OAK RIDGE National Laboratory

The AMPX/SCALE Capability with the AMPX 1597-g Library for Advanced Reactor Analysis

2018 SCALE Users' Group Workshop

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U.S. DEPARTMENT OF ENERGY

Backgrounds and Objective

- **AMPX code package**
  - Cross section processing for multigroup (MG) and continuous energy (CE)
  - AMPX MG and CE libraries for the SCALE code package
  - Developed by Oak Ridge National Laboratory
  - Similar to NJOY at LANL
- **SCALE code package**
  - Compute problem-dependent MG cross sections
  - Both deterministic and Monte Carlo
  - Resonance self-shielding for deterministic:
    - Pointwise slowing down (CENTRM) & Bondarenko (ESSM) approaches
- **Application of the SCALE deterministic MG procedure**
  - Light water reactor: PWR, BWR
  - High temperature gas cooled rector
  - Fast spectrum systems
- **Limitations and objective**
  - Large reactivity bias for fast spectrum systems due to coarse energy group structure and poor unresolved resonance treatment
  - Resolve the reactivity bias issue

AMPX Library Generation Procedure

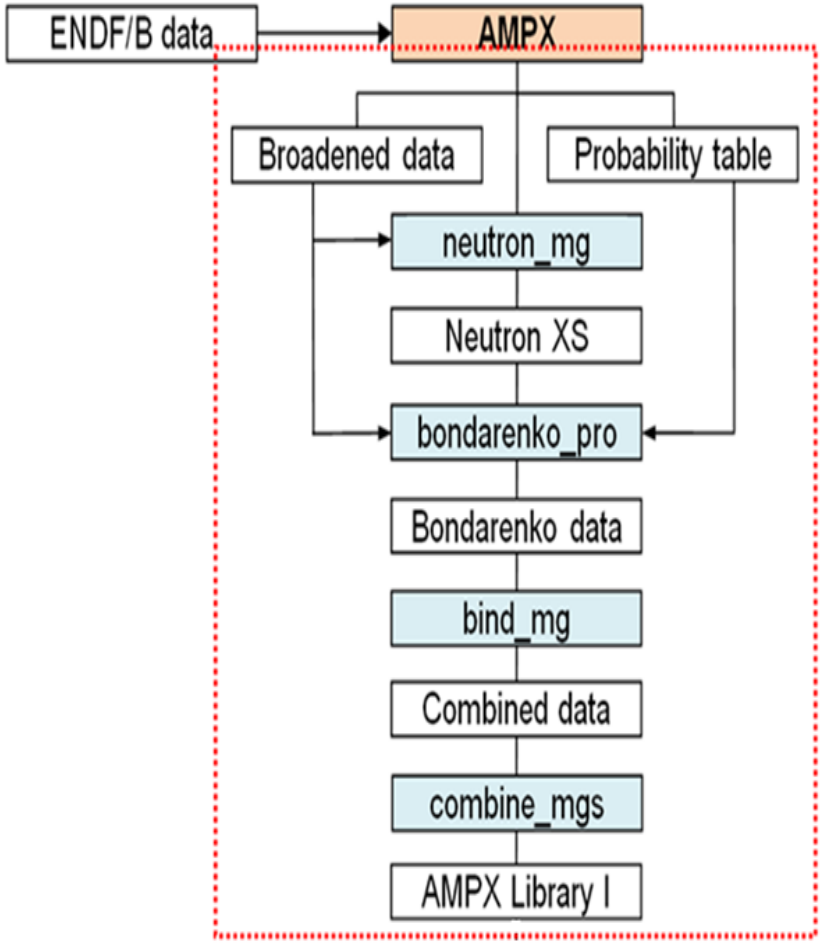
- **Pointwise XS data generation**
  - Doppler broadening
  - Probability table
- **Multigroup XS generation**
  - Flux weighting options
    - Maxwellian+1/E+Fission spectrum
    - Pointwise PWR spectra
  - Self-shielded resonance data
    - Narrow resonance approximation

$$\sigma_{i,g}(T,\sigma_0)=\frac{\int_g \frac{\sigma_i(T,E)\sigma_0}{\sigma_t(T,E)+\sigma_0}dE}{\int_g \frac{\sigma_0}{\sigma_t(T,E)+\sigma_0}dE}$$

    - Scattering matrix

$$\sigma_{s,l,gg'}=\frac{1}{\int_g \phi(E)dE}\int_g y(E)\sigma_s(E)\phi(E)dE\int_{g'} f_l(E,E')dE'$$

  - AMPX MG libraries
    - 252-group (default), 56-group (coarse) structure



Unresolved Resonance Treatment – AMPX

- **Probability Table Method with NR Approximation**
  - Continuous energy

$$\sigma_{x,g,i} = \frac{\int_g \sum_m p_i^m \sigma_{x,i}^m(E)\phi^m(E)dE}{\int_g \sum_m p_i^m \phi^m(E)dE} \qquad \phi^m(E) = \frac{W(E)}{N_i\sigma_{t,i}^m(E) + \sum_{j\neq i} N_j\sigma_{t,j}(E) + \Sigma_e(E)}$$

σ_x^m = a cross section level m of reaction x in the URR probability table,
p^m = a probability of the level m,
$\sigma_{x,g}$ = a self-shielded cross section of reaction x, and
$\phi^m(E)$ = scalar flux at the level m.

  - MG self-shielded resonance data & calculation
    - Compute pre-calculated resonance table using arbitrary background XSs (σ_0)

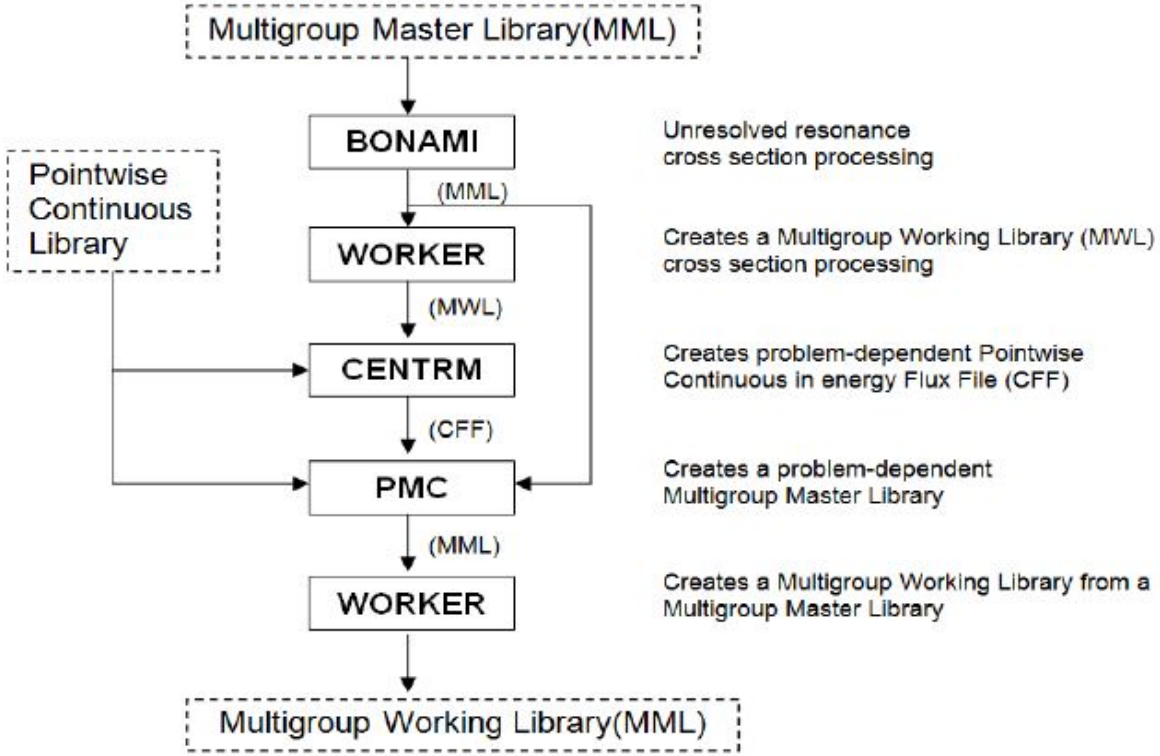
$$\sigma_{x,g,i} = \frac{\sum_m \frac{p_i^m \sigma_{x,i,g}^m}{\sigma_{t,i,g}^m + \sigma_{0,i,g}}}{\sum_m \frac{p_i^m}{\sigma_{t,i,g}^m + \sigma_{0,i,g}}}$$

    - Problem-dependent background XS (σ_0) can be determined by the following equation where Σ_e can be obtained by Dancoff factor.

$$\sigma_{0,i,g} = \frac{1}{N_i}\left(\sum_{j\neq i} N_j\sigma_{t,j,g} + \Sigma_{e,g}\right)$$

SCALE MG Procedure

- **Cross section processing procedure**
  - BONAMI: resonance self-shielding based on Bondarenko approach
  - CENTRM: pointwise slowing down calculation for thermal + resolved energy groups
  - PMC: obtain multigroup cross sections and scattering matrices
  - Deliver XS to the transport codes XSDRN, NEWT & KENO



Ultra-Fine Group Structure

- **An AMPX 1597-group test library was generated for this study using the AMPX/SCALE code packages and the ENDF/B-VII.1 data**
  - 0.1 keV ~ 20 MeV: 1323 groups based on MC^2-3 of ANL
    - To represent broad resonances of intermediate weight nuclides explicitly
  - < 0.1 keV: 274 groups based on the AMPX 252-group structure

- **To verify the probability table generated by the AMPX code package and the AMPX/SCALE MG cross section processing procedure, an intensive reaction rate analysis was performed for various fast reactor problems**

Reaction Rate Analysis

- **Reaction rate analysis procedure**
  - SCALE-MG vs. CE KENO
    - Edit MG microscopic cross sections & scalar fluxes
  - Convert reaction rate difference into reactivity difference
    - Reactivity differences for each energy group, nuclide and reaction type
    - Identify the reactions causing the observed reactivity difference
    - Two options: [1] Only by cross section difference
      [2] By both cross section and flux differences

$$\Delta\rho^{K}_{a,g,J} = \left(\frac{1}{k^{KENO}_{eff}} - \frac{\sum_{j}\sum_{i}\sum_{g'} N_{i,j}\sigma^{KENO}_{a,g',i,j}\varphi^{KENO}_{g',j}V_j - N_{K,J}(\sigma^{KENO}_{a,g,K,J} - \sigma^{MG}_{a,g,K,J})\hat{\varphi}_{g,J}V_J}{\sum_{j}\sum_{i}\sum_{g'} N_{i,j}\nu\sigma^{KENO}_{f,g',i,j}\varphi^{KENO}_{g',j}V_j} \right) \cdot 10^5$$

$$\Delta\rho^{K}_{\nu f,g,J} = \left(\frac{1}{k^{KENO}_{eff}} - \frac{\sum_{j}\sum_{i}\sum_{g'} N_{i,j}\sigma^{KENO}_{a,g',i,j}\varphi^{KENO}_{g',j}V_j}{\sum_{j}\sum_{i}\sum_{g'} N_{i,j}\nu\sigma^{KENO}_{f,g',i,j}\varphi^{KENO}_{g',j}V_j - N_{K,J}(\nu\sigma^{KENO}_{f,g,K,J} - \nu\sigma^{MG}_{f,g,K,J})\hat{\varphi}_{g,J}V_J} \right) \cdot 10^5$$

$$\Delta\rho_g = \sum_{j}\sum_{K}\sum_{g}(\Delta\rho^{K}_{a,g,j} + \Delta\rho^{K}_{\nu f,g,j})$$

Benchmark Problems

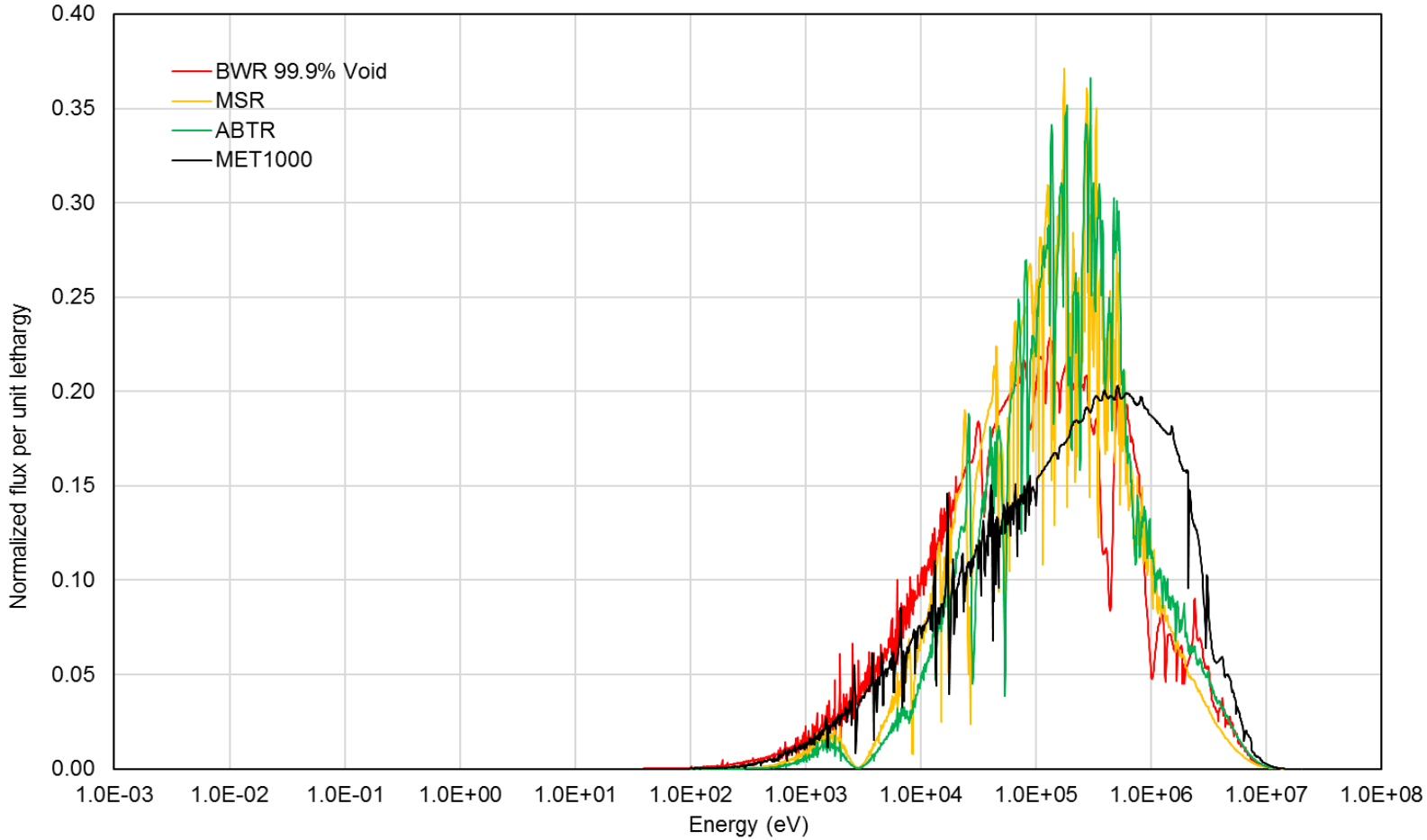
- **BWR, MSR, ABTR, MET1000, SNU**

Fuel type	Material	Radius	Atomic number density	Void %
BWR	Fuel	0.60579	^{235}U 7.18132E-04 ^{16}O 4.57642E-02 ^{238}U 2.21546E-02	
	Clad	0.62103	^{27}Al 6.02611E-02	
	Mod.	1.87452	^{1}H 6.72142E-02 ^{16}O 3.36071E-02	*
			^{1}H 4.41459E-02 ^{16}O 2.20729E-02	0.0
			^{1}H 1.32438E-02 ^{16}O 6.62187E-03	70.0
			^{1}H 4.41459E-03 ^{16}O 2.20729E-03	90.0
			^{1}H 4.41459E-04 ^{16}O 2.20729E-04	99.0
			^{1}H 4.41459E-05 ^{16}O 2.20729E-05	99.9
MSR	Fuel	-	^{235}U 3.10000E-05 ^{238}U 4.27500E-03 ^{239}Pu 4.04000E-04 ^{240}Pu 5.40000E-05 ^{241}Pu 2.70000E-05 ^{242}Pu 5.40000E-05 ^{23}Na 5.38300E-03 ^{35}Cl 1.50100E-02 ^{37}Cl 4.83320E-03	
ABTR	Fuel	0.35010	^{235}U 3.22479E-05 ^{238}U 2.02220E-02 ^{239}Pu 3.49907E-03 ^{240}Pu 3.73979E-04 ^{90}Zr 3.75264E-03	
	Inner	0.48750	^{23}Na 2.22720E-02	
	Clad	0.50900	^{54}Fe 4.08237E-03 ^{56}Fe 6.40845E-02	
	Outer	1.04500	^{23}Na 2.22720E-02	
MET1000	Fuel	-	^{nat}C 1.00000E-02 ^{62}Ni 4.01013E-06 ^{90}Zr 1.46077E-03 ^{91}Zr 3.18559E-04 ^{92}Zr 4.86924E-04 ^{94}Zr 4.93454E-04 ^{239}Pu 8.48385E-04 ^{240}Pu 5.03166E-04 ^{241}Pu 7.22184E-05 ^{242}Pu 1.12387E-04	
SNU	Fuel	-	^{nat}C 1.00000E-02 ^{239}Pu 1.00000E-03	
	Fuel	-	^{23}Na 7.14528E-03 ^{56}Fe 1.34500E-02 ^{239}Pu 1.56532E-03	
	Fuel	-	^{23}Na 7.14528E-03 ^{56}Fe 1.34500E-02 ^{235}U 1.44262E-05 ^{238}U 9.04638E-03 ^{239}Pu 1.56532E-03	

*Moderator temperature: 293.6 K

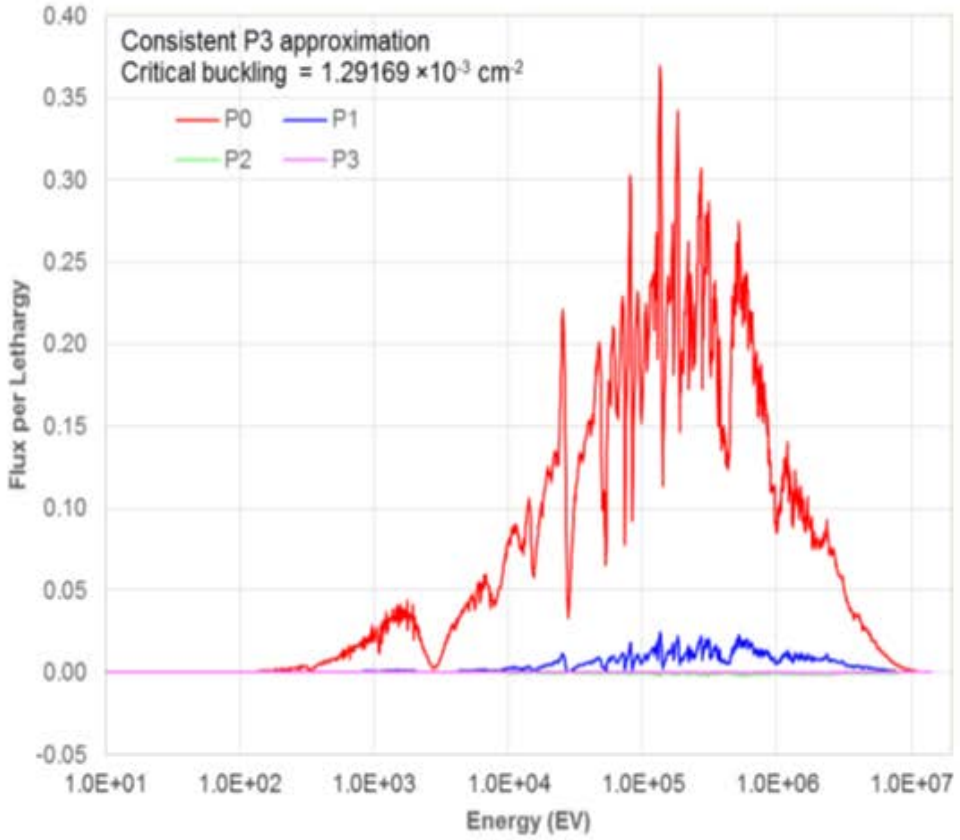
Benchmark Problems

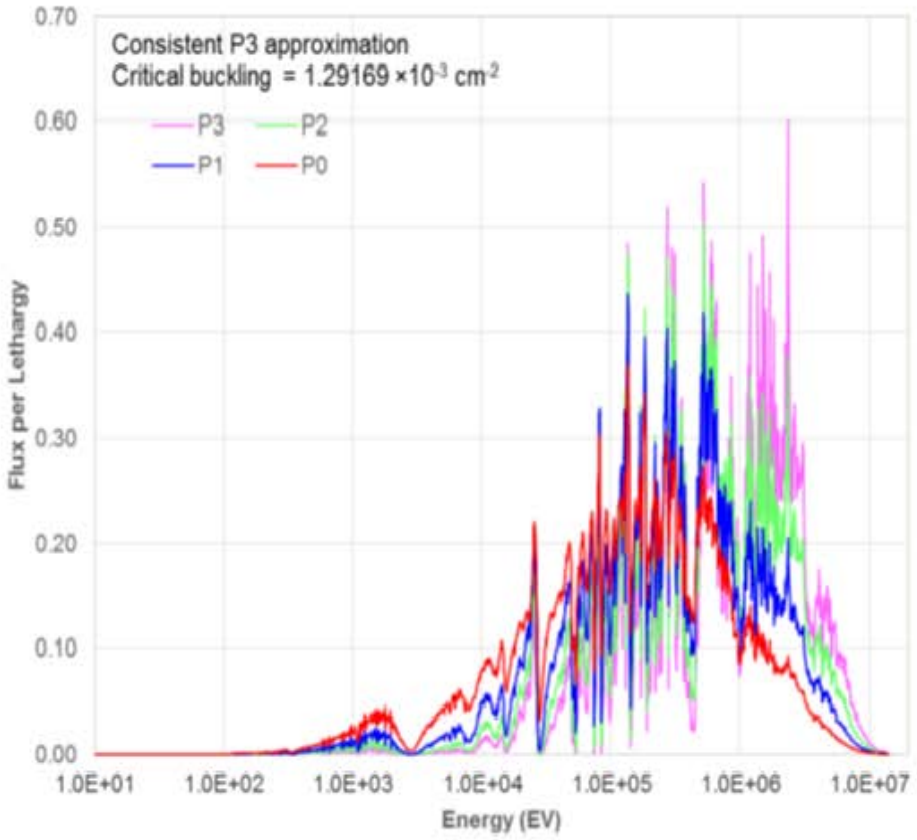
- **Comparisons of the Neutron Spectra**
  - From SCALE



Anisotropic Effect

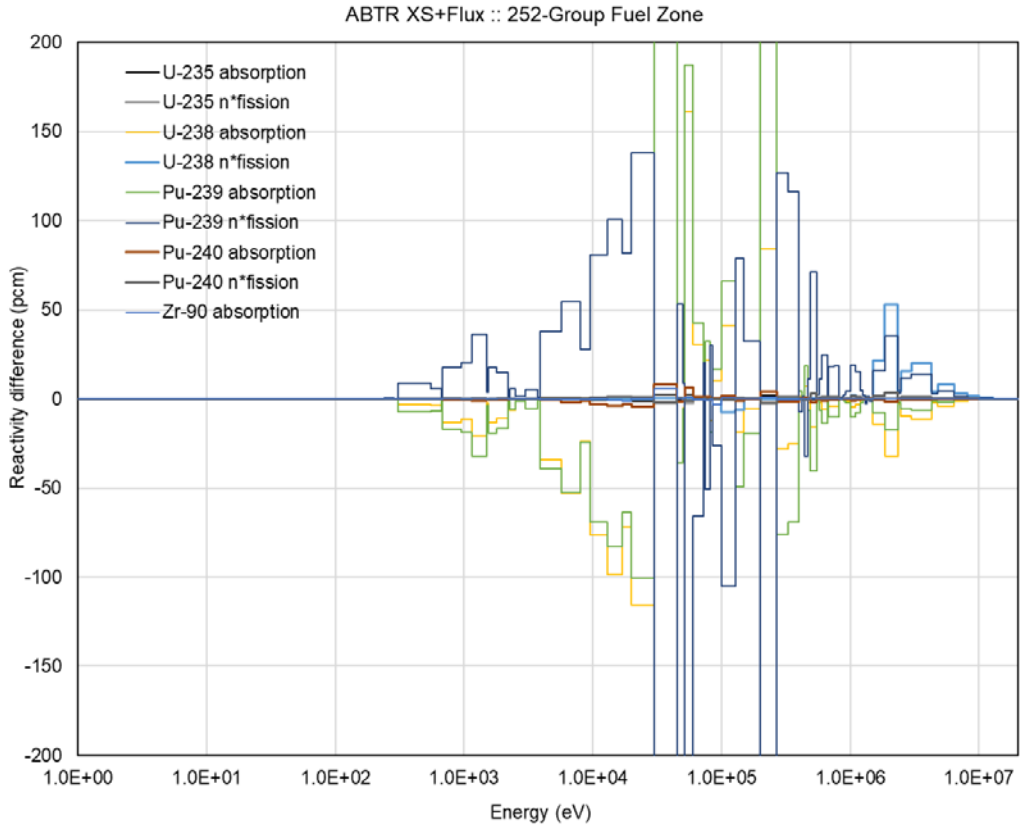
- **Comparisons of high order flux moments**
  - Thermal vs. Fast
  - Require high order transport calculation
  - Require high order flux moment weighting for group collapsing

