OAK RIDGE
National Laboratory

CASL VERA Benchmark Results with ENDF/B-VII.1 and VIII.0 for the Pressurized Water Reactors

November 4, 2019

Kang Seog Kim, Erik Walker, Andrew Godfrey

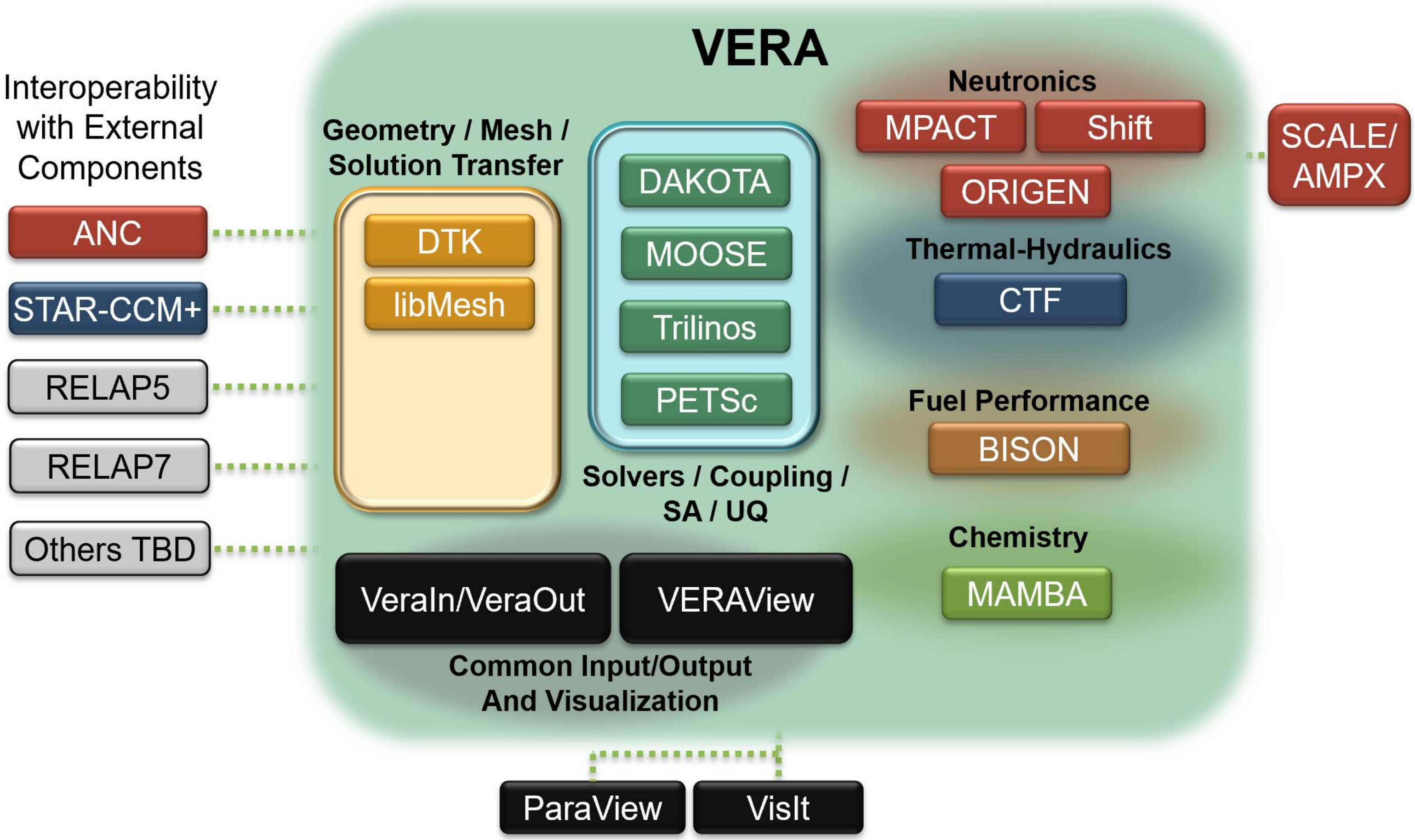
U.S. DEPARTMENT OF
ENERGY

Overview

- **Contents**
  - CASL VERA overview
    - VERA & MPACT
  - MPACT library generation procedure
    - AMPX MG & MPACT 51-group library generation
    - Subgroup method and subgroup data
  - PWR Benchmarks
    - Hot Zero Power Benchmark Results
    - ITC Benchmark Results
    - Hot Full Power Benchmark Results
  - Epithermal Upscattering Consideration
    - Reactivity Bias
  - ENDF/B-VII.1 vs. VIII.0
    - Burnup Calculation
  - Conclusion & Discussion

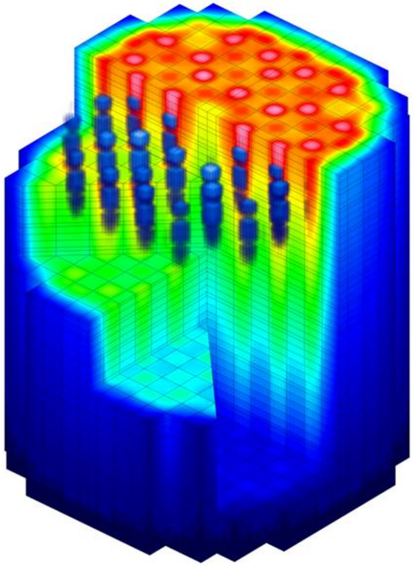
CASL and VERA

- **CASL ::** Consortium for the Advanced Simulation of Light Water Reactors
- **VERA ::** Virtual Environment for Reactor Application



VERA Multiphysics Coupling

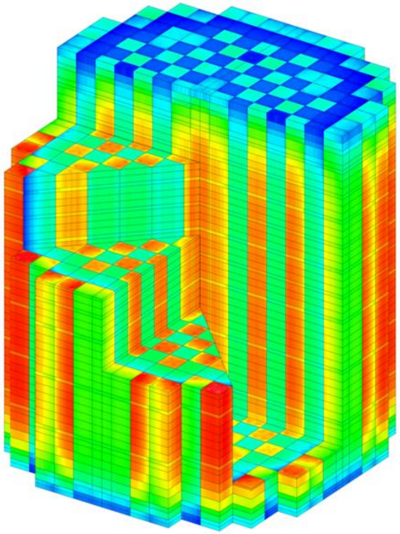
WB1C11 Middle-of-Cycle Coolant Temperature Distribution



MPACT

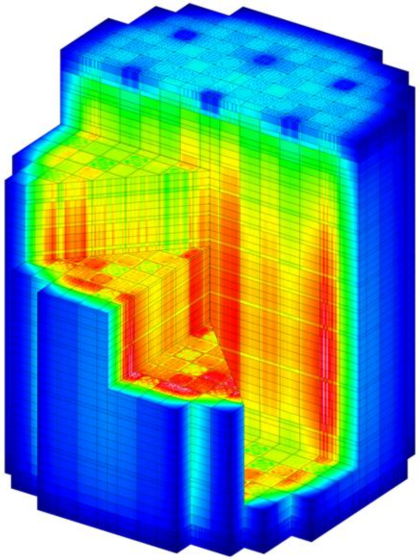
Advanced pin-resolved 3-D whole-core neutron transport in 51 energy groups and >5M unique cross section regions

