Journal of Computational Physics 330 (2017) 134–155

Contents lists available at ScienceDirect

Journal of Computational Physics

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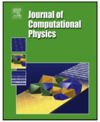

Resonance treatment using pin-based pointwise energy slowing-down method

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Guillermo Ibarra

Nuclear Engineering Research Seminar, April 28th, 2020

Introduction

- Equivalence theory used resonance calculations.
- Cao reported overestimation of multi-group ^{238}U absorption XS (2015).
- Present paper proposes a new resonance self-shielding method using a pointwise energy slowing-down solution (PSM).

Equivalence Theory

Transport equation with collision probabilities:

$$\Sigma_{t,F}(E)\phi_F(E)V_F = P_{FF}V_F Q_{s,F}(E) + P_{MF}(E)V_M Q_{s,M}(E), \tag{1}$$

Equivalence Theory

Transport equation with collision probabilities:

$$\Sigma_{t,F}(E)\phi_F(E)V_F = P_{FF}V_FQ_{s,F}(E) + P_{MF}(E)V_MQ_{s,M}(E), \tag{1}$$

where

$$Q_{s,F}(E) = \sum_{r\in F} N^r \int_E^{E/\alpha^r} \sigma_s^r(E')\phi_F(E')\frac{1}{1-\alpha^r}\frac{dE'}{E'} \tag{2}$$

$$Q_{s,M}(E) = \sum_{r\in M} N^r \int_E^{E/\alpha^r} \sigma_s^r(E')\phi_M(E')\frac{1}{1-\alpha^r}\frac{dE'}{E'} \tag{3}$$

Scattering Source

IR approximation

$$\int_{E}^{E/\alpha^r} \sigma_s^r(E')\phi_F(E')\frac{1}{1-\alpha^r}\frac{dE'}{E'} \approx \lambda^r \sigma_p^r \frac{1}{E} + (1-\lambda^r)\sigma_s^r(E)\phi_F(E), \tag{4}$$

$$\int_{E}^{E/\alpha^r} \sigma_s^r(E')\phi_M(E')\frac{1}{1-\alpha^r}\frac{dE'}{E'} \approx \lambda^r \sigma_p^r \frac{1}{E} \tag{5}$$

Updated Collision Probabilities

Rewriting Eq. 1 using the approximate scattering source and a reciprocity theorem:

$$\Sigma_{t,F}(E)\phi_F(E)V_F = P_{FF}\left[\lambda_F\Sigma_{p,F}\frac{1}{E} + (1-\lambda_F)\Sigma_{s,F}(E)\phi_F(E)\right] + P_{FM}(E)\Sigma_{t,F}(E)V_F\frac{1}{E}, \tag{6}$$

Updated Collision Probabilities

Rewriting Eq. 1 using the approximate scattering source and a reciprocity theorem:

$$\Sigma_{t,F}(E)\phi_F(E)V_F = P_{FF}\left[\lambda_F\Sigma_{p,F}\frac{1}{E} + (1-\lambda_F)\Sigma_{s,F}(E)\phi_F(E)\right] + P_{FM}(E)\Sigma_{t,F}(E)V_F\frac{1}{E}, \tag{6}$$

where $\lambda_X\Sigma_{p,X} = \sum_{r\in X}\lambda^r N^r\sigma_p^r$, ($X = F$ or M); and the reciprocity theorem:

$$P_{FM}(E)\Sigma_{t,F}(E)V_F = P_{MF}(E)\Sigma_{t,M}V_M \approx P_{MF}(E)\lambda_M\Sigma_{p,M}V_M. \tag{7}$$

Updated Collision Probabilities

Rewriting Eq. 1 using the approximate scattering source and a reciprocity theorem:

$$\Sigma_{t,F}(E)\phi_F(E)V_F = P_{FF}\left[\lambda_F\Sigma_{p,F}\frac{1}{E} + (1-\lambda_F)\Sigma_{s,F}(E)\phi_F(E)\right] + P_{FM}(E)\Sigma_{t,F}(E)V_F\frac{1}{E}, \tag{6}$$

where $\lambda_X\Sigma_{p,X} = \sum_{r\in X}\lambda^r N^r\sigma_p^r$, $(X = F$ or $M)$; and the reciprocity theorem:

$$P_{FM}(E)\Sigma_{t,F}(E)V_F = P_{MF}(E)\Sigma_{t,M}V_M \approx P_{MF}(E)\lambda_M\Sigma_{p,M}V_M. \tag{7}$$