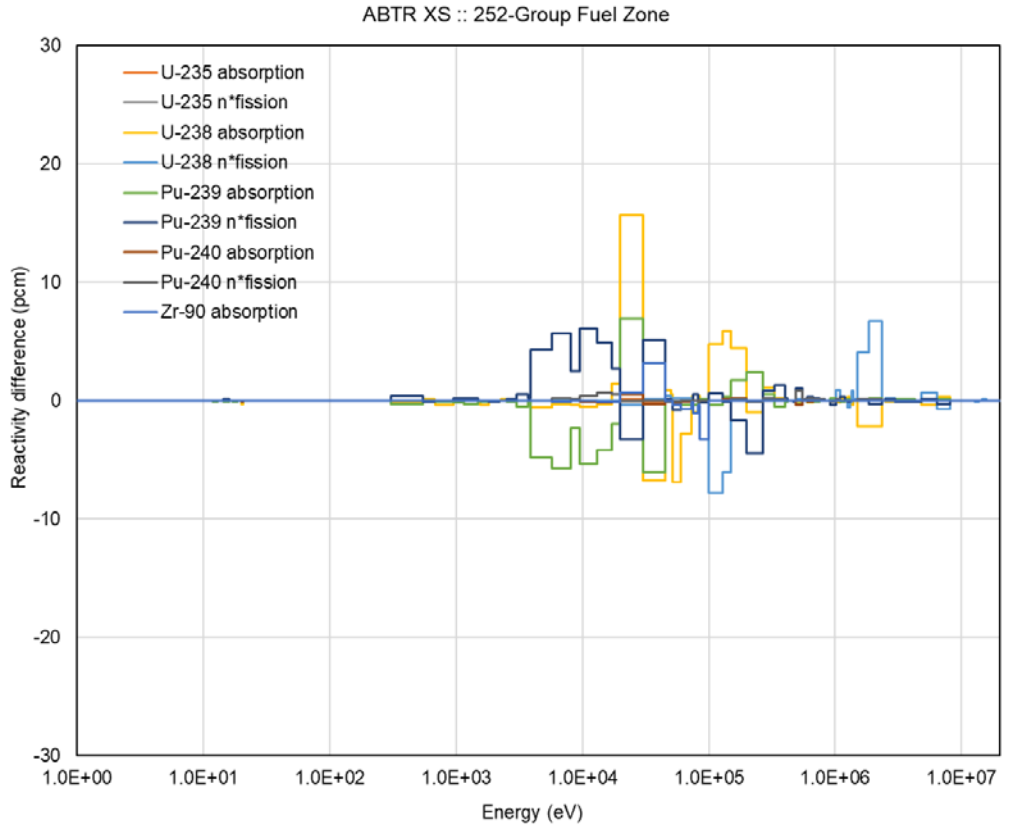




Limitation of the AMPX 252-Group Library

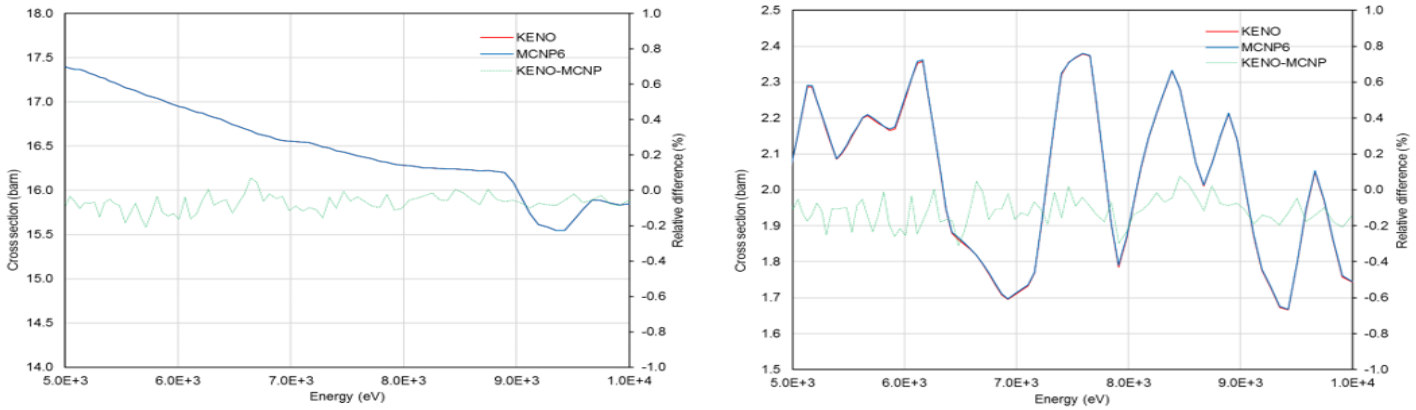
- **Reaction rate analysis for ABTR**
  - Self-shielded cross sections seems to be fine
  - Reaction rates are very bad. Scalar fluxes are bad.
  - Bad scattering matrices :: no high order flux moment weighting, resonances due to structure nuclides





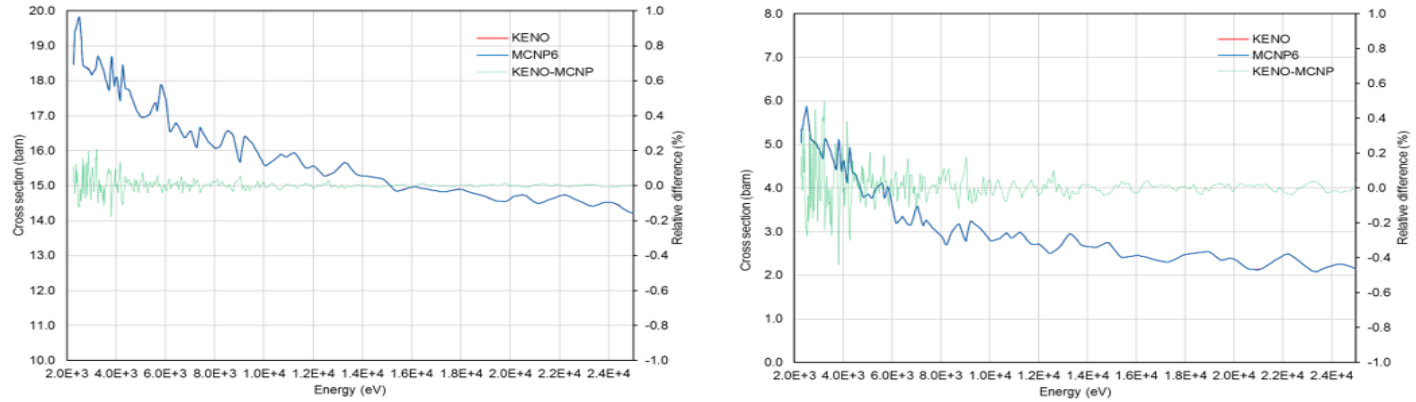
Verification of the AMPX Probability Table

- **Comparisons of the MG Tallied URR XSs: CE-KENO vs. MCNP**
  - A normalization issue in the AMPX Probability Table was identified and fixed



(a) Total (b) Fission

Comparison of the URR MG Cross Sections between KENO and MCNP for ^{239}Pu.



(a) Total (b) Fission

Comparison of the URR MG Cross Sections between KENO and MCNP for ^{235}U.

Benchmark Results Using the AMPX 1597-g Library

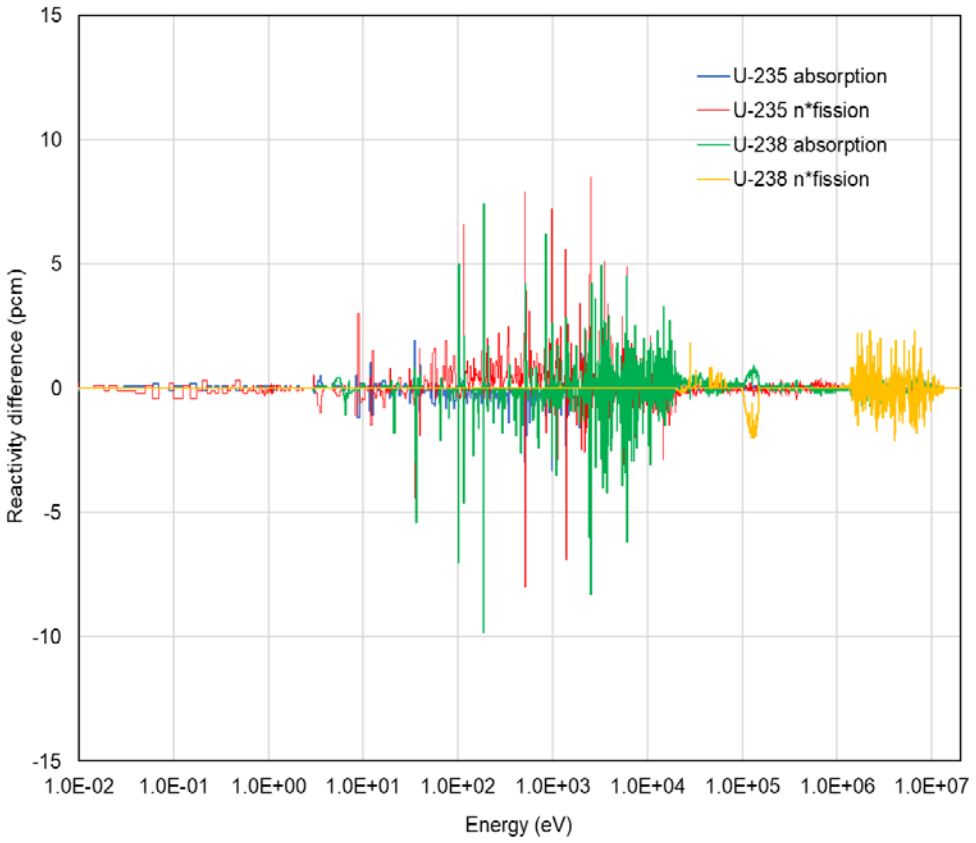
- **Comparisons of the Multiplication Factors**
  - CE-KENO, MCNP, SERPENT, and MG-KENO
  - CE-KENO with old and new probability tables

Type	Temp. (K)		Void (%)	CE KENO	Δk_{eff} (pcm)			
	Mod.	Fuel			Old-KENO	MCNP	SERPENT	MG-KENO
BWR	600	600	90.0	0.92499	7	40	11	99
			99.0	0.75990	25	-20	-18	-6
			99.9	0.72988	31	-13	-1	-1
	600	900	90.0	0.90996	25	24	22	132
			99.0	0.74916	15	-39	-40	-14
			99.9	0.72207	25	-27	-20	-9
	600	1200	90.0	0.89815	20	-16	-27	129
			99.0	0.74185	24	-38	-33	-2
			99.9	0.71692	15	-21	-13	-4
MSR	-	293.6	-	1.13987	-697	62	62	36
		600.0	-	1.13228	-669	83	77	66
		900.0	-	1.12835	-651	78	81	89
		1200.0	-	1.12562	-662	66	77	79
ABTR	293.6	293.6	-	1.60101	-489	-46	-60	39
	600.0	600.0	-	1.59471	-480	-69	-68	39
	600.0	900.0	-	1.59166	-494	-71	-70	59
	600.0	1200.0	-	1.58964	-461	-85	-96	56
MET1000	-	293.6	-	2.22285	-782	-104	-99	74
		600.0	-	2.21827	-812	-119	-123	21
		900.0	-	2.21620	-805	-105	-110	9
		1200.0	-	2.214994	-786	-99	-98	6

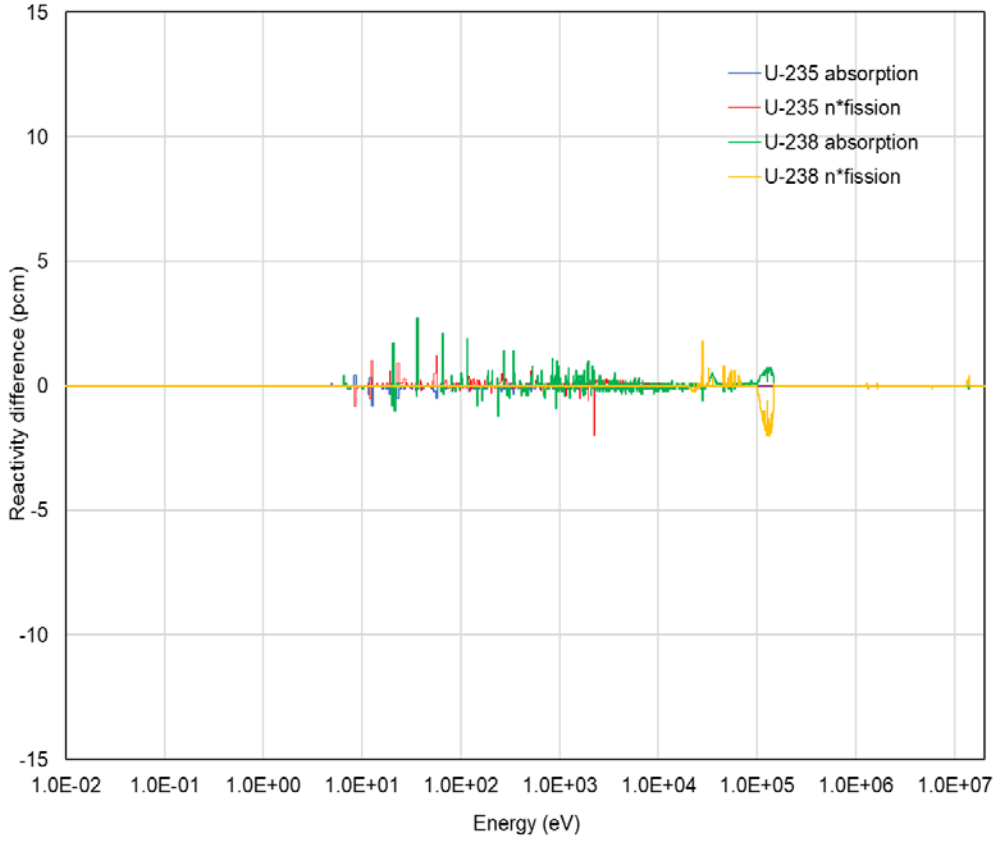
* standard deviation for Monte Carlo: <10 pcm

Reaction Rate Analysis: BWR

- **Comparisons of the Reaction Rates**
  - CE-KENO vs. MG-KENO 1597-g
  - BWR fuel with 99.0% void



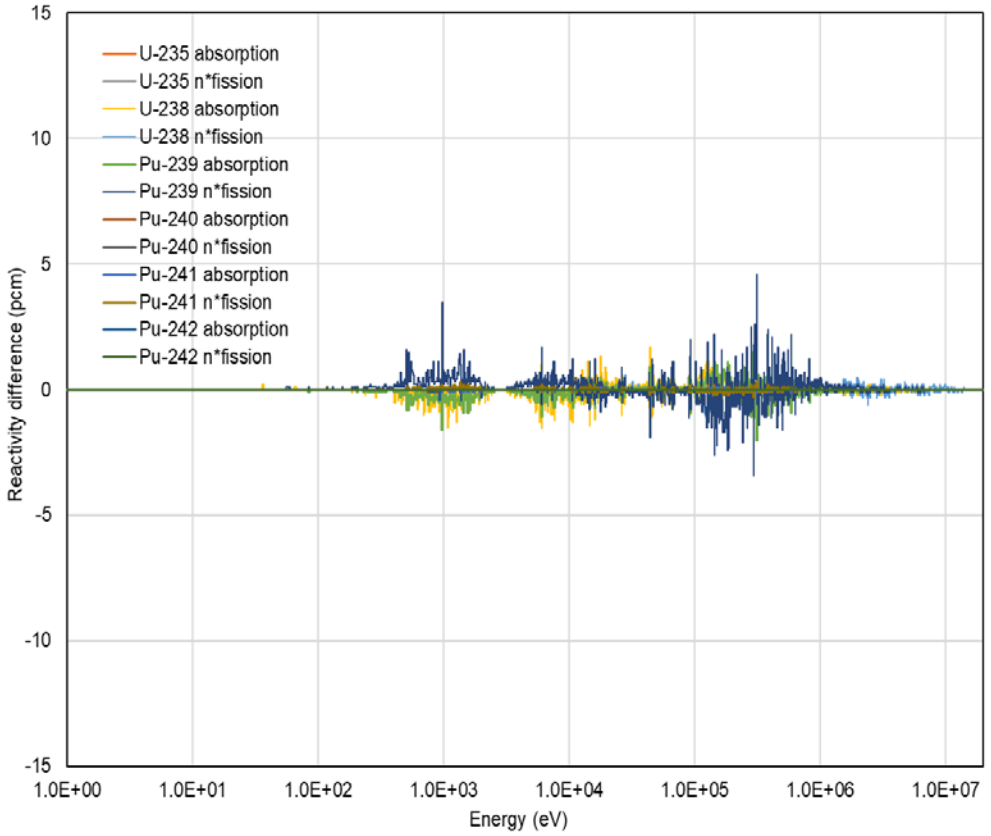
Reaction rate differences



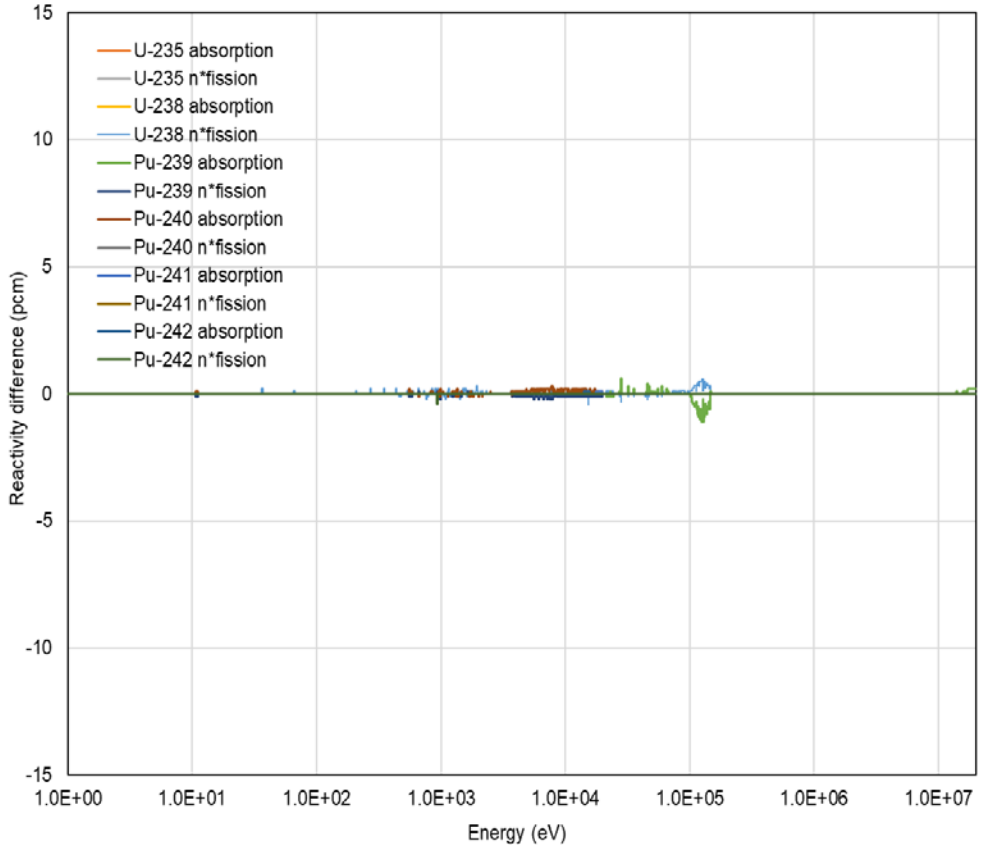
Cross section differences

Reaction Rate Analysis: MSR

- **Comparisons of the Reaction Rates**
  - CE-KENO vs. MG-KENO 1597-g
  - MSR fuel