WB1C11 End-of-Cycle Pin Exposure Distribution



CTF

Subchannel thermal-hydraulics with transient two-fluid, three-field (i.e., liquid film, liquid drops, and vapor) solutions in 14,000 coolant channels with crossflow



WB1C11 ***Beginning-of-Cycle Pin Power Distribution***

ORIGEN

Isotopic depletion and decay in >2M regions tracking 263 isotopes

CASL Neutronics Simulators

- **Neutronics simulators**
  - **MPACT** : Deterministic 1D (NEM or SPN)/2D (MOC) 3D CMFD Framework
  - **SHIFT** : Continuous energy Monte Carlo

- **MPACT**
  - Development
    - U. of Michigan & Oak Ridge National Laboratory
  - Methodology
    - Neutron flux solver
      - 3D CMFD framework with 2D radial MOC & 1D axial NEM or SPN
      - Transport corrected P0 and High order scattering
    - Resonance self-shielding method :: Bondarenko approach
      - Subgroup method for intra pin non-uniform temperature profile
      - Embedded Self-Shielding Method (ESSM) and/or Quasi 1D (under development)
    - Depletion
      - Internal module with Matrix exponential method (510 burnup chain)
      - ORIGEN-API with ORIGEN depletion libraries (2237 and 255 burnup chains)
    - T/H feedback
      - Internal T/H & COBRA-TF

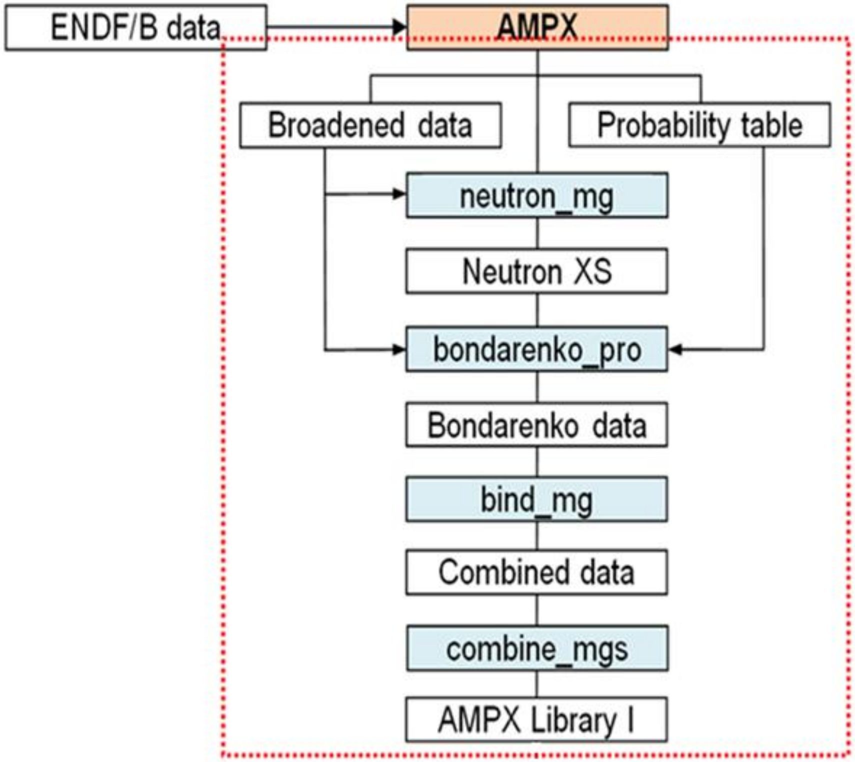
AMPX/SCALE Procedure I

- **Pointwise XS data generation**
  - Doppler Broadening / Probability Table Data
- **Multigroup XS data generation**
  - Flux weighting
  - Weighting function
  - Conventional
    - Maxwellian : thermal
    - 1/E : slowing down
    - Fission spectrum : fast
  - Practical spectra
    - Pointwise typical PWR fuel pin
    - SCALE-CENTRM
  - Self-shielded data
    - Narrow resonance approximation

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

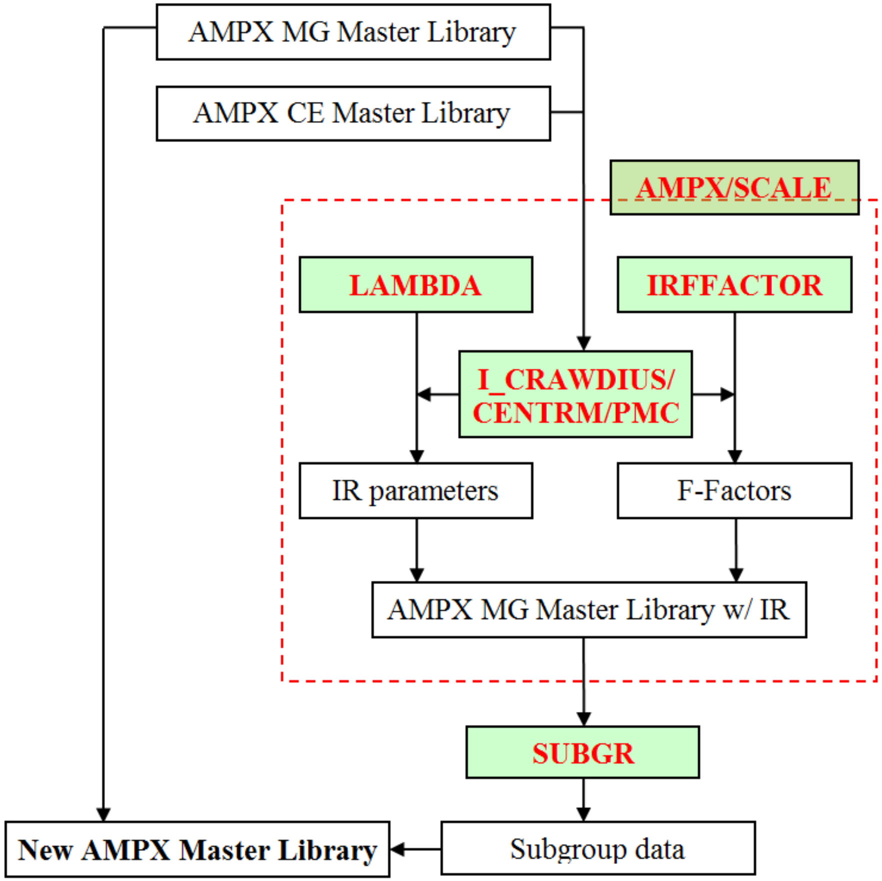
  - Scattering matrix

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



AMPX/SCALE Procedure II

- **Improvement of Resonance data**
  - Intermediate resonance parameter
    - LAMBDA
  - Homogeneous models
    - H-1 + Target isotope
    - Homogeneous slowing down
  - Heterogeneous models
    - Heterogeneous slowing down
    - ESSM to obtain background XS
    - Important nuclides
  - Introduce within-group correctior
    - Adjusting scattering matrices
    - Homogeneous & heterogeneous


