Generation of Subgroup Weights by Extended Fitting Using Region-wise Resonance Cross Sections

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Subgroup Method Background

Resonance Treament Method in Lattice Physics Codes

- One of the major methods with the Equivalence Theory
- Interpin effect is treated by performing explicit transport calculations(SubGroup Fixed Source Problem), which makes it possible to consider space-dependent resonance self-shielding as well.
- Reasonably accurate with much fewer groups than Ultrafine Energy Group Calculation methods.
- Subgroup parameters should be pre-generated.
  - Physical Probability Table approach
  - Mathematical Probability Table approach

$$\sigma_{eff,x,g}^{SG} = \sum_{n=1}^{N} \frac{\omega_{x,g,n}\sigma_{x,g,n}\sigma_{b,n}}{\sigma_{a,g,n}+\sigma_{b,n}} \Big/ \sum_{n=1}^{N} \frac{\omega_{g,n}\sigma_{b,n}}{\sigma_{a,g,n}+\sigma_{b,n}}$$

Physical Probability Table Approach (nTRACER)

- A set of **effective XSs** are fitted through subgroup parameters.
  - Homogeneous one .vs. Heterogeneous one
- **"Slowing down" effect** is incorporated.

Mathematical Probability Table Approach

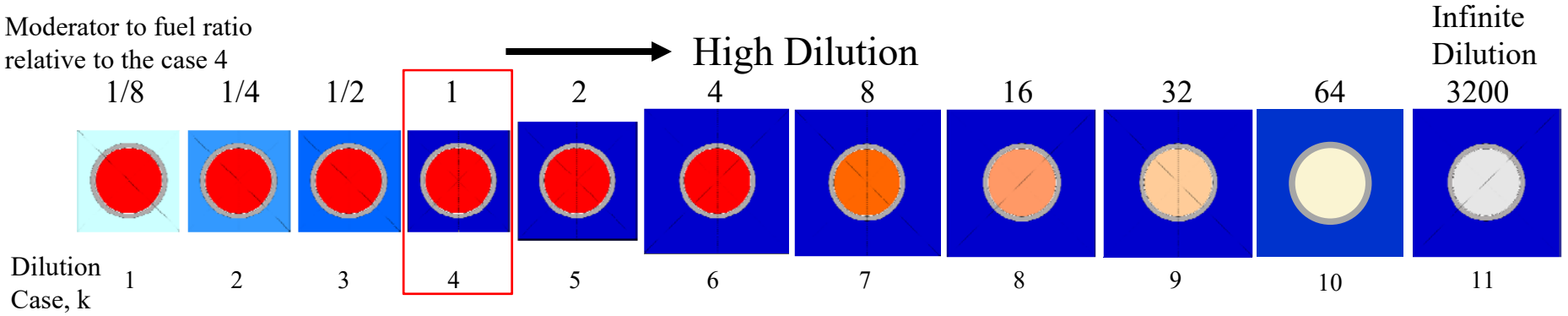
- Subgroup parameters are chosen in such a way that a set of moments of a cross section is preserved.

$$m_{x,g,p} = \frac{\int_{E_g}^{E_{g-1}} dE\sigma(E)^p}{\int_{E_g}^{E_{g-1}} dE} = \sum_{n=1}^{N} \sigma_{x,g,n}^{p}\omega_{x,g,n} \quad for \quad p = 0, \dots, 2N-1$$

Subgroup Parameter Generation in SNU

☐ Physical Probability Table Approach

- **Fits subgroup parameters (levels & weights) over effective XSs of 2-D heterogeneious pin-cells at various dilutions.**



- **Methametical Statement :**

Fit $\bar{\sigma}^{ref}_{eff,g,k}$, k = 1 … K by determining subgroup parameters, σ_g, ω_g, by

minimizing $$F_g(\boldsymbol{\sigma_g}, \boldsymbol{\omega_g}) = \sum_{k=1}^{K}\left(1-\frac{\sigma^{SG}_{eff,g,k}}{\bar{\sigma}^{ref}_{eff,g,k}}\right)^2 = \sum_{k=1}^{K}\left(1-\frac{1}{\bar{\sigma}^{ref}_{eff,g,k}}\sum_{n=1}^{N}\frac{\omega_{g,n}\sigma_{g,n}\sigma_{b,n,k}}{\sigma_{a,g,n}+\sigma_{b,n,k}}\Big/\sum_{n=1}^{N}\frac{\omega_{g,n}\sigma_{b,n,k}}{\sigma_{a,g,n}+\sigma_{b,n,k}}\right)^2$$

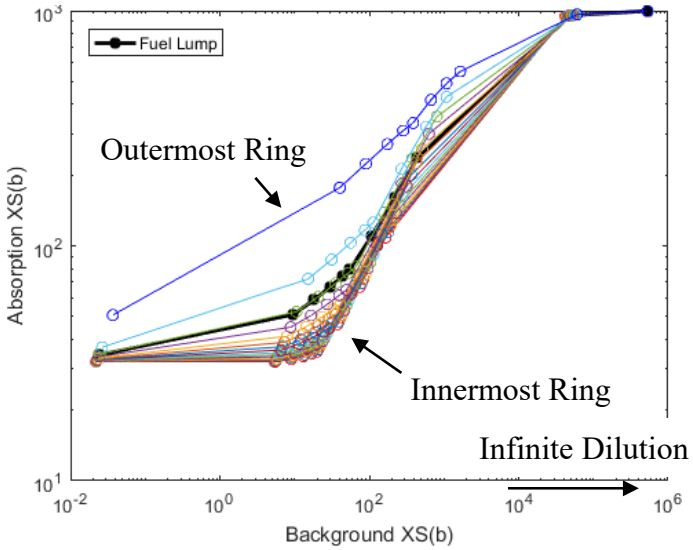
with the Simulated Annealing method(for level) and the Lagrange Multiplier method(for weight).

→ $\boldsymbol{\sigma_g}$ *and* $\boldsymbol{\omega_g}$ lose their physical meaning. They are just a parameter solution of the least square method.

Limitation of the Current Method

☐ S.G. Parameter Fitting only to Pellet Average XS

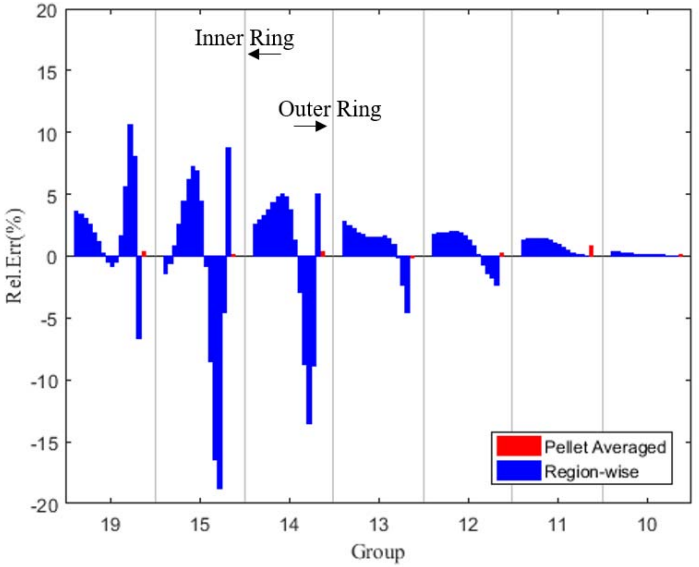
U238 Absorption Effective XSs over 11 Dilutions in G19



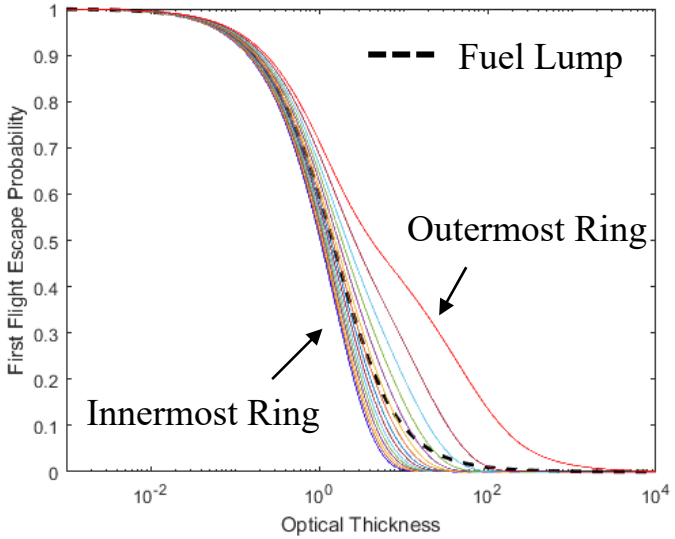
$\sigma_{a,eff}$

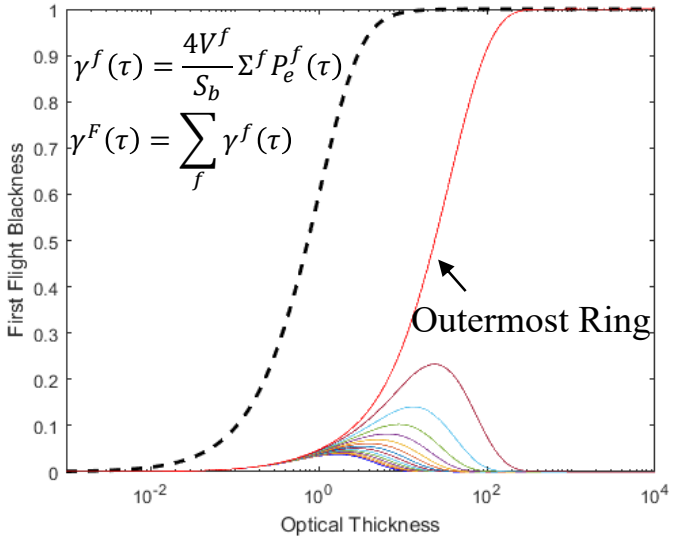
$$\sigma_b = \sigma_{a,eff} \frac{\phi}{1-\phi}$$

U238 Absorption Effective XS Errors in Major Resonance Groups



Different Behavior of Region-wise Escape Probability





$\tau \to \infty, \gamma \to 1$

For fuel lump & outermost ring

$\tau \to \infty, \gamma \to 0$

$(\gamma \to e^{-X\tau})$

For inner rings

- In the Equivalence Theory, the fuel to fuel first flight collision probability is approximated by a rational form.

$$P_{ff}(\tau) \sim 1 - e^{-\tau} \Rightarrow \sum_{n=1}^{N} \beta_n \frac{\tau}{\tau + \alpha_n}$$

$(\sum_{n=1}^{N} \beta_n = 1)$ for black limit of P_{FF}

$(\sum_{n=1}^{N} \alpha_n \beta_n = 1)$ for black limit of $\frac{dP_{FF}}{d\tau}$

$$\gamma(\tau) = \tau P_{esc,f}(\tau) \Rightarrow \sum_{n=1}^{N} \beta_n \frac{\alpha_n \tau}{\tau + \alpha_n} \longrightarrow$$

Cannot achieve exponential decay behavior of partial blackness of inner regions!

Subgroup Method in Multi-region Problem

- In the Subgroup method, the fuel to fuel first flight collision probability is just converted to a rational form, and escape XS (escape probability) is explicitly evaluated through SGFSP.

$$P_{FF}(\tau) = \frac{\tau}{\tau + a(\tau)} \quad \rightarrow \quad P_{esc}^{F}(\tau) = \frac{a^{F}(\Sigma^{F})/l^{F}}{\Sigma^{F} + a^{F}(\Sigma^{F})/l^{F}} = \frac{\Sigma_{e}^{F}(\Sigma^{F})}{\Sigma^{F} + \Sigma_{e}^{F}(\Sigma^{F})}$$

$$l^{F} = average\ chord\ length$$

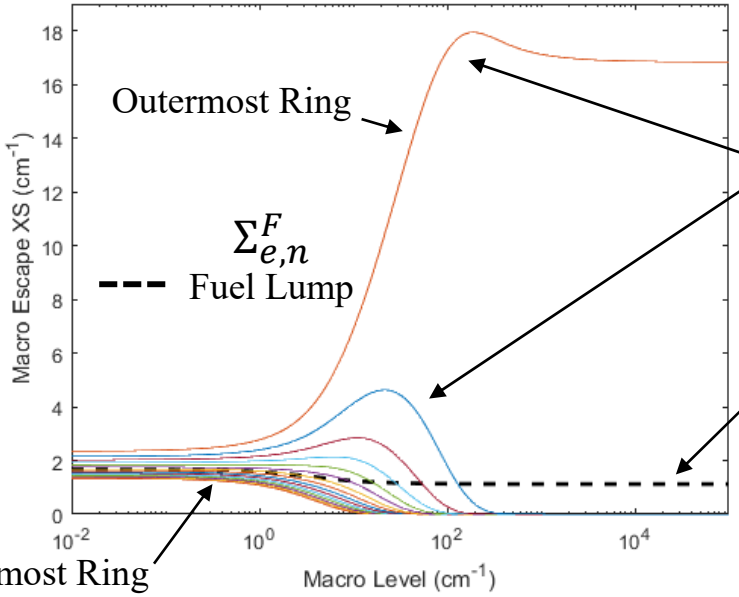
- Likewise, the same form of escape probability is used for all sub-regions.

$$P_{esc}^{f}(\tau) = \frac{a^{f}(\Sigma^{F})/l^{F}}{\Sigma^{F} + a^{f}(\Sigma^{F})/l^{F}} = \frac{\Sigma_{e}^{f}(\Sigma^{F})}{\Sigma^{F} + \Sigma_{e}^{f}(\Sigma^{F})}$$

Different Function!

$$\Sigma_{e,n}^{f} = \frac{\frac{S_b}{4V^f}\gamma^f \Sigma_n}{\Sigma_n - \frac{S_b}{4V^f}\gamma^f}$$

$$\Sigma_n \rightarrow \infty, \Sigma_{e,n}^{f} \rightarrow \frac{S_b}{4V^f}\gamma^f$$



New Approach

Original Function : $$F_g(\boldsymbol{\sigma_g}, \boldsymbol{\omega}_g) = \sum_{k=1}^{K} \left(1 - \frac{\sigma_{eff,g,k}^{(F)SG}(\boldsymbol{\sigma_g}, \boldsymbol{\omega}_g)}{\bar{\sigma}_{eff,g,k}^{(F)ref}} \right)^2$$

☐ Region-wise Subgroup Weights Scheme

Modified Function : $$F_g(\boldsymbol{\sigma_g}, \{f \in F | \boldsymbol{\omega}_g^f\}) = \sum_{f \in F} w_g^f \sum_{k=1}^{K} \left(1 - \frac{\sigma_{eff,g,k}^{(f)SG}(\boldsymbol{\sigma_g}, \boldsymbol{\omega}_g^f)}{\bar{\sigma}_{eff,g,k}^{(f)ref}} \right)^2$$

- **Rationale : Mathematical weights, $\boldsymbol{\omega}_g$, IS NOT PHYSICALLY A WEIGHT, BUT JUST A PARAMETER in the least square method.**
- Advantage : # of parameters ↑ → **Accurate**
- Shortcoming : There should be a provision for the spatial interpolation of weigths in the usage step.

☐ Extended Fitting Scheme

Modified Function : $$F_g(\boldsymbol{\sigma_g}, \boldsymbol{\omega}_g) = \sum_{f \in F} \sum_{k=1}^{K} \left(1 - \frac{\sigma_{eff,g,k}^{(f)SG}(\boldsymbol{\sigma_g}, \boldsymbol{\omega}_g)}{\bar{\sigma}_{eff,g,k}^{(f)ref}} \right)^2$$

$$\sigma_{eff,x,g}^{(f)SG} = \frac{\sum_{n=1}^{N} \frac{\omega_{x,g,n} \sigma_{x,g,n} \sigma_{b,n}^{(f)}}{\sigma_{a,g,n} + \sigma_{b,n}^{(f)}}}{\sum_{n=1}^{N} \frac{\omega_{a,g,n} \sigma_{b,n}^{(f)}}{\sigma_{a,g,n} + \sigma_{b,n}^{(f)}}}$$