Reaction rate differences

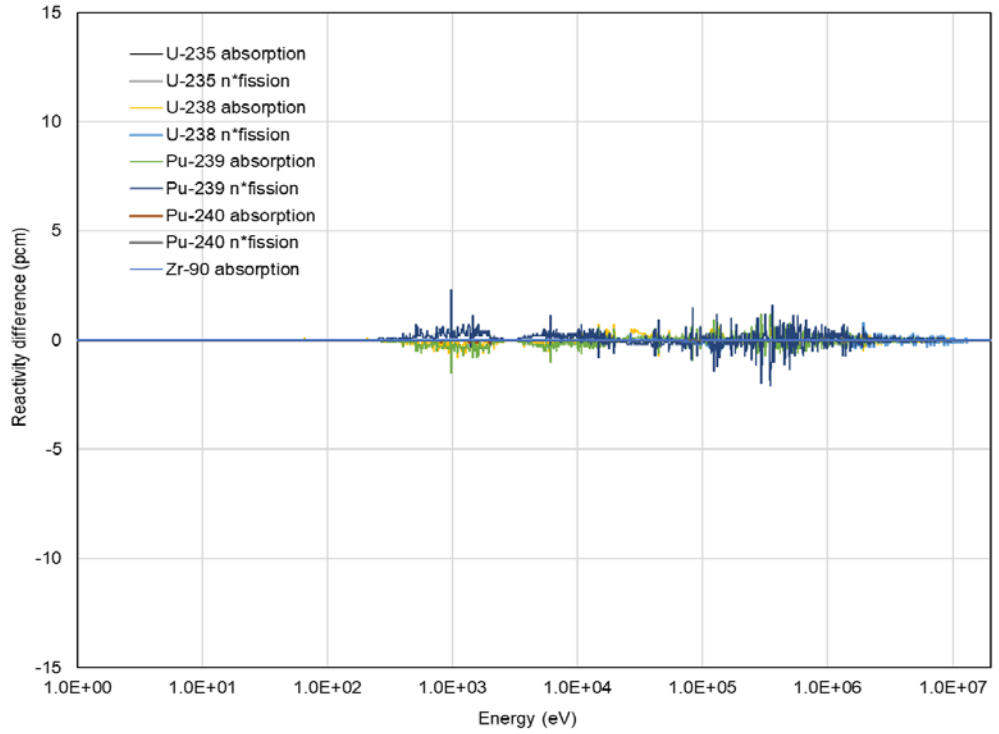


Cross section differences

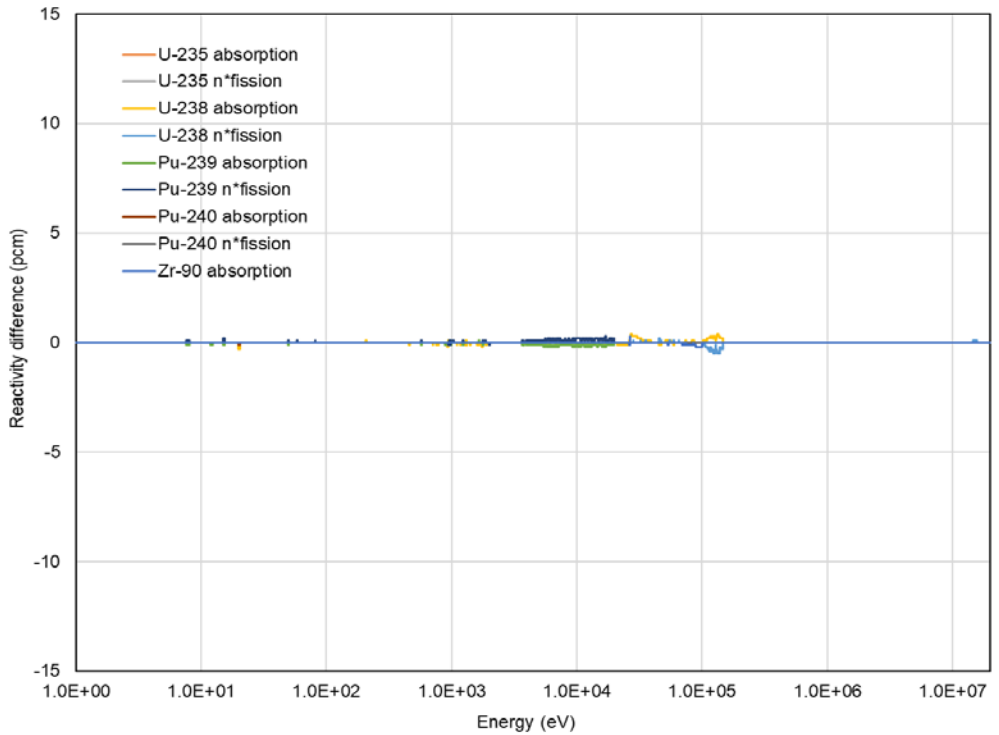
Reaction Rate Analysis: ABTR

- **Comparisons of the Reaction Rates**
  - CE-KENO vs. MG-KENO 1597-g

Case	Group	^{235}U		^{238}U		^{239}Pu		^{240}Pu		^{90}Zr	Sum
		R_a	R_{nf}	R_a	R_a	R_a	R_{nf}	R_a	R_{nf}	R_a	
Reaction rate	Fast	0	0	-5	5	-7	13	-1	1	0	6
	URR	0	0	21	-13	-18	10	0	2	-5	-3
	RR	0	0	-21	0	-35	35	-1	0	0	-22
	Thermal	0	0	0	0	0	0	0	0	0	0
	Sum	0	0	-5	-8	-60	58	-2	3	-5	-19
Cross section	Fast	0	0	0	0	0	0	0	0	3	0
	URR	0	0	15	-13	-26	27	-1	2	-5	-1
	RR	0	0	-2	0	-2	2	0	0	0	-2
	Thermal	0	0	0	0	0	0	0	0	0	0
	Sum	0	0	13	-13	28	29	-1	2	-5	-2



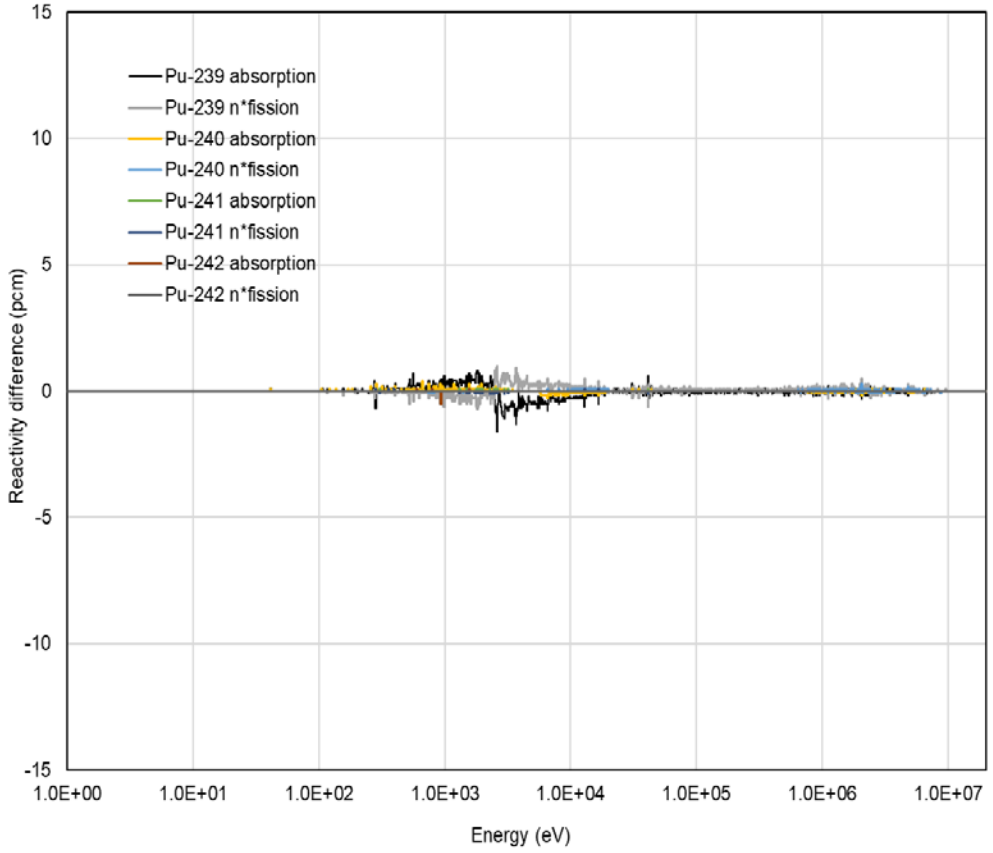
Reaction rate differences



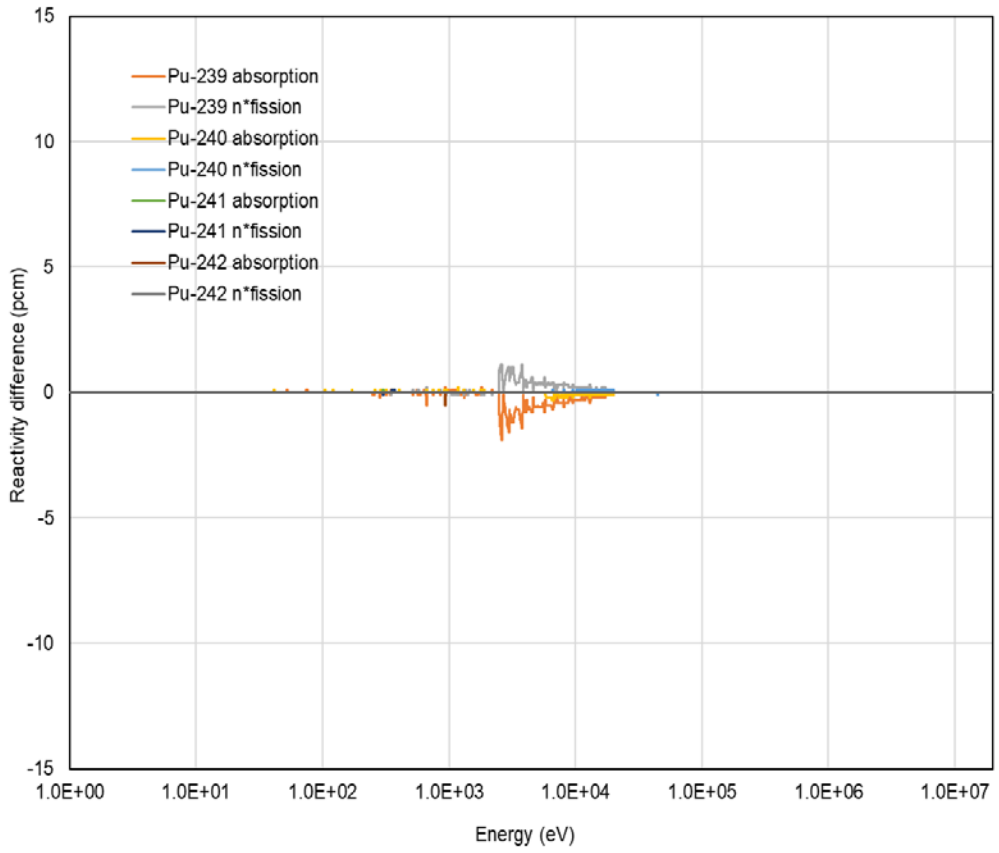
Cross section differences

Reaction Rate Analysis: MET-1000

- **Comparisons of the Reaction Rates**
  - CE-KENO vs. MG-KENO 1597-g
  - MET-1000 fuel



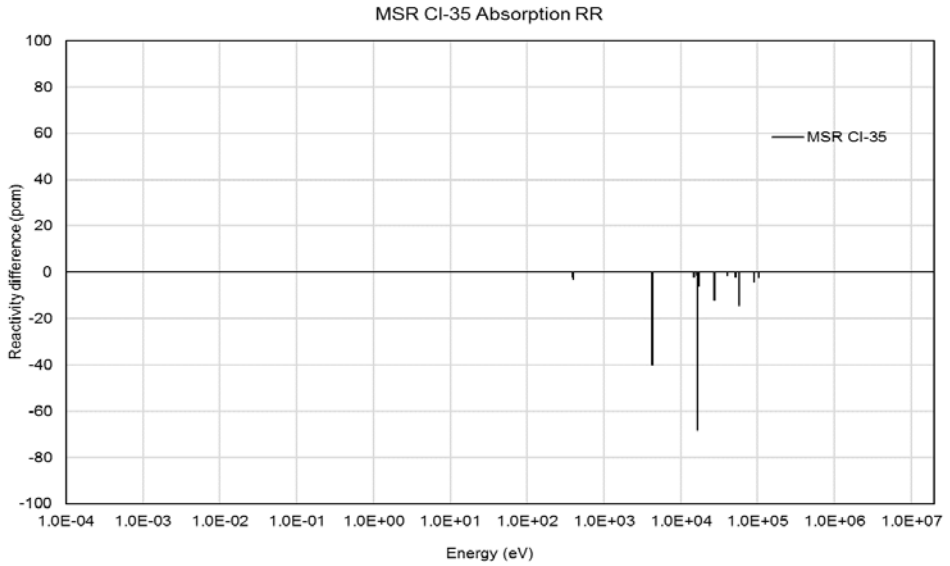
Reaction rate differences

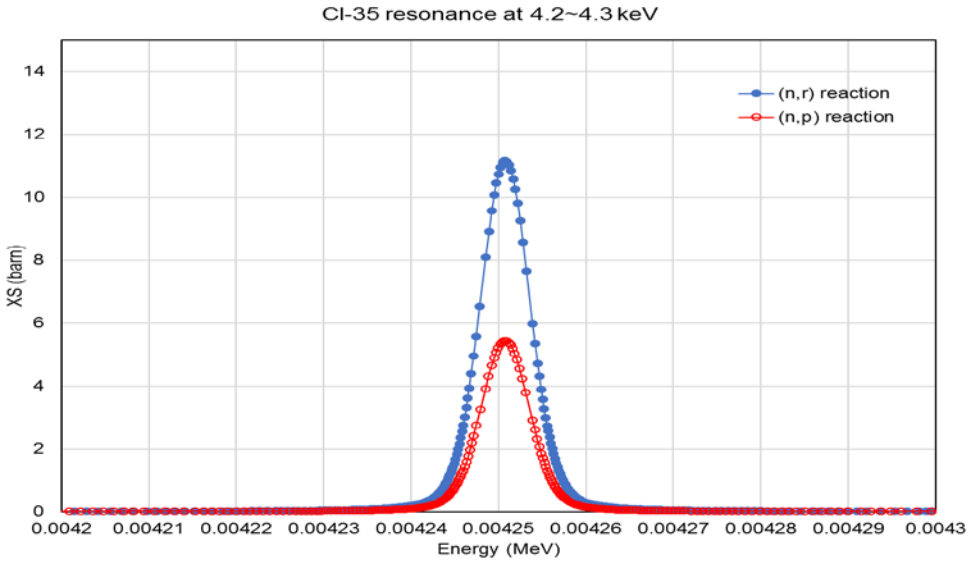


Cross section differences

Issue: MSR Cl-35

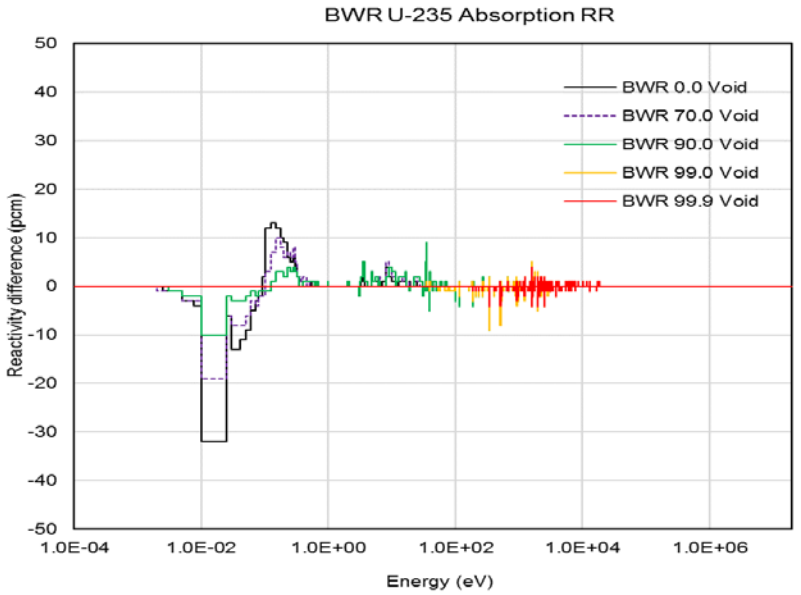
- **Reaction Rate Analysis**
  - ^{35}Cl introduces > 100 pcm
  - ^{35}Cl includes (n,p) resonances
- **AMPX/SCALE**
  - Includes resonance data for ^{35}Cl (n,p) reaction in the AMPX MG library
  - The issue has been fixed.

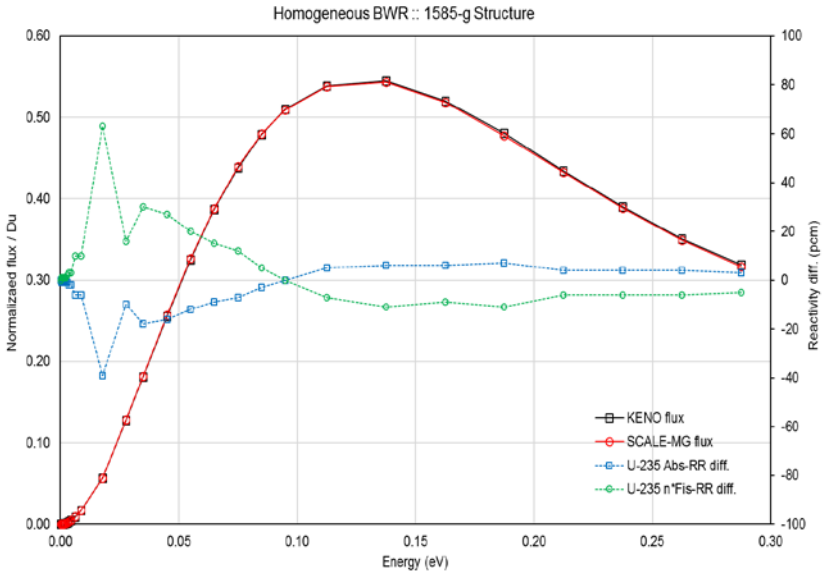


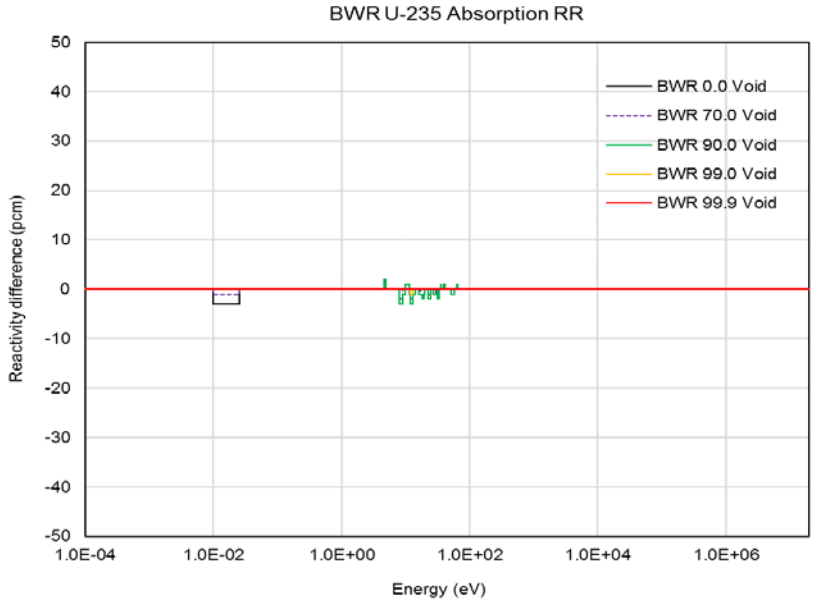


Issue: Thermal Spectrum

- **Reaction Rate Analysis**
  - XSs are fine.
  - Scalar fluxes are poor at thermal
  - Error cancellation between absorption and ν*fission
  - Common to deterministic MG transport

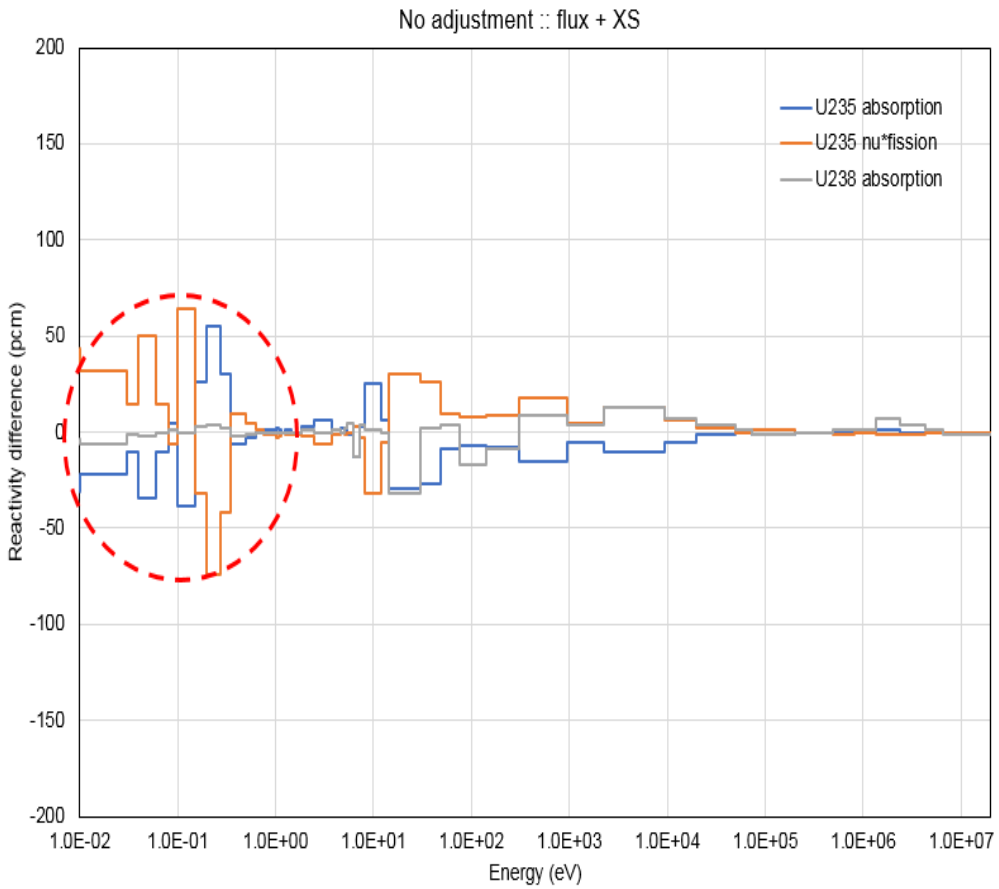


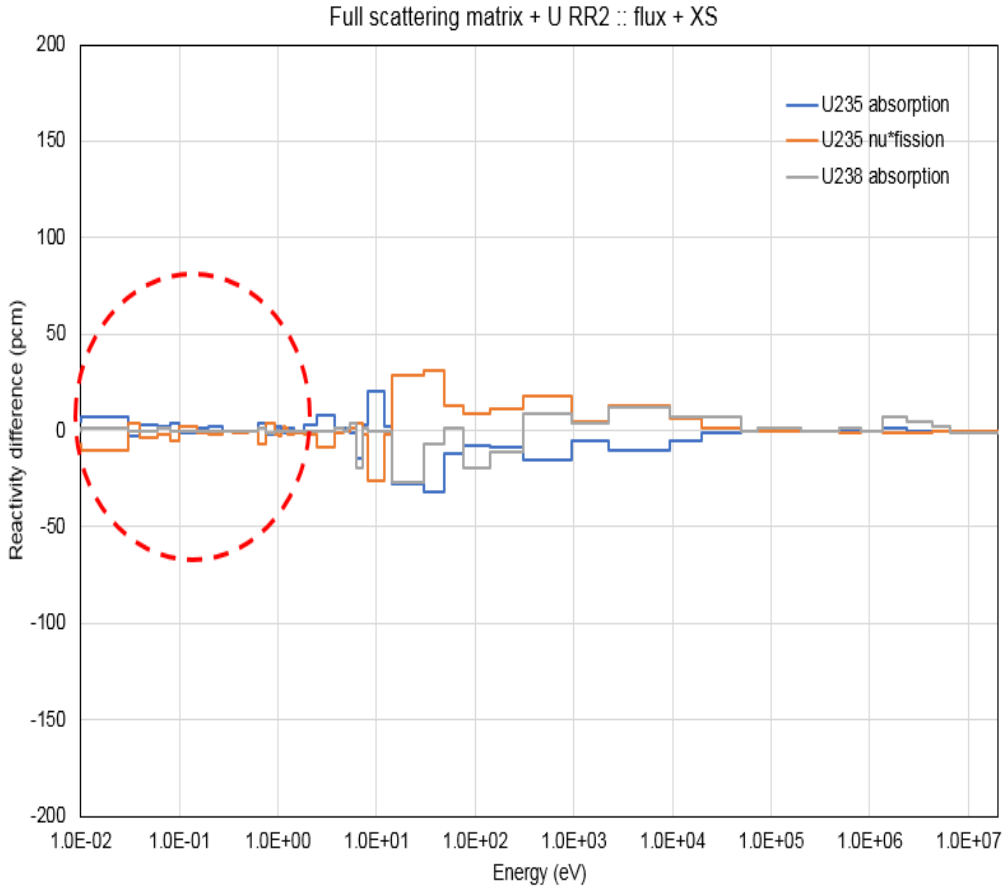




Issue: Thermal Spectrum

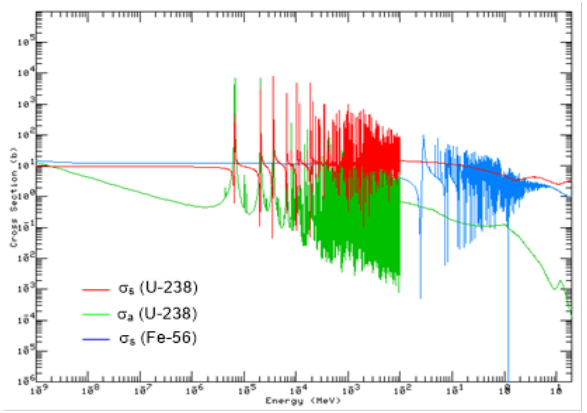
- **Resolution**
  - CE Monte Carlo based P_0 scattering matrices
  - SPH factor application
- **Trial**
  - CASL VERA MPACT





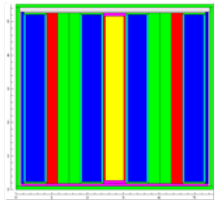
Fast Reactor Analysis Procedure Using AMPX/SCALE

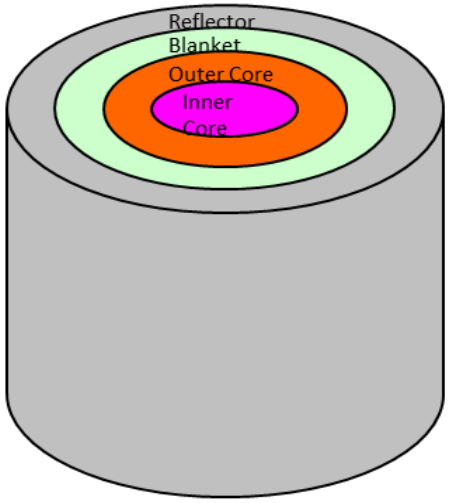
- **AMPX vs. MC^2-3**



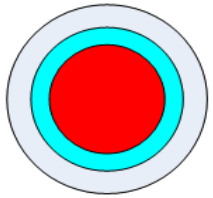
Nuclear Data (ETOE/MC2-3 vs AMPX)

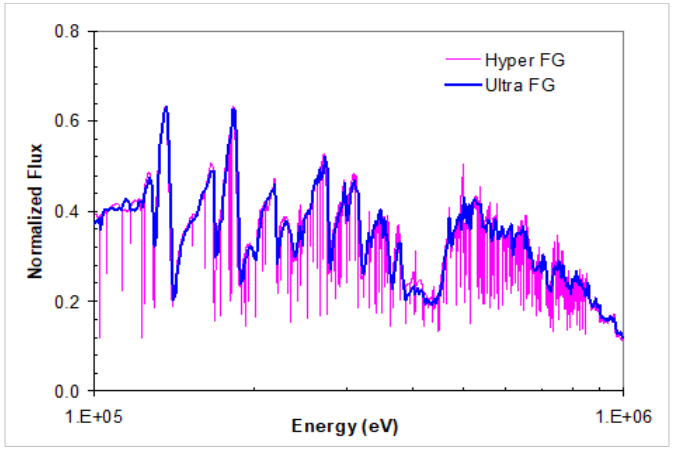
Resonance self-shielding for specific composition and geometry (UFG only) (MC2-3/SCALE-XSPROC)





0D / 1D unit cell calculation (MC2-3 0D/1D vs SCALE-CENTRM)





MC2-3 UFG/HFG transport calculation vs SCALE-CENTRM

2D R-Z core calculation (TWODANT)

Region-wise broad group cross sections MC2-3 vs SCALE-XSDRN or NEWT

Conclusion

- **URR Treatment**
  - AMPX probability table is consistent with NJOY probability table
  - AMPX's analytic probability table method is adequate

- **Group structure**
  - AMPX/SCALE 252-group + MC^2 ultra-fine group
  - 1597-group structure is adequate for general application

- **Ongoing Work**
  - Neutron leakage model for fast reactor application
  - Internal energy group collapsing for computational efficiency
  - Apply the AMPX library for the Bondarenko approach
    - SCALE-Polaris: Embedded Self-Shielding Method (ESSM)

- **Pending Issue**
  - Thermal spectrum & scattering matrix issue in CENTRM
    - Poor thermal spectrum same as other transport codes (resolved)
    - No high order flux moment weighting
    - Energy group structure optimization for memory and speed efficiency