AMPX MG Master Library

AMPX CE Master Library

AMPX/SCALE

LAMBDA

IRFFACTOR

I_CRAWDIUS/ CENTRM/PMC

IR parameters

F-Factors

AMPX MG Master Library w/ IR

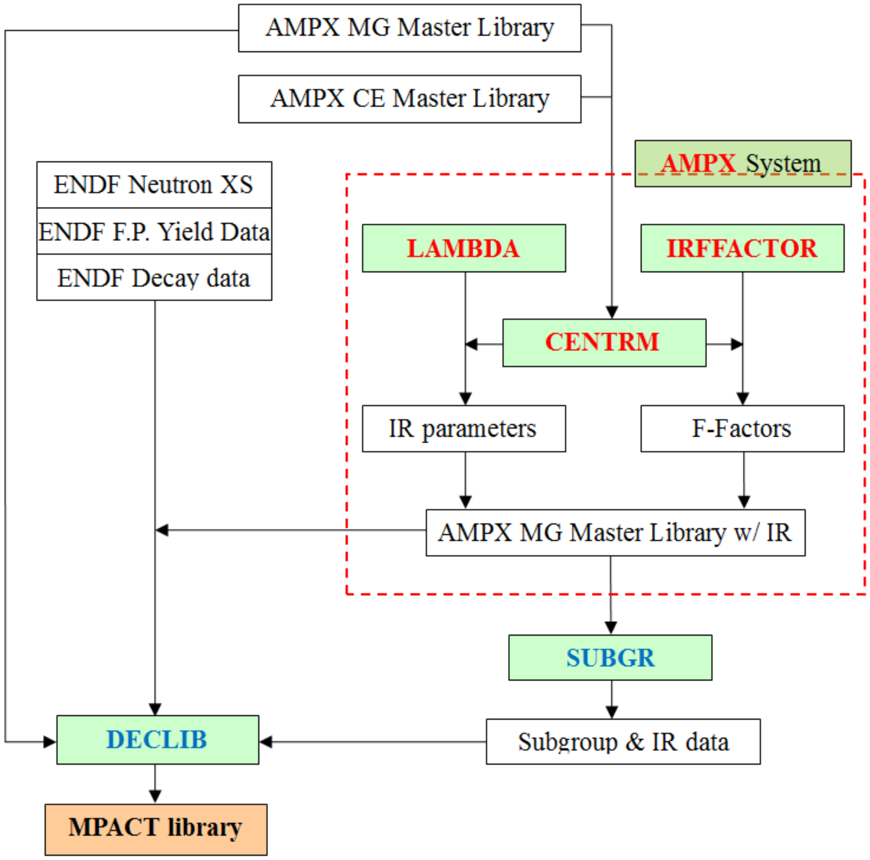
SUBGR

New AMPX Master Library

Subgroup data

The MPACT 51-Group Library

- **Development of the 51-group library**
  - Group structure
    - 51-group
    - Resonance: 10-31
  - Key characteristics
    - ENDF/B-VII.0, VII.1 and VIII.0
    - Pointwise PWR weighting function
    - NLC transport cross section for ^{1}H
    - Within-group correction factor
    - Resonance data
      - Intermediate resonance parameters
      - Heterogeneous models
        - Important nuclides
      - Homogeneous models
        - > A=40
      - Narrow resonance
    - Subgroup data: 51 nuclides
    - Resonance upscattering data for ^{238}U
    - Transient data



Subgroup Method

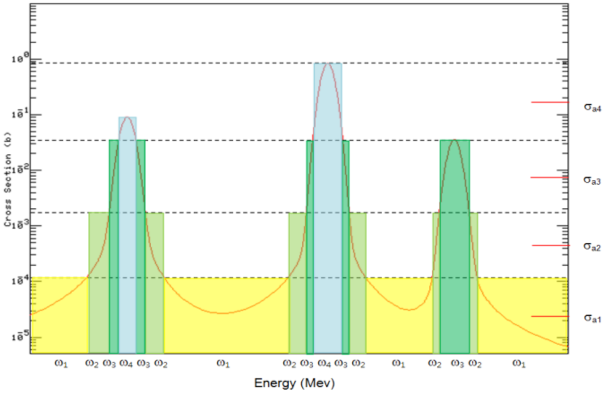
- **Subgroup data generation**
  - Real data method
    - Given subgroup levels ? obtain width (or weights)
  - Physical method
    - Resonance self-shielded XS table
    - Given subgroup levels ? obtain width (or weights)
    - Non-linear least square fitting

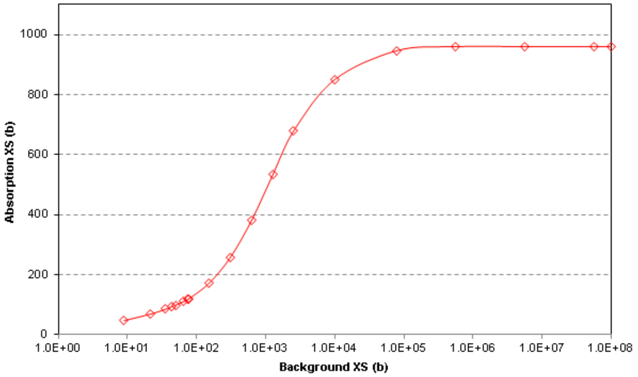
$$\sigma_x = \frac{\sum_n w_{xn}\sigma_{xn}\phi_n}{\sum_n w_{an}\phi_n} = \frac{\sum_n w_{xn}\sigma_{xn}\dfrac{\sigma_{bn}}{\sigma_{an}+\sigma_{bn}}}{\sum_n w_{an}\dfrac{\sigma_{bn}}{\sigma_{an}+\sigma_{bn}}}$$

- **Subgroup method**
  - Background XS for each subgroup level
    - Fixed source transport equation: MOC

$$\hat{\Omega}\cdot\nabla\psi_{g,n} + (\Sigma_{r,g,an} + \sum_i \lambda_{i,g}\Sigma_{i,p})\psi_{g,n}(\hat{\Omega}) = \sum_i \lambda_{i,g}\Sigma_{i,p}$$

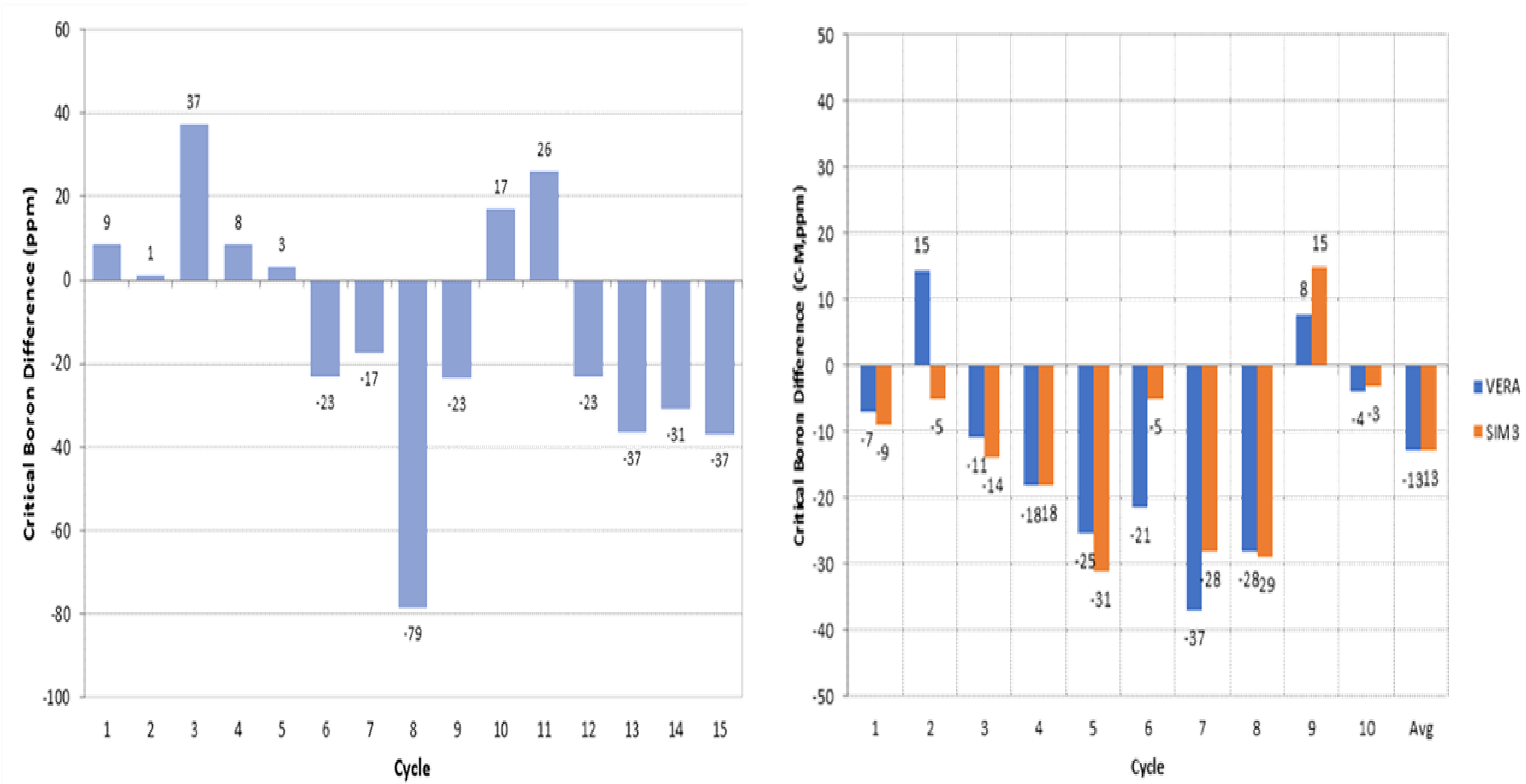
$$\sigma_{g,bn} = \frac{\Sigma_{g,bn}}{N_R} = \frac{\sum_i N_i\lambda_i\sigma_{i,g,p} + \Sigma_{g,en}}{N_R} = \frac{\sigma_{g,an}\phi_{g,n}}{1-\phi_{g,n}}$$





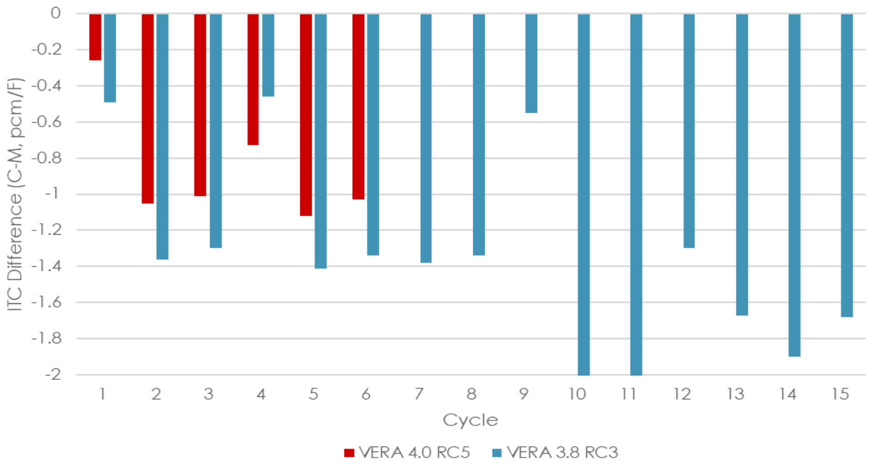
Hot Zero Power Benchmark Results (Old)

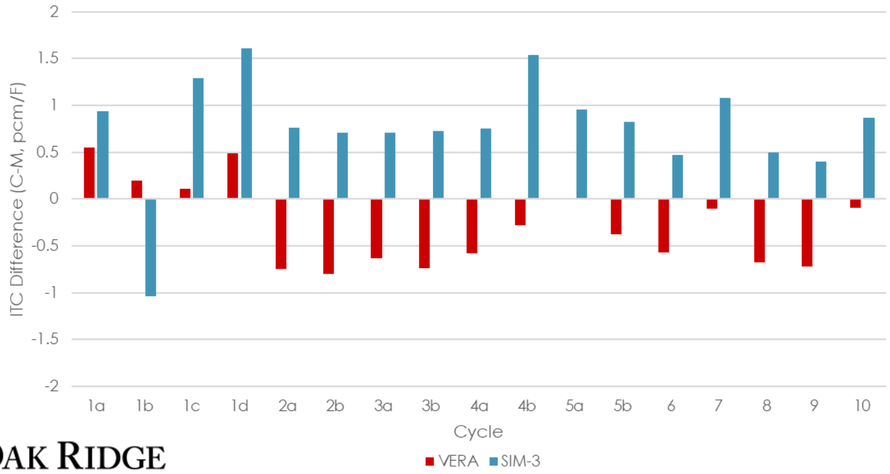
- **Critical boron concentration at HZP (Old): ENDF/B-VII.1**
  - Watts Bar unit I (left), TMI unit I (right)
    - Lower reactivity
    - No epithermal upscattering



Isothermal Temperature Coefficients (Old)

- **Hot Zero Power ITC: : ENDF/B-VII.1**
  - Watt Bar I (left top), TMI 1 (left bottom), Krsko/Davis/Watt Bar II/Votgle I
    - More negative: similar trend with HFP causing low reactivity at HFP
    - No epithermal upscattering

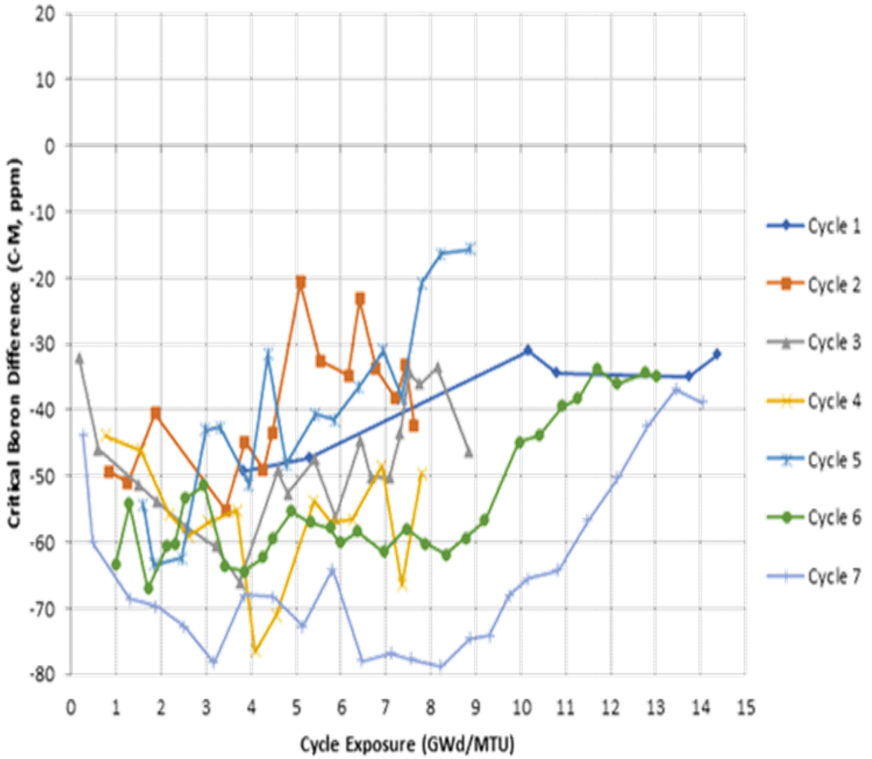




Plant	Cycle	ITC Difference [pcm/F]
Krsko	1	-0.13
	2	-2.18
	3	-2.08
Davis-Besse	15	-0.29
Watts Bar 2	1	-0.80
Votgle 1	9	-0.87
	10	-0.35
	11	-0.85
	12	-1.29
	13	-0.61

Hot Full Power Benchmark Results (Old)

- **PWR plant simulation: ENDF/B-VII.1**
  - Watt Bar unit I (left), TMI unit I (right): no epithermal upscattering
  - Low reactivity error sources
    - ENDF/B nuclear data
    - Fuel temperature estimation: however, ITC indicates more suspect for data
    - Other sources



Plants & Fuel Types Analyzed (New)

- **Westinghouse's simulation**
  - Gary Mangham, "VERA industry validation by Westinghouse"
  - CASL IC/SC meeting on 10/15-17
  - No epithermal upscattering with ENDF/B-VII.1
- **Eleven plants (27 cycles)**
  - Includes seven initial cycles
- **Core and Fuel types**
  - Availability and reliability of measured data
  - Measured - Predicted

Parameter	**Selection**
Core size (# of assemblies)	2-loop (121), 3-loop (157), 4-loop (193), AP1000® (157)
Fuel Lattice Size (N x N)	14, 15, 16, 17 (small diameter), 17 (large diameter)
Rod Diameter (inch)	0.360, 0.374, 0.422
Enrichment (w/o U235)	0.71 – 4.95
Burnable Absorber	IFBA(ZrB_2), WABA, Gadolinia, Pyrex
Cycle Energy (GWD/MTU)	9 - 25
RCCA Material	Ag-In-Cd, hafnium, tungsten

Hot Zero Power Benchmark Results (New)

- **Critical boron concentration at HZP: ENDF/B-VII.1**
  - Measured – Predicted for 27
    - Mean = -6 ppm
    - S.D. = 17 ppm

Plant	Mean (ppm)	Number of Measurements	Minimum Difference (ppm)	Maximum Difference (ppm)
A	-17	3	-27	-9
B	-15	4	-29	10
C	-12	4	-37	2
D	-7	3	-44	12
E	7	2	-5	18
F	1	3	-7	13
G	-10	4	-24	5
H	13	1	13	13
I	-6	1	-6	-6
J	14	1	14	14
K	14	1	14	14
Combined	**-6**	**27**	**-44**	**18**

Standard Deviation (ppm)	**17**

Isothermal Temperature Coefficients (New)

- **ITC at HZP: ENDF/B-VII.1**
  - Measured – Predicted for 26
    - Mean = +0.3 pcm/F
    - S.D. = 0.6 pcm/F

Plant	Mean (pcm/°F)	Number of Measurements	Minimum Difference (pcm/°F)	Maximum Difference (pcm/°F)
A	0.3	3	-0.1	0.6
B	-0.6	4	-0.9	0.1
C	0.5	4	-0.7	1.3
D	0.7	3	0.3	1.0
E	0.4	1	0.4	0.4
F	0.7	3	0.6	0.9
G	0.7	4	0.4	1.1
H	0.3	1	0.3	0.3
I	0.5	1	0.5	0.5
J	0.2	1	0.2	0.2
K	-0.1	1	-0.1	-0.1
Combined	**0.3**	**26**	**-0.9**	**1.3**

Standard Deviation (pcm/°F)	**0.6**

Hot Full Power Benchmark Results (New)

- **Critical Boron vs. burnup: ENDF/B-VII.1**
  - 21 measurement
  - Measured – Predicted

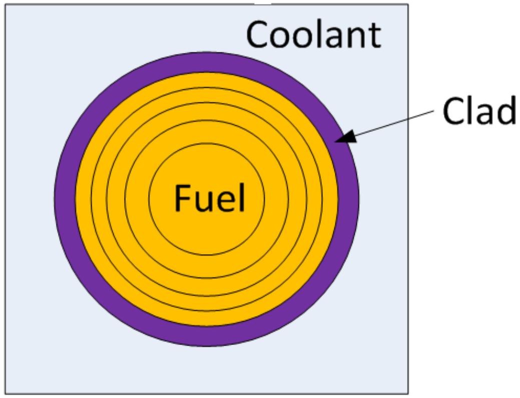
- **Beginning of cycle**
  - Measured – Predicted
    - Mean = -14 ppm
    - S.D. = 21 ppm

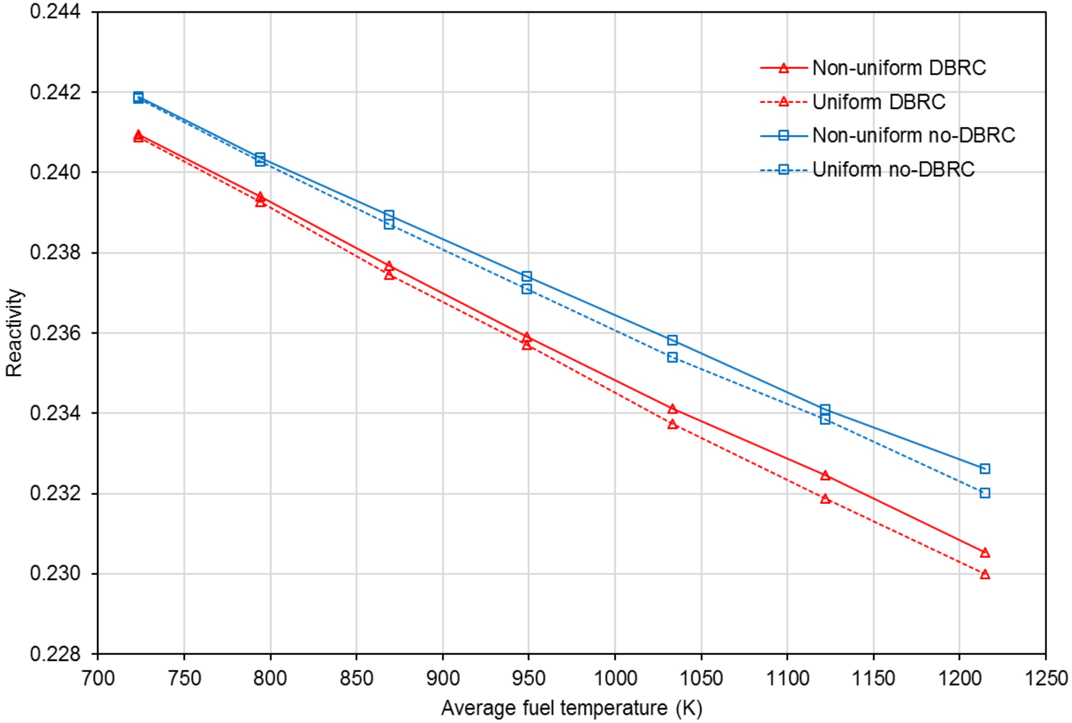
- **End of cycle**
  - Measured – Predicted for 26
    - Mean = 27 ppm
    - S.D. = 21 ppm

Plant	Cycle	Near-BOC M-P (ppm)	Near-EOC M-P (ppm)
A	**18**	-27	2
	19	-22	1
B	**1**	12	34
	2	11	32
	3	-14	34
	4	-25	25
C	**21**	-11	21
	22	-3	21
	23	0	4
D	**1**	-72	2
	2	41	26
	3	-19	26
E	**25**	-19	59
	26	-16	59
F	**28**	-30	61
	29	-20	63
	30	-10	51
G	**24**	6	29
	25	-13	-13
	26	-36	17
	27	-22	21
Mean (ppm)		**-14**	**27**
SD (ppm)		**21**	**21**

Epithermal Upscattering

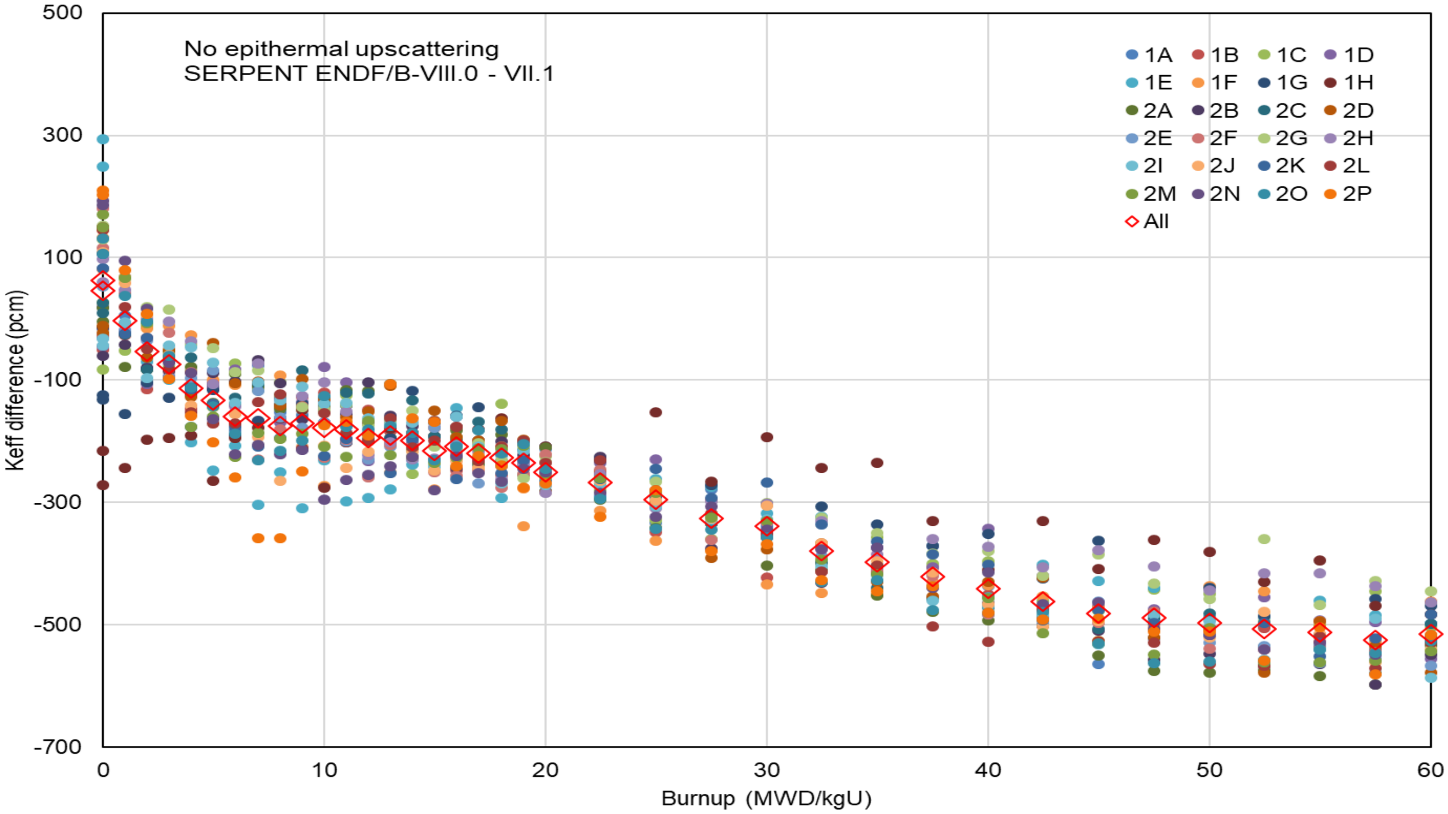
- **Epithermal upscattering**
  - Thermal motion of heavy target nuclei: theoretically correct
  - Significant impact on eigenvalue (150~200 pcm lower for HFP)
  - Monte Carlo codes: Doppler Broadening Rejection Correction (DBRC)
    - Non-default options: KENO, Serpent, MC21, (MCNP not yet)
  - VERA MPACT MG library
    - Options: only for U-238 (dominant for PWR)