Then, fuel-to-fuel collision probability is approximated by rational equation:

$$P_{FF}(E) = 1 - P_{FM}(E) = \sum_{n=1}^{N}\frac{\beta_n\Sigma_{t,F}(E)}{\Sigma_{t,F}(E)+\alpha_n\Sigma_e}, \tag{8}$$

Total Flux

Using a multi-term rational approximation, total flux is formulated as a linear combination:

$$\phi_F(E) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(E) = \sum_{n=1}^{N} \beta_n \frac{\lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e}{\Sigma_{a,F}(E) + \lambda_F \Sigma_{rs,F}(E) + \lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e} \frac{1}{E}, \quad (9)$$

Total Flux

Using a multi-term rational approximation, total flux is formulated as a linear combination:

$$\phi_F(E) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(E) = \sum_{n=1}^{N} \beta_n \frac{\lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e}{\Sigma_{a,F}(E) + \lambda_F \Sigma_{rs,F}(E) + \lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e} \frac{1}{E}, \tag{9}$$

Dividing by N^r

$$\phi_F(E) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(E) = \sum_{n=1}^{N} \beta_n \frac{\sigma^r_{b,n}}{\sigma^r_a(E) + \lambda^r \sigma^r_{rs}(E) + \sigma^r_{b,n}} \frac{1}{E}, \tag{10}$$

Total Flux

Using a multi-term rational approximation, total flux is formulated as a linear combination:

$$\phi_F(E) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(E) = \sum_{n=1}^{N} \beta_n \frac{\lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e}{\Sigma_{a,F}(E) + \lambda_F \Sigma_{rs,F}(E) + \lambda_F \Sigma_{p,F} + \alpha_n \Sigma_e} \frac{1}{E}, \tag{9}$$

Dividing by N^r

$$\phi_F(E) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(E) = \sum_{n=1}^{N} \beta_n \frac{\sigma^r_{b,n}}{\sigma^r_a(E) + \lambda^r \sigma^r_{rs}(E) + \sigma^r_{b,n}} \frac{1}{E}, \tag{10}$$

with the background XS:

$$\sigma^r_{b,n} = \frac{1}{N^r}(\lambda_F \Sigma_{p,F} + \alpha \Sigma_e). \tag{11}$$

Lethargy Form

$$\phi_F(u) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(u) = \sum_{n=1}^{N} \beta_n \frac{\sigma_{b,n}^r}{\sigma_a^r(u) + \lambda_r^r \sigma_s^r(u) + \sigma_{b.n}^r} \tag{12}$$

Multi-group XS definition:

$$\sigma_{x,g} = \frac{\int_{\Delta u_g} \sigma_x^r(u)\phi_F(u)du}{\int_{\Delta u_g} \phi_F(u)du} = \frac{\int_{\Delta u_g} \sigma_x^r(u)\sum_{n=1}^{N} \beta_n \frac{\sigma_{b.n}}{\sigma_a^r(u)+\sigma_{b.n}} du}{\int_{\Delta u_g} \sum_{n=1}^{N} \beta_n \frac{\sigma_{b.n}}{\sigma_a^r(u)+\sigma_{b.n}} du}$$

$$= \frac{\sum_{n=1}^{N} \beta_n \int_{\Delta u_g} \sigma_x^r(u) \frac{\sigma_{b.n}}{\sigma_a^r(u)+\sigma_{b.n}} du}{\sum_{n=1}^{N} \beta_n \int_{\Delta u_g} \frac{\sigma_{b.n}}{\sigma_a^r(u)+\sigma_{b.n}} du} = \frac{\sum_{n=1}^{N} \beta_{n,g} \sigma_{x,n,g}^r(u)\phi_{n,g}}{\sum_{n=1}^{N} \beta_{n,g}\phi_{n,g}} \tag{13}$$

Lethargy Form

$$\phi_F(u) = \sum_{n=1}^{N} \beta_n \phi_{F,n}(u) = \sum_{n=1}^{N} \beta_n \frac{\sigma^r_{b,n}}{\sigma^r_a(u) + \lambda^r_{r s}(u) + \sigma^r_{b.n}} \tag{12}$$

Multi-group XS definition:

$$\begin{aligned}\sigma_{x,g} &= \frac{\int_{\Delta u_g} \sigma^r_x(u)\phi_F(u)du}{\int_{\Delta u_g} \phi_F(u)du} = \frac{\int_{\Delta u_g} \sigma^r_x(u) \sum_{n=1}^{N} \beta_n \frac{\sigma_{b.n}}{\sigma^r_a(u)+\sigma_{b.n}} du}{\int_{\Delta u_g} \sum_{n=1}^{N} \beta_n \frac{\sigma_{b.n}}{\sigma^r_a(u)+\sigma_{b.n}} du} \\ &= \frac{\sum_{n=1}^{N} \beta_n \int_{\Delta u_g} \sigma^r_x(u) \frac{\sigma_{b.n}}{\sigma^r_a(u)+\sigma_{b.n}} du}{\sum_{n=1}^{N} \beta_n \int_{\Delta u_g} \frac{\sigma_{b.n}}{\sigma^r_a(u)+\sigma_{b.n}} du} = \frac{\sum_{n=1}^{N} \beta_{n,g} \sigma^r_{x,n,g}(u) \phi_{n,g}}{\sum_{n=1}^{N} \beta_{n,g} \phi_{n,g}}\end{aligned} \tag{13}$$

where,

$$\sigma^r_{x,n,g} = \sigma^r_{x,g}\left(\sigma^r_{b,n,g}\right), \quad x = a, s, f, \tag{14}$$

$$\phi_{n,g} = \phi_g\left(\sigma^r_{b,n,g}\right) = \frac{\sigma^r_{b,n,g}}{\sigma^r_{a,n,g} + \sigma^r_{b,n,g}} \tag{15}$$

$$\sigma^r_{b,n,g} = \frac{1}{N^r}\left(\sum_r \lambda^r_g N^r \sigma^r_p + \alpha_{n,g}\Sigma_e\right) \tag{16}$$

Resonance Integral Form

$$\sigma^r_{x,g} = \frac{\sum_{n=1}^{N} \beta_{n,g} RI^r_{x,n,g}}{1 - \sum_{n=1}^{N} \beta_{n,g} \frac{RI^r_{a,n,g}}{\sigma^r_{b,n,g}}}, \tag{17}$$

Resonance Integral Form

$$\sigma^r_{x,g} = \frac{\sum_{n=1}^{N} \beta_{n,g} RI^r_{x,n,g}}{1 - \sum_{n=1}^{N} \beta_{n,g} \frac{RI^r_{a,n,g}}{\sigma^r_{b,n,g}}}, \tag{17}$$

where

$$RI^r_{x,n,g} = \frac{\int_{\Delta u_g} \sigma^r_x(u)\phi_{F,n}(u)du}{\int_{\Delta u_g} du} = RI^r_{x,n}\left(\sigma^r_{b,n,g}\right) = \sigma^r_{x,n,g}\phi_{n,g}. \tag{18}$$

Modified Forms of Equivalence Theory

WIMS

$$\sigma^r_{x,g} = \frac{\sum_{n=1}^{N} \beta_{n,g} RI^r_{x,n,g}}{1 - \sum_{n=1}^{N} \beta_{n,g} \frac{\lambda RI^r_{rs,n,g} + RI^r_{a,n,g}}{\sigma^r_{b,n,g}}}, \tag{19}$$

Modified Forms of Equivalence Theory

Yamamoto

$$\tilde{\sigma}^r_{a,g} \sum_{n=1}^{N} \beta_{n,g} \frac{\sigma^r_{b,n,g}}{\tilde{\sigma}^r_{a,g} + \sigma^r_{b,n,g}} = \sum_{n} \beta_n \frac{\sigma^r_{a,n,g}\sigma^r_{b,n,g}}{\sigma^r_{a,n,g} + \sigma^r_{b,n,g}}, \tag{20}$$

$$\sigma^r_{x,g} = \frac{\sum_{n=1} \beta_{n,g} \sigma^r_{x,n,g} \frac{\sigma^r_{b,n,g}}{\sigma^r_{a,n,g} + \sigma^r_{b,n,g}}}{\sum_{n=1}^{N} \beta_{n,g} \frac{\sigma^r_{b,n,g}}{\tilde{\sigma}^r_{a,g} + \sigma^r_{b,n,g}}} \tag{21}$$

$$\sigma^r_{x,g} = \frac{\sum_{n=1} \beta_{n,g} \sigma^r_{x,n,g} \phi^{SD}_{n,g}}{\sum_{n=1}^{N} \beta_{n,g} \phi^{SD}_{n,g}} \tag{22}$$

Numerical Test with Equivalence Theory

Table 1
Material composition of base pin-cell problem.

Material	Nuclide	Number density (#/barn-cm)
Fuel	^{238}U	2.22265E−02
	^{16}O	4.55881E−02
Moderator	^{1}H	6.67232E−02
	^{16}O	3.33616E−02

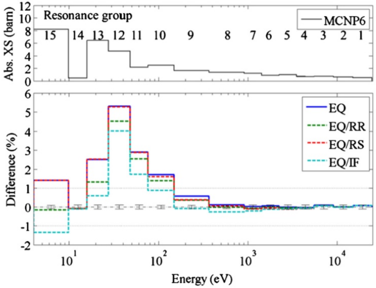

Fig. 1. Comparison of ^{238}U absorption XSs from equivalence theory (base pin-cell problem).

Pointwise Energy Approach

$$\Sigma_{t,F}(u)\phi_F(u) = P_{FF}(u)Q_{s,F} + P_{FM}(u)\Sigma_{t,F}(u) \tag{23}$$

Pointwise Energy Approach

$$\Sigma_{t,F}(u)\phi_F(u) = P_{FF}(u)Q_{s,F} + P_{FM}(u)\Sigma_{t,F}(u) \tag{23}$$

Flux specified as a rational approximation:

$$\phi_F(u) = \sum_{n=1}^{N} \beta_n \frac{Q_{s,F}(u) + \alpha_n \Sigma_e}{\Sigma_{t,F}(U) + \alpha_n \Sigma_e} \tag{24}$$

Pointwise Energy Approach

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Flux specified as a rational approximation:

$$\phi_F(u) = \sum_{n=1}^{N} \beta_n \frac{Q_{s,F}(u) + \alpha_n \Sigma_e}{\Sigma_{t,F}(U) + \alpha_n \Sigma_e} \tag{24}$$

Assuming that total flux is a linear combination and the IR approximation:

$$\phi_F(u) = \sum_{n=1}^{N} \beta_n \frac{\lambda \Sigma_{p,F} + \alpha_n \Sigma_e}{\Sigma_{t,F}(U) + \alpha_n \Sigma_e} = \sum_{n=1}^{N} \beta_n \phi_{F,n}(u) \tag{25}$$

Pointwise Energy Approach

separated fluxes

$$\Sigma_{t,F}(u)\phi_{F,n}(u) = \frac{\Sigma_{t,F}(u)}{\Sigma_{t,F}(u) + \alpha_n \Sigma_e} Q_{s,F,n}(u) + \left(1 - \frac{\Sigma_{t,F}(u)}{\Sigma_{t,F}(u) + \alpha_n \Sigma_e}\right), \quad n = 1, \ldots, N, \tag{26}$$

$$\sigma^r_{x,g} = \frac{\int_{\Delta u_g} \sigma^r_x(u) \sum_{n=1}^N \beta_n \phi_{F,n}(u)\, du}{\int_{\Delta u_g} \sum_{n=1}^N \beta_n \phi_{F,n}(u)\, du}, \tag{27}$$

where

$$Q_{s,F,n}(E) = \sum_{r \in F} N^r \int_E^{E/\alpha^r} \sigma^r_s(E')\phi_{F,n}(E') \frac{1}{1-\alpha^r} \frac{dE'}{E'} \tag{28}$$

Pointwise Energy Approach

separated fluxes

$$\Sigma_{t,F}(u)\phi_F(u) = \sum_{n=1}^{N} \beta_n \frac{\Sigma_{t,F}(u)}{\Sigma_{t,F}(u) + \alpha_n \Sigma_e} Q_{s,F}(u) + \left(1 - \sum_{n=1}^{N} \beta_n \frac{\Sigma_{t,F}(u)}{\Sigma_{t,F}(u) + \alpha_n \Sigma_e}\right) \Sigma_{t,F}(u) \tag{29}$$

$$\sigma^r_{x,g} = \frac{\int_{\Delta u_g} \sigma^r_x(u)\phi_F(u)du}{\int_{\Delta u_g} \phi_F(u)du} \tag{30}$$

Difference between fluxes:

$$\phi^S_F(u) - \phi^C_F(u) = \sum_{n=1}^{N} \beta_n \frac{Q_{F,n}(u) - Q_F(u)}{\Sigma_{t,F}(u) + \alpha_n \Sigma_e} \neq 0 \tag{31}$$

Numerical Test with Pointwise Energy Approach

Table 2
Coefficients of three-term rational equation.

n	α_n	β_n
1	1.422510	1.491740
2	3.464850	−0.699455
3	5.131570	0.207720

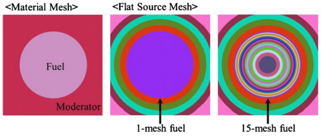

Fig. 2. Flat source mesh divisions of pointwise energy MOC.

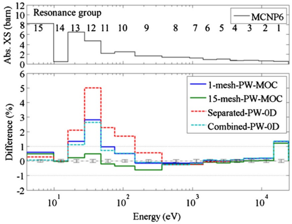

Fig. 3. Comparison of fuel region averaged ^{238}U absorption XSs from pointwise energy approaches (base pin-cell problem).

Numerical Test with Pointwise Energy Approach

Collision Probability

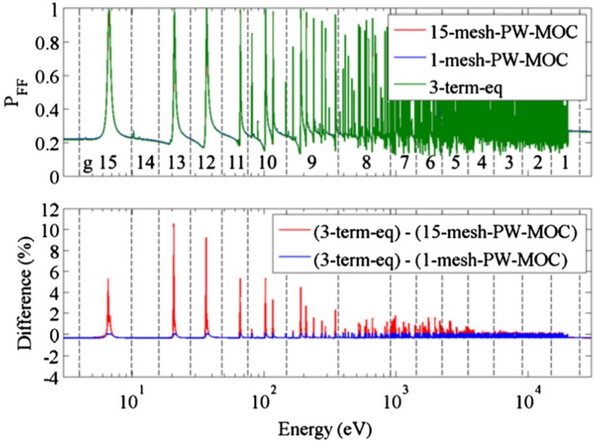

Fig. 4. Comparison of fuel-to-fuel collision probability (base pin-cell problem).

Numerical Test Without Resonance Scattering Cross Section

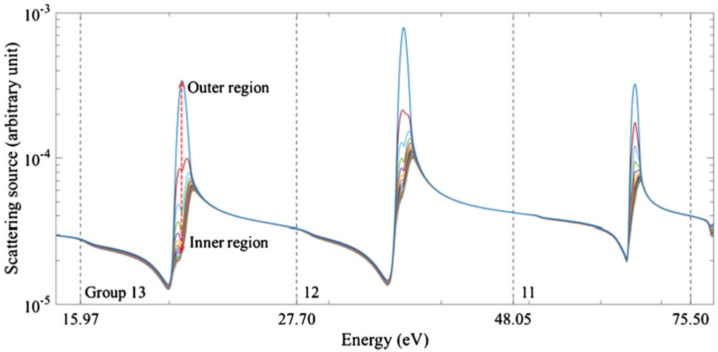

Fig. 5. Scattering source distribution in fuel pellet from 15-mesh-PW-MOC.

Numerical Test Without Resonance Scattering Cross Section

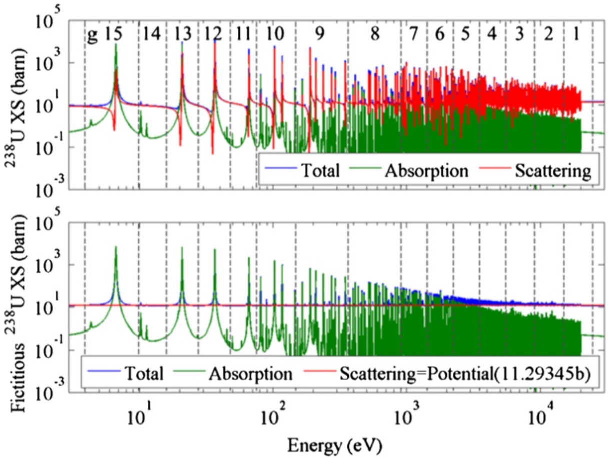

Fig. 6. Cross sections of ^{238}U and fictitious ^{238}U.

Numerical Test Without Resonance Scattering Cross Section

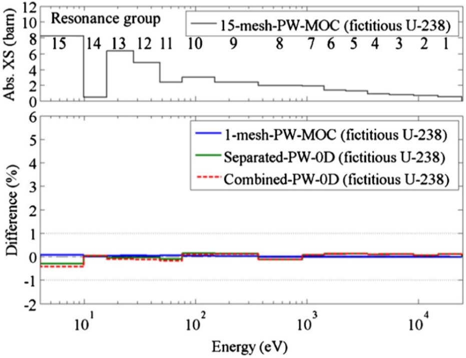

Fig. 7. Comparison of fictitious ^{238}U absorption XSs from pointwise energy approaches (base pin-cell problem).

New Resonance Self-Shielding Method

- Comteporary spatially dependent methods
  - SDDM
  - ESSM
- Pin-based pointwise energy slowing-down method (PSM)

PSM Collision Probability

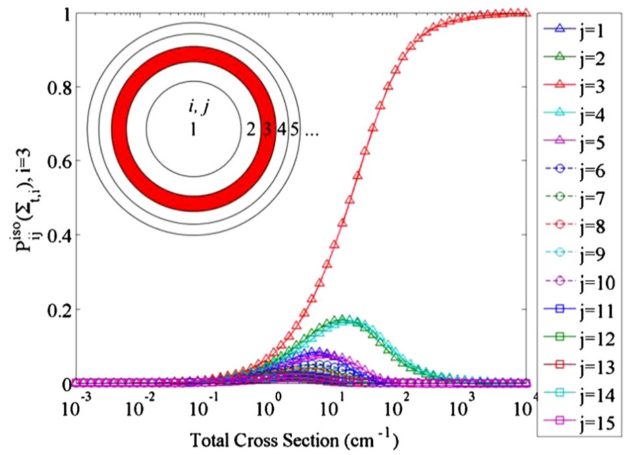

Fig. 8. Example for fuel collision probability of neutron born in submesh 3.

PSM Escape Probability

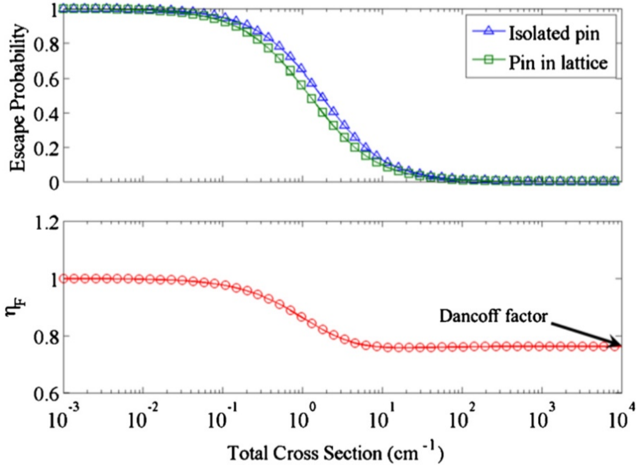

Fig. 9. Example for fuel escape probability of fuel lump and ratio.

PSM Calculation Flowchart

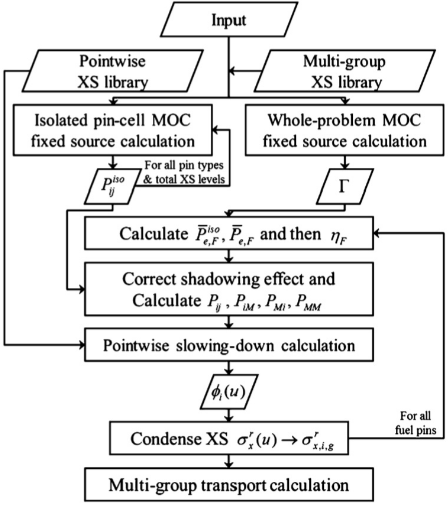

Fig. 10. Flowchart of the pin-based pointwise energy slowing-down solution method.

Verification

base pin problem

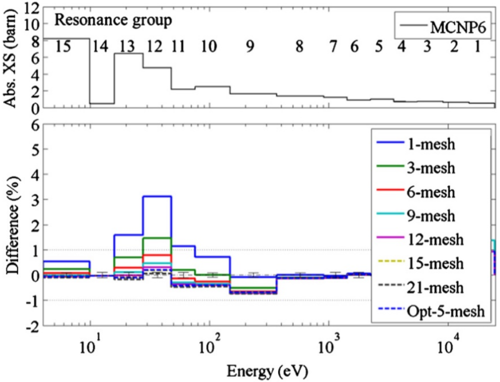

Fig. 11. Comparison of fuel region averaged ^{238}U absorption XS for PSM submesh sensitivity test (base pin-cell problem).

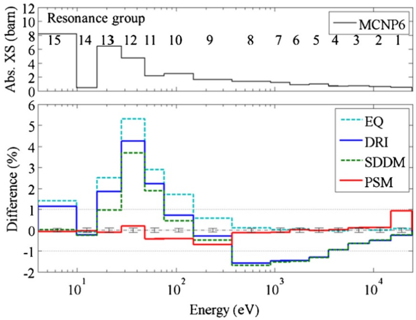

Fig. 12. Comparison of fuel region averaged ^{238}U absorption XS with spatially dependent resonance self-shielding method (base pin-cell problem).

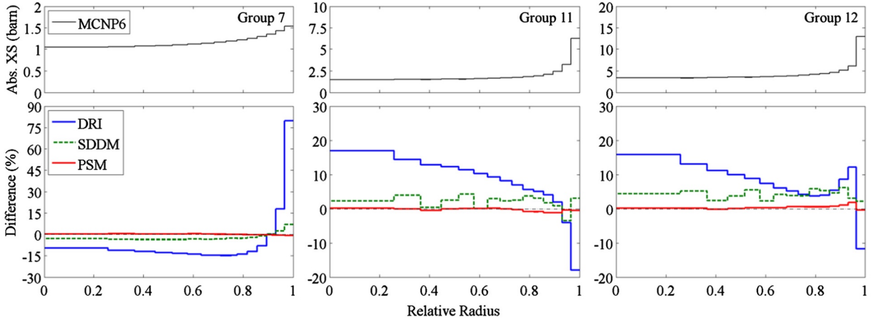

Fig. 13. Comparison of region-wise ^{238}U absorption XS of resonance groups 7, 11 and 12 (base pin-cell problem; relative radius = outer radius of sub-mesh/radius of fuel pellet).

Verification

additional tests

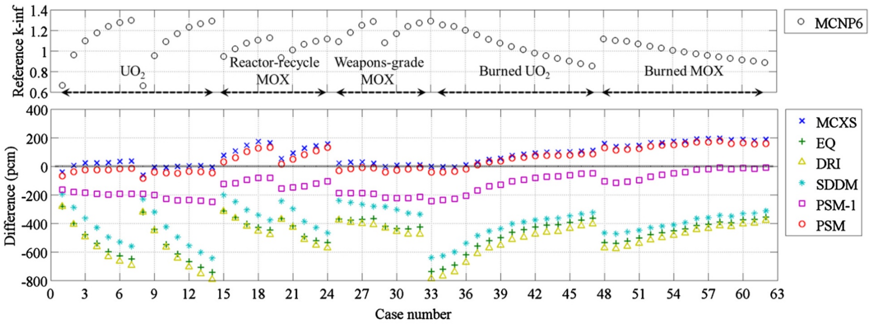

Fig. 14. Pin-cell comparison results.

Verification

additional tests

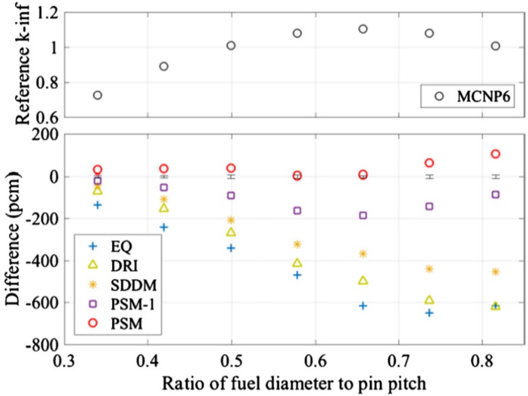

Fig. 15. Sensitivity test result for ratio of fuel diameter to pin pitch.

Verification

additional tests

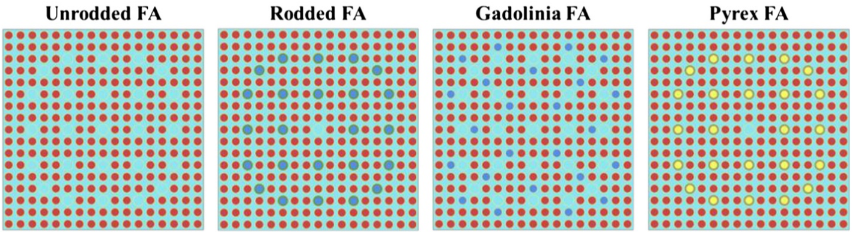

Fig. 16. Configurations of 17 × 17 fuel assembly problems.

Verification

additional tests

Table 3
Unrodded and rodded FA analyses results.

Method	Unrodded FA 3.1 wt.% UO_2 fuel			Rodded FA 3.1 wt.% UO_2 fuel		
	k-inf difference (pcm)	Pin power difference (%) RMS	Max	k-inf difference (pcm)	Pin power difference (%) RMS	Max
MCNP6	1.18309 ±4	±0.07	±0.09	0.78728 ±4	±0.09	±0.09
EQ	−630	0.11	0.30	−264	0.16	0.40
DRI	−634	0.11	0.30	−269	0.16	0.40
SDDM	−492	0.11	0.30	−188	0.16	0.40
PSM-1	−158	0.16	0.50	57	0.19	0.50
PSM	10	0.11	0.30	158	0.17	0.50

Table 4
Gadolinia FA and Pyrex FA analyses results.

Method	Gadolinia FA 3.1 wt.% UO_2 fuel			Pyrex FA 3.1 wt.% UO_2 fuel		
	k-inf difference (pcm)	Pin power difference (%) RMS	Max	k-inf difference (pcm)	Pin power difference (%) RMS	Max
MCNP6	0.92690 ±5	±0.08	±0.09	0.97530 ±4	±0.08	±0.09
EQ	−583	0.11	0.30	−499	0.12	0.40
DRI	−582	0.11	0.30	−505	0.12	0.40
SDDM	−484	0.12	0.30	−395	0.12	0.40
PSM-1	−174	0.12	0.40	−97	0.13	0.40
PSM	8	0.12	0.40	34	0.13	0.40

Comparison of Computing Time

Table 5
Comparison of computing time in 17 × 17 FA analysis between EQ and PSM.

MOC ray condition[a]	Method	Elapsed time (sec)					
		MOC FSP for fuel[b]	MOC FSP for clad[c]	Using MG library[d]	PW energy calculation[e]	XS total[f]	Total[g]
Coarse	EQ	2.3	2.2	1.4	–	8.1	50.9
(0.05/48/3)	PSM	0.2	2.2	0.4	4.9	8.9	51.9
Rigorous	EQ	31.5	29.8	1.4	–	64.8	627.4
(0.01/128/3)	PSM	2.2	29.8	0.3	5.0	38.7	580.9

[a] Ray distance (cm)/the number of azimuthal angels/the number of polar angles.
[b] Elapsed time in whole problem MOC fixed source calculation for the fuel.
[c] Elapsed time in whole problem MOC fixed source calculation for the clad.
[d] Elapsed time in using MG XS and RI look-up table.
[e] Elapsed time for PSM such as pointwise XS interpolation, pointwise flux calculation, XS condensation and etc.
[f] Elapsed time in all of multi-group XS calculations including ‘MOC FSP’, ‘Using MG library’, ‘PW energy calculation’ and etc.
[g] Total elapsed time including multi-group XS calculation and eigenvalue calculation.

Conclusions

- PSM eliminates the limitations of conventional equivalence methods.
- Spatially dependent pointwise energy slowing down equation
- Shadowing effect correction factors
- Good agreement of PSM with MCNP6 ($<$ 100 pcm) and 1% difference in absorption XSs

Thanks!
Questions?