NCSP	Nuclear Criticality Safety Program
ORNL	Oak Ridge National Laboratory
OU	Ohio University
UND	University of Notre Dame
RRR	Resolved Resonance Region
URR	Unresolved Resonance Region

- **ENDF8** is ENDF/B-VIII.0 nuclear data library
- **LANL2024** is ENDF8 including new evaluation LANL+TerraPower collaboration for ^{35}Cl
  - MF=2 is ENDF8 + MF=3 for MT=600 extending below RRR limit that is 1.2 MeV
- **ORNL2025** is ENDF8 including new RRR evaluation up to 1.2 MeV (MF=2)
- **ORLA2025** is ORNL2025+LANL2024 without background MF=3 for MT=600

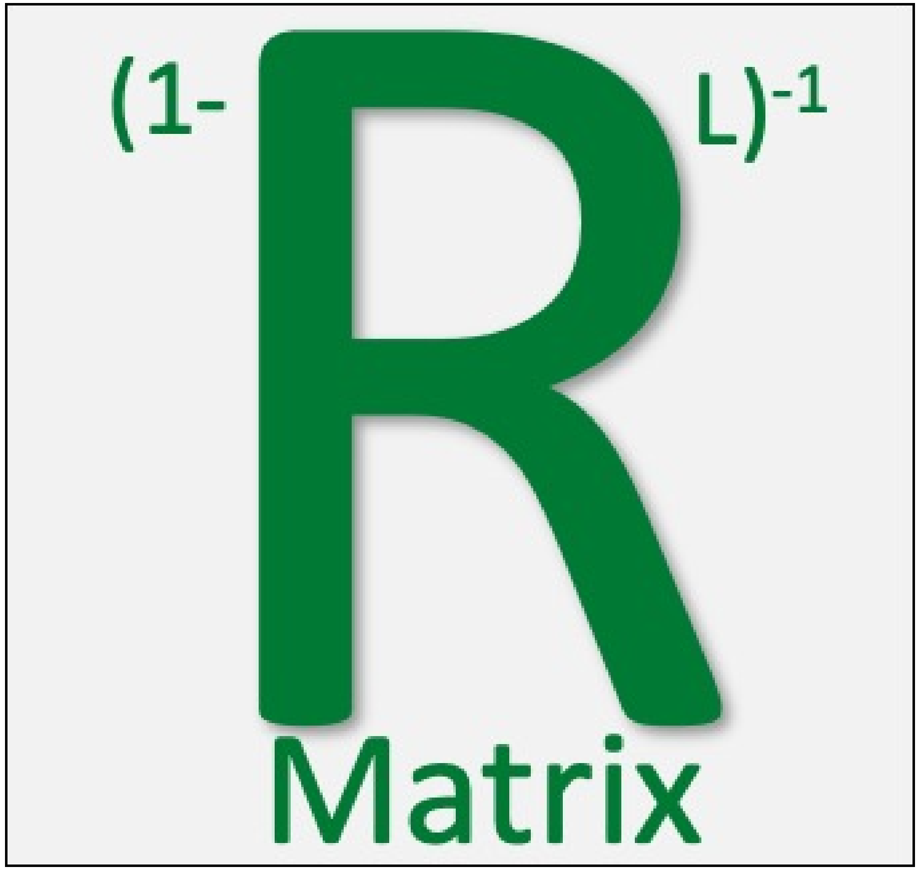
ANNOUNCEMENT

Nuclear data school on nuclear data evaluation with SAMMY and AZURE2 R-matrix Codes

- Where : FY2025 at ORNL
- When : 2–6 June 2025
- Topic : Neutron induced nuclear data library
- 2-Day or 5-Day options
- SAMMY and AZURE2 training classes

R-matrix team

- Marco Pigni and Dorothea Wiarda (ORNL)
- James deBoer (UND)
- Carl Brune (OU)



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