- **Rationale : Region-wise effective XSs are used with region-wise escape XSs.**
- Advantage : Simple implementation

Optimization Result (U238 Absorption)

RMS(Root Mean Square) Error * (%)

Group	Reg. Wgt.	Ext. Fit.
10	0.08	0.09
11	0.09	0.26
12	**0.13**	**1.05**
13	**0.27**	**1.50**
14	**0.16**	**1.15**
15	**0.26**	**1.23**
16	0.00	0.00
17	0.01	0.01
18	0.01	0.01
19	**0.13**	**1.53**
20	0.10	0.44
21	0.02	0.01
22	0.01	0.00
23	0.01	0.00
24	0.01	0.00
25	0.01	0.00

$$* \; RMS\ Error_g = \sqrt{\frac{\sum_{f \in F}^{N} \sum_{k=1}^{K} \left(1 - \frac{\sigma_{eff,g,k}^{(f)SG}}{\bar{\sigma}_{eff,g,k}^{(f)ref}} \right)^2}{K \cdot N}}$$

Obviously “Reg. Wgt.” scheme is better for fitting.

Stoker Weiss Approach Implementation for Comparison

☐ Combination with Subgroup Method

- **Fuel Average XS : by Subgroup Method**
- **Intra-pellet Correction : by Stoker-Weiss[1] Method**

$$\sigma_g^{(f)} = \sigma_g^{(F)SG} \boxed{\frac{\sigma_g^{(f)SW}}{\sigma_g^{(F)SW}}}$$

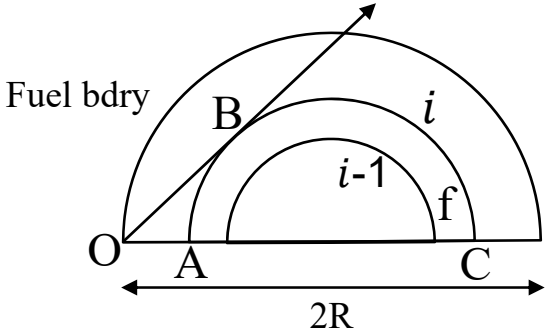
Inter-pin Dancoff Effect

Intra-pin Correction

1) C. Stoker and Z. Weiss, "Spatially Dependent Resonance Cross Sections In a Fuel Rod," Ann. Nucl. Energy, 23, 765 (1996)

※ Stoker-Weiss Method

- Correct region-wise escape probabilities as follow by utilizing the additivity of blackness.



γ_i = (Fraction of incoming neutrons which see the "OAB" or "OBC" region) $\times (\gamma_{OBC}^i - \gamma_{OAB}^i)$

$$\gamma^{(f)} = \gamma_i - \gamma_{i-1} = \rho_i(\gamma_{OBC}^i - \gamma_{OAB}^i) - \rho_{i-1}(\gamma_{OBC}^{i-1} - \gamma_{OAB}^{i-1})$$

$$P_e^{(f)} = \frac{S_b}{4V_f}\frac{1}{\Sigma_f}\gamma^{(f)} = \frac{\rho_i}{\rho_i^2 - \rho_{i-1}^2}\frac{1}{\bar{l}_F}\left(\bar{l}_{BC}^i \sum_{n=1}^{N}\beta_n \frac{\alpha_n/l_{BC}^i}{\Sigma + \alpha_n/l_{BC}^i} - \bar{l}_{AB}^i \sum_{n=1}^{N}\beta_n \frac{\alpha_n/l_{AB}^i}{\Sigma + \alpha_n/l_{AB}^i}\right) - \frac{\rho_{i-1}}{\rho_i^2 - \rho_{i-1}^2}\frac{1}{\bar{l}_F}\left(\bar{l}_{BC}^{i-1} \sum_{n=1}^{N}\beta_n \frac{\alpha_n/l_{BC}^{i-1}}{\Sigma + \alpha_n/l_{BC}^{i-1}} - \bar{l}_{AB}^{i-1} \sum_{n=1}^{N}\beta_n \frac{\alpha_n/l_{AB}^{i-1}}{\Sigma + \alpha_n/l_{AB}^{i-1}}\right)$$

$$= \sum_{m=1}^{4} F_m \sum_{n=1}^{N} \beta_n \frac{\alpha_n/l_m}{\Sigma + \alpha_n/l_m} \qquad \left(\sum_{m=1}^{4} F_m = 1, \sum_{n=1}^{N} \beta_n = 1\right)$$

$$\sigma_{x,g,f} = \frac{\sum_{m=1}^{4} F_m \sum_{n=1}^{N} \beta_n I_{x,g}(\sigma_{bnm})}{1 - \sum_{m=1}^{4} F_m \sum_{n=1}^{N} \beta_n \frac{I_{a,g}(\sigma_{bnm})}{\sigma_{bnm}}}$$

nTRACER Pin-cell Calculation

☐ Problem Description

- **0.7w/o UOX Pin-cell (to minimize resonance interference effect)**
- **OPR1000 Pin-cell Geometry**
- **HZP (600K at all regions)**

☐ Calculation Condition

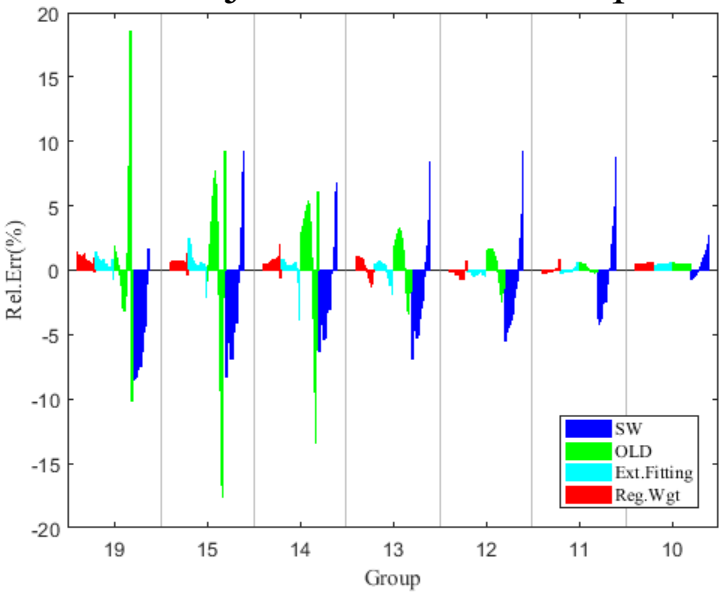
- **nTRACER (Direct Whole Core MG Transport code in SNU)**
  - Ray spacing : 0.01/ # of azimuthal angles in a quadrant : 32/ # of polar angles in the upper hemisphere : 4
  - 15 equi-volumetric subrings in a fuel
  - Resonance interference treatment : RIFL method by UNIST (S.Y.Choi)
  - Resonance MG XS angle dependency treatment : PSSL method by SNU (H.Park)
- **McCARD (C.E. Monte Carlo code in SNU)**
  - 20,000 particles/cycle, 500/50 active/inactive cycles

0.7% UOX Pin-cell Reactivity Result

Code		K-eff	Δρ (pcm)	Δρ Component (pcm)		
McCARD		0.88491	±9	Thermal	Resonance	Fast
nTRACER	S.W.	0.88486	-6	-33	+26	+4
	Old	0.88389	-130	-35	-100	+9
	Ext. Fit.	0.88448	-55	-34	-23	+6
	Reg. Wgt.	0.88401	-115	-36	-84	+8

nTRACER Pin-cell Result Comparison

U238 Absorption Effective XS Errors in Major Resonance Groups



"Reg.Wgt." does not have more benefits than "Ext.Fit.", because "Reg.Wgt." should provide a proper spatial interpolation method for region-wise subgroup weights.

Pellet Average Absorption XS Error (%)

Grp.	S.W.	Old	Ext.Fit.	Reg.Wgt.
10	0.47	0.48	0.46	0.51
11	0.09	0.13	0.04	0.06
12	-0.17	-0.11	-0.30	-0.21
13	-0.31	0.10	-0.31	0.01
14	-0.33	0.73	-0.44	0.58
15	-0.01	0.60	0.12	0.47
19	-2.95	0.46	0.21	0.58

Much Better

RMS Error (%) of Region-wise Absorption XSs

Grp.	S.W.	Old	Ext.Fit.	Reg.Wgt.
10	1.10	0.48	0.47	0.51
11	3.65	0.32	0.24	0.30
12	4.24	1.48	0.30	0.44
13	4.44	2.44	0.77	0.81
14	4.25	5.86	1.13	0.85
15	5.73	8.11	1.15	0.69
19	6.22	7.47	0.74	0.93

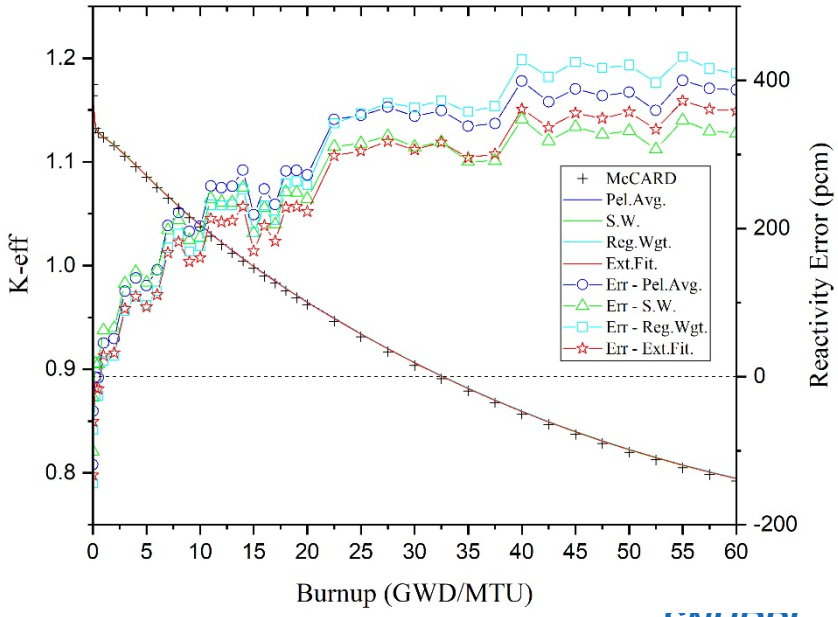
nTRACER Pin-cell Burnup Calculation

☐ Problem Description

- **VERA 1C HFP Pin-cell (No T-H Feedback)**

☐ Calculation Condition

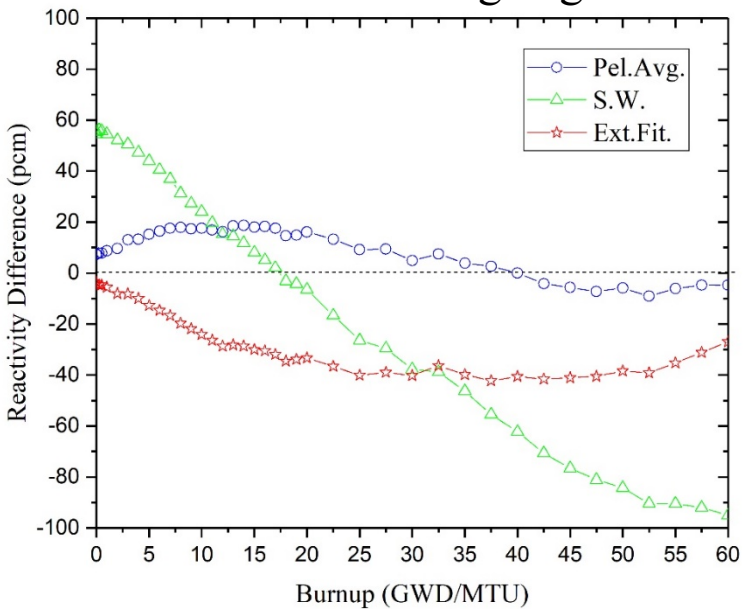
- **nTRACER**
  - Ray spacing : 0.01/ # of azimuthal angles in a quadrant : 32/ # of polar angles in the upper hemisphere : 4
  - Depletion : Krylov subspace
  - 373 isotopes, 238 fission products, 8 fissionable isotopes
  - Resonance interference treatment : RIFL method by UNIST (S.Y.Choi)
  - Resonance MG XS angle dependency treatment : PSSL method by SNU (H.Park)
- **McCARD**
  - 100,000 particles/cycle, 100/20 active/inactive cycles
  - Depletion : Exponential Matrix
  - 1307 isotopes, 880 fission products, 31 fissionable isotopes
- **Common**
  - 15 equi-volumetric subrings in a fuel
  - Transient Xe



SNURPL

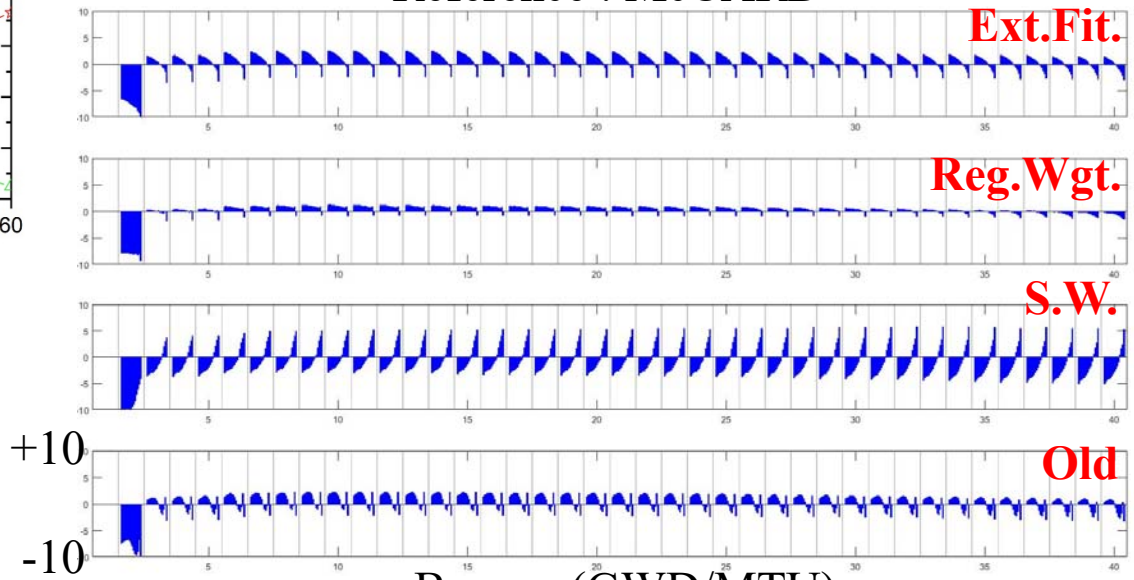
nTRACER Pin-cell Burnup Result Comparison

Reactivity Difference (pcm)
Reference : “Reg.Wgt.”



- The ‘Ext.Fit.’ result is as good as the “Reg.Wgt” one as well as the “Old” one..
- ‘S.W.’ burns faster due to stronger rim effect.

Region-wise Pu239 Number Density Error(%) over Burnup
Reference : McCARD



SNURPL

Conclusion

☐ Limitation of the Current Subgroup Method

- Inconsistency of the escape XS behavior between in the subgroup parameter generation step and in the usage step induces large region-wise effective XS errors.

☐ Suggestion of Extended Fitting Scheme

- **With only one set of subgroup parameters, region-wise effective XSs were successfully evaluated by using region-wise reference effective XSs with corresponding region-wise escape XSs in the fitting.**
- As accurate as region-wise subgroup weights scheme.
- Obviously better than Stoker Weiss (SDDM) method in the Equivalence Theory both for steady state and burnup calculations.