ENDF/B-VII.1 vs. ENDF/B-VIII.0

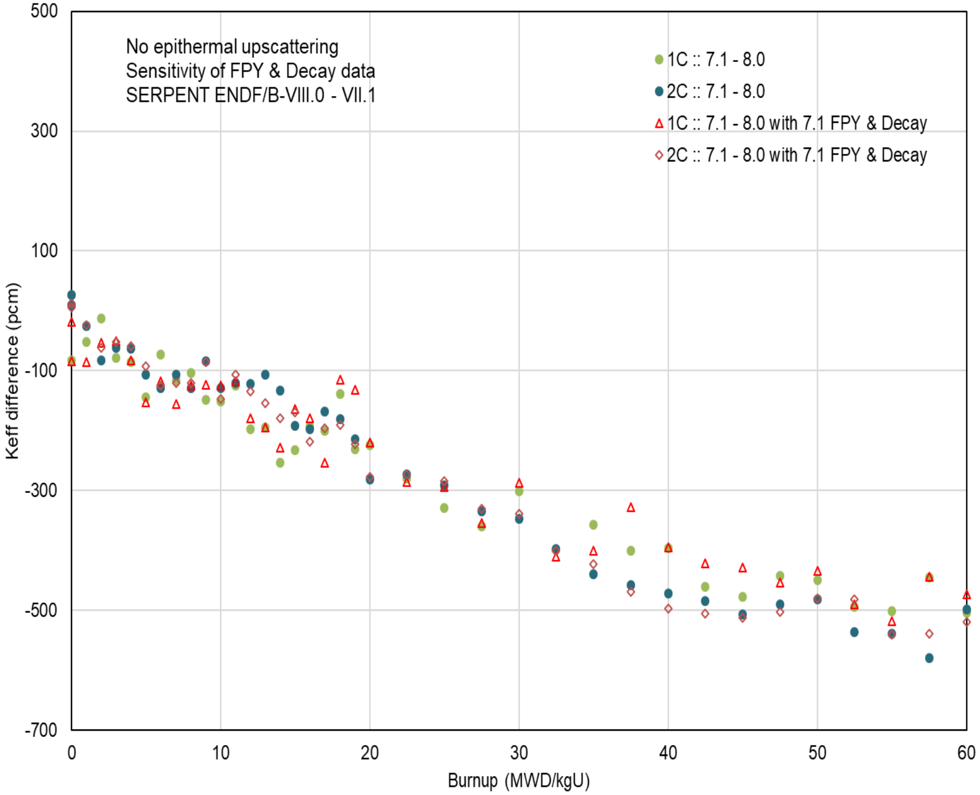
- **Depletion**
  - VERA Depletion Benchmark Problems
    - PWR single pins and assemblies
    - SERPENT2
  - ENDF/B-VIII.0 reactivities are much lower



ENDF/B-VII.1 vs. ENDF/B-VIII.0

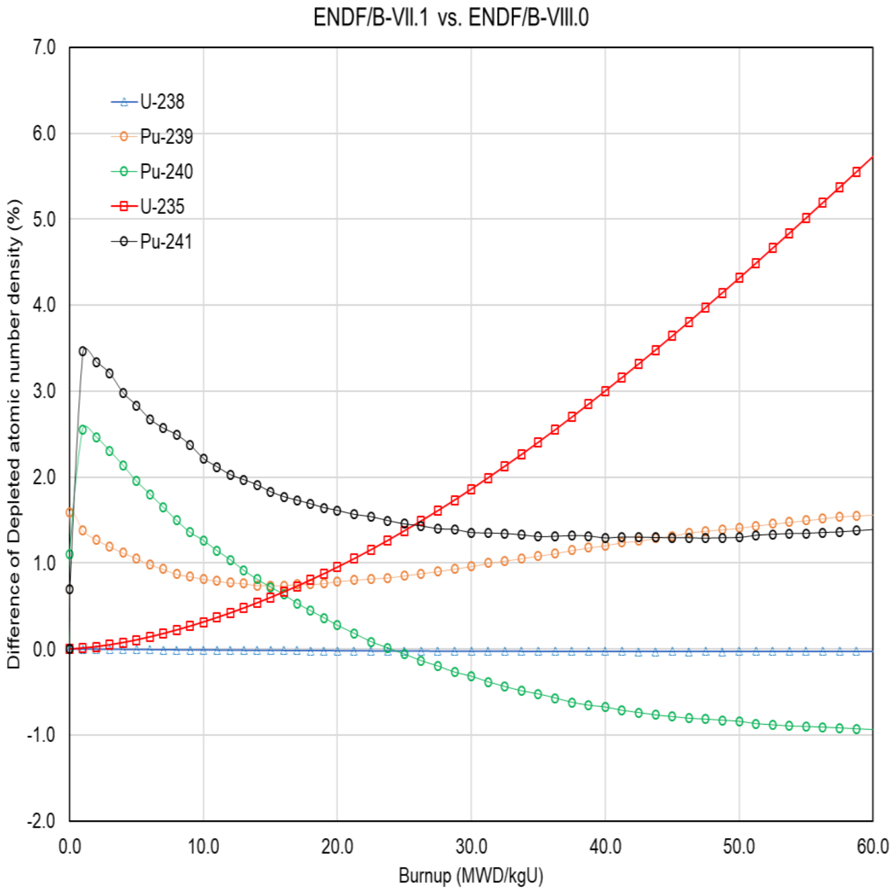
- **Bias Source**
  - Snapshot burnup calculations
  - Fission product yields and decay data: VIII.0 XS + VII.1 FPY & decay
    - Minor impact on reactivity

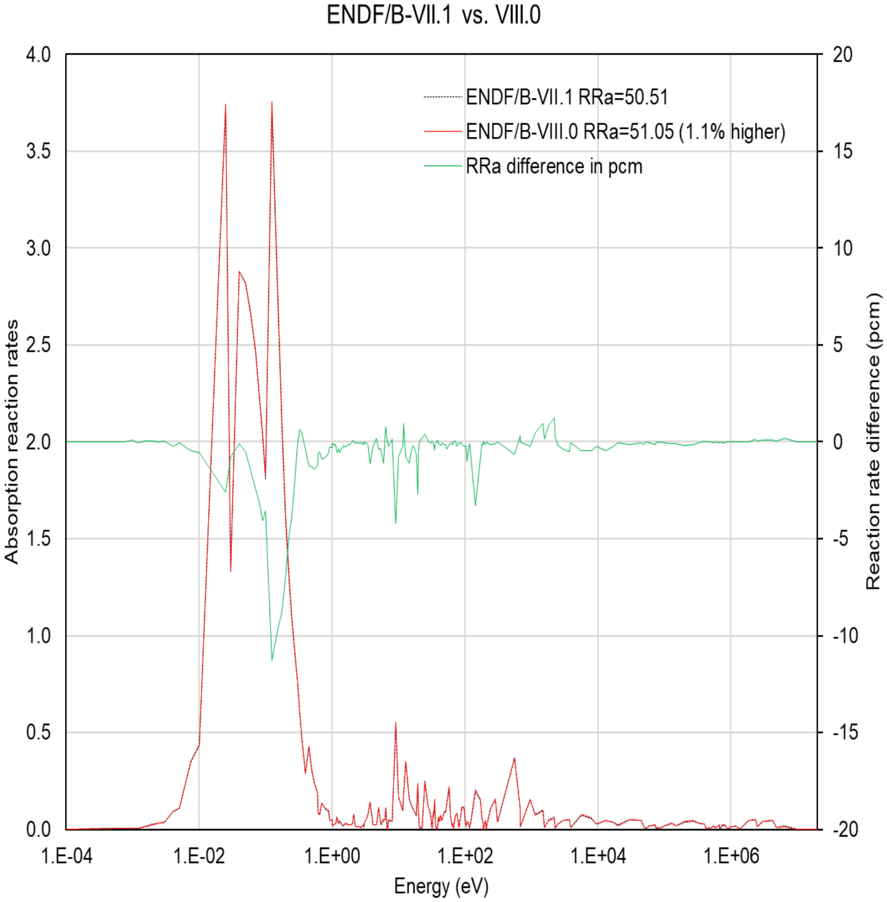
Case	Burnup	FPY	ENDF/B		Δρ (pcm)
			VII.1	VIII.0	
b01_burn_S00	0	no	1.24587	1.24720	86
b02_burn_S10	10	yes	1.08699	1.08738	33
b03_burn_S20	20	yes	1.00292	1.00297	5
b04_burn_S40	40	yes	0.88318	0.88297	-27
b05_burn_S60	60	yes	0.80886	0.80869	-26
b06_burn_S10x	10	no	1.17320	1.17394	54
b07_burn_S20x	20	no	1.11657	1.11647	-8
b08_burn_S40x	40	no	1.03682	1.03614	-63
b09_burn_S60x	60	no	0.98941	0.98849	-94



ENDF/B-VII.1 vs. ENDF/B-VIII.0

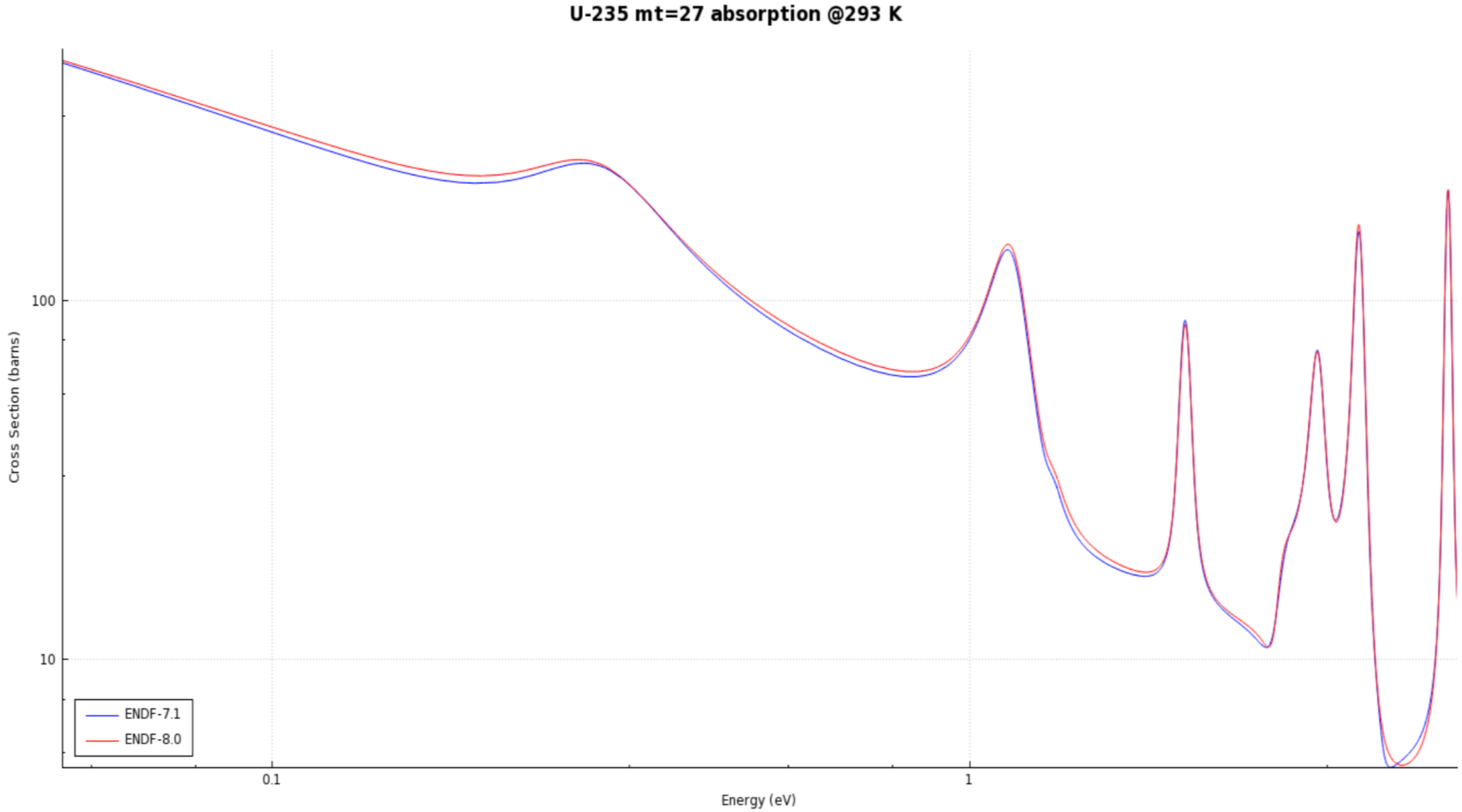
- **Bias Source**
  - Depleted atomic number densities: U-235 & Pu-241
  - U-235 absorption reaction rate comparison
    - 0.01~1 eV → lower





ENDF/B-VII.1 vs. ENDF/B-VIII.0

- **Bias Source**
  - Depleted atomic number densities: U-235 & Pu-241
  - U-235 absorption reaction rate comparison
    - 0.01~1 eV → lower



Discussion & Conclusion

- **ENDF/B-VII.1**
  - Overall good for the PWR HZP & HFP core reactivity
    - ITC is also good, but slightly more negative
    - BOC is more positive reactivity, but EOC is more negative reactivity
  - Reactivity as a function of burnup
    - Lower at high burnup
    - CASMO-5 is using JEFF-3 data for Pu's
  - Epithermal upscattering would result in more negative reactivity
    - 150-200 pcm more negative
    - Theoretically better, but can not be used

- **ENDF/B-VIII.0**
  - Significant reactivity bias for depletion
    - ~500 pcm lower at 50 MWD/kgU compared to ENDF/B-VII.1
    - Much bigger thermal absorption reaction rates for U-235 and other Pu's
  - ENDF/B-VIII.0 + epithermal upscattering
    - >500 pcm bias may be bigger than the covariance based uncertainty
    - Cannot be used for the PWR simulation