CBZLIB and advanced Bondarenko model

This material is a summary of the following paper:

G. Chiba, et al., "Advanced Bondarenko method for resonance self-shielding calculations in deterministic reactor physics code system CBZ," Ann. Nucl. Energy, 96, p.277-286 (2016).

CBZ and CBZLIB

- CBZ is a general-purpose reactor physics code system being developed at Nuclear Reactor Engineering Laboratory of Hokkaido University.

- CBZ is based on the deterministic method, so multi-group representations for neutron flux and reaction cross sections are adopted.

- CBZLIB is a multi-group library, and is used to calculate multi-group (effective) cross sections of medium in homogeneous and heterogeneous systems.

- CBZLIB is based on the Bondarenko-type library*; it consists of infinite-dilution cross sections, scattering matrices and self-shielding factors dependent on background cross sections.

** Bondarenko, I. I., "Group constants for nuclear reactor calculations," Consultants Bureau, New York (1964).*

Concept of CBZLIB

- Nowadays, advanced energy group structure like SHEM 281-group structure and CASMO 586-group structure has been adopted in many reactor physics code systems.

- When we use these fine-group libraries, energy group collapsing (or condensation) of cross sections is sometimes required in assembly calculations or subsequent whole-core calculations.

- The concept of CBZLIB is to improve calculation accuracy of effective cross sections WITHOUT increasing the number of energy groups; the SRAC-107 group structure is continuously utilized.

Basic theory of the Bondarenko model

- Bondarenko-type libraries are applied to resonance self-shielding calculations based on the equivalence theory.

- The key point of the equivalence theory is how to accurately evaluate background cross sections in arbitrary heterogeneous systems.

- Escape probability from a single fuel pin is generally approximated by the rational approximation.

- Lattice effect can be taken into account by the neutron current method proposed by Yamamoto and Sugimura*.

** N. Sugimura, A. Yamamoto, "Evaluation of Dancoff factors in complicated geometry using the method of characteristics," J. Nucl. Sci. Technol., **43**, p.1182 (2006).*

Escape probability representation in CBZLIB

- Accuracy of the escape probability can be improved by increasing the number of terms considered in the rational approximation: multi-term rational approximation.

- CBZLIB adopts a different approach: Bell factor optimization.

$$\phi^F(E) = \frac{\Sigma_0^F}{\Sigma_t^F(E)}\left(1 - P_{esc}(E)\right) + P_{esc}(E) \quad \Rightarrow \quad \tilde{\phi}^F(E) \propto \frac{1}{\sigma_t^i(E) + \sigma_0 + a/\left(N_i \bar{l}\right)}$$

$$P_{esc}(E) \approx \frac{a}{\bar{l}\Sigma_t^F(E) + a}$$

- Optimized Bell factor a can be calculated so as to satisfy the following equation. The energy integration is carried out by the sub-group method.

$$\frac{\left\langle \sigma_x^i(E)\phi^F(E)\right\rangle}{\left\langle \phi^F(E)\right\rangle} = \frac{\left\langle \sigma_x^i(E)\tilde{\phi}^F(E)\right\rangle}{\left\langle \tilde{\phi}^F(E)\right\rangle}$$

Further improvement in CBZLIB: resonance interference

- Theoretically the equivalence theory cannot consider the resonance interference effect because when one resonant nuclide is a target of calculation, other nuclides are assumed non-resonant.

- The TIMS code can provide self-shielding factors calculated by solving neutron slowing-down equation with considering two different resonant nuclides.

- With this capability, we can consider resonance interference with one-specific other nuclide. Generally resonance interference with uranium-238 are considered.

Further improvement in CBZLIB: resonance interference

- In CBZLIB, a pair of nuclides where resonance interference is considered can be dependent on nuclide and energy group.

- If we need to consider important resonance interferences of several nuclide pairs in the same energy group, multiple correction is adopted:

$$\sigma_g = \left(\prod_{j=1}^{J} \frac{\sigma_g^j}{\sigma_g^{w/oRI}} \right) \cdot \sigma_g^{w/oRI}$$

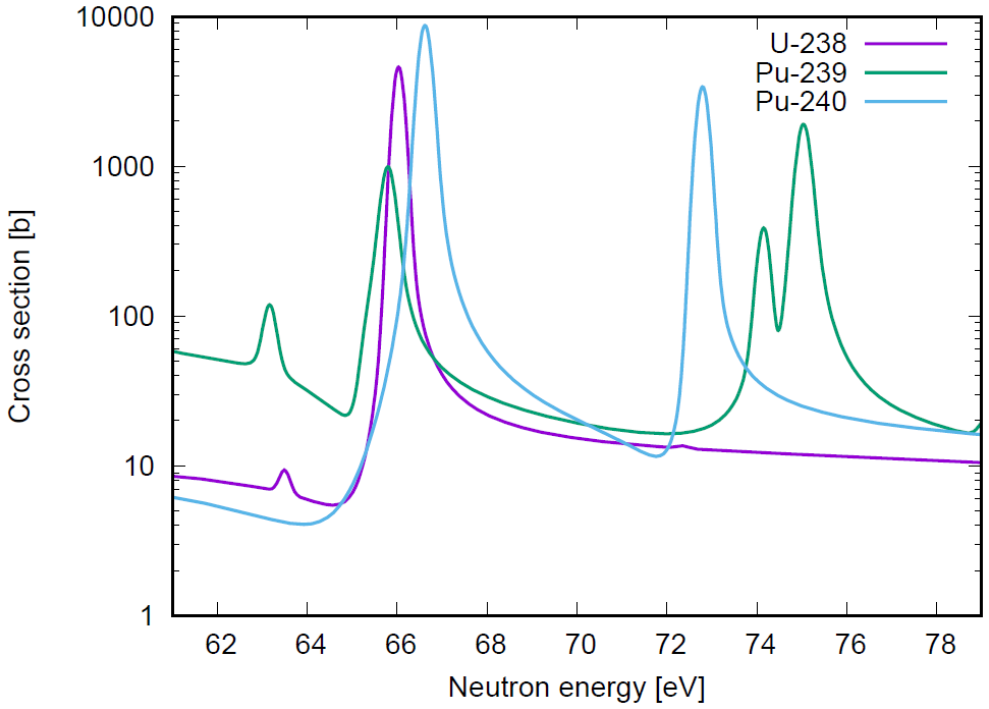
Target nuclides with which resonance interference is taken into account.

Nuclide	Target nuclide (Energy group)
Uranium-235	Uranium-238 (All)
Uranium-238	Uranium-235 (57, 58) Plutonium-240 (48[a], 50, 51, 53) Plutonium-239 (Other groups, 48[a])
Plutonium-239	Plutonium-240 (47, 50[a], 53[a]) Plutonium-241 (53[a], 54, 55, 56) Plutonium-242 (49) Uranium-238 (Other groups, 50[a], 53[a])
Plutonium-240	Plutonium-239 (47, 50) Uranium-238 (Other groups)
Plutonium-241	Plutonium-239 (52, 54, 55, 56) Americium-241 (59) Uranium-238 (Other groups)
Plutonium-242	Plutonium-239 (49) Americium-241 (61) Uranium-238 (Other groups)
Americium-241	Plutonium-241 (59) Uranium-238 (Other groups)

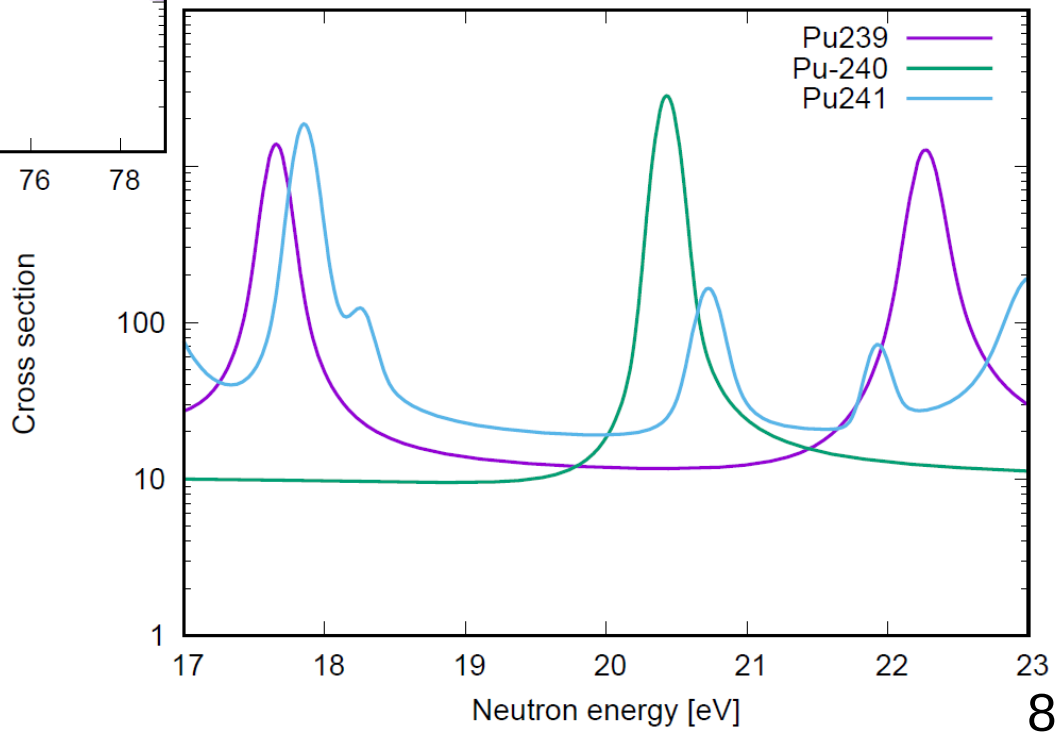
[a] Multiple resonance interference factors are adopted.

Further improvement in CBZLIB: resonance interference

(a) SRAC 48th group (61.4 - 78.9 eV)



(b) SRAC 53th group (17.6 – 22.6 eV)



Further improvement in CBZLIB: current-weight total XS

- It has been well known that neutron current-weighted total cross sections should be considered in energy group collapsing in the neutron transport equation*.

- If we do not consider this, group collapsing errors affect numerical results. To avoid this, the SPH factors are sometimes used.

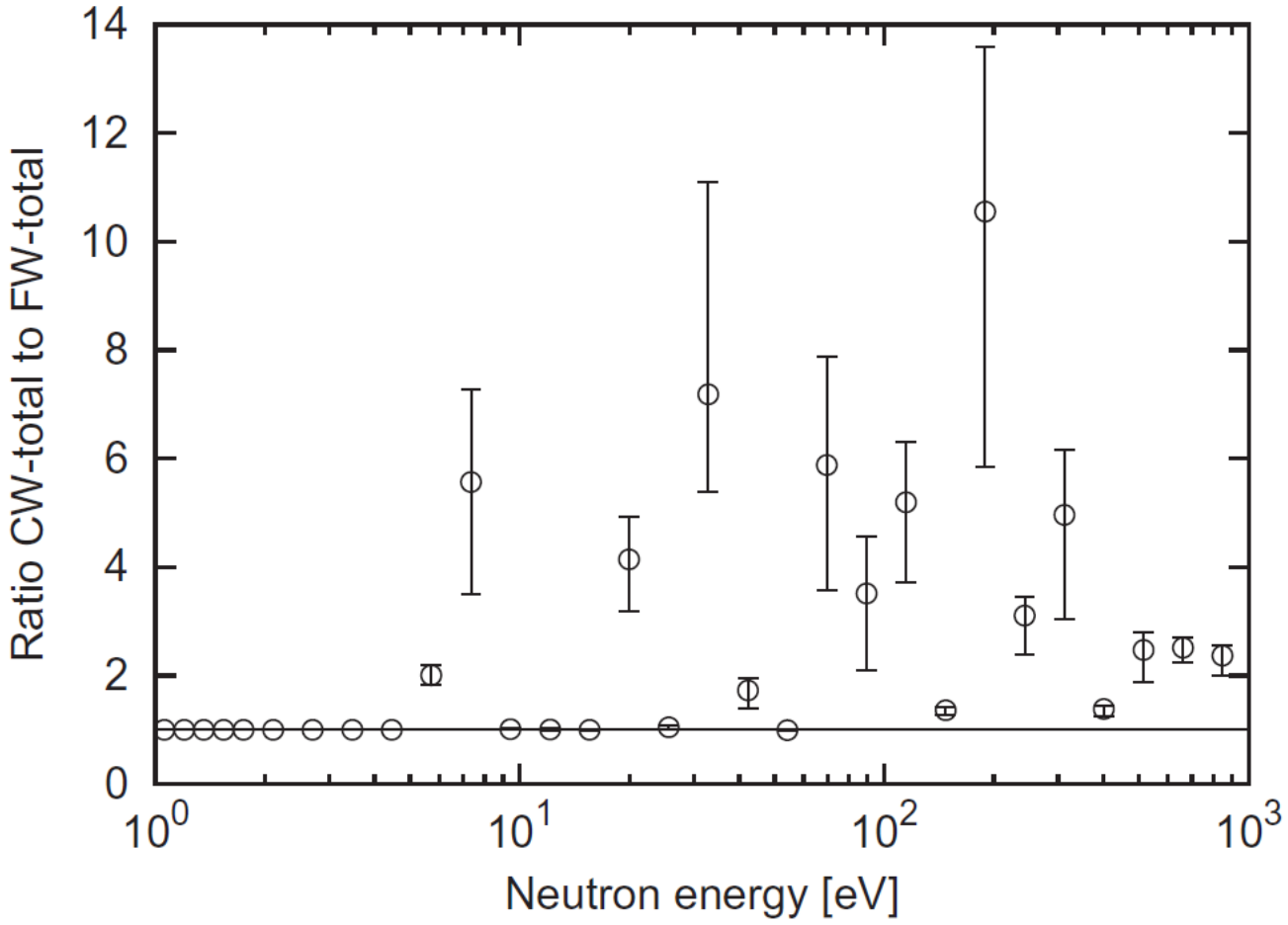
- NJOY can calculate current-weighted total cross sections based on the homogeneous P1 approximation and narrow resonance approximation, but this is applicable to limited problems and not to light water reactor pin-cell problems.

- In CBZLIB, current-weight total cross sections are calculated with some representative pin-cell problems with a fine-group library.

** T. Takeda, T. Kitada, "Direction and region dependent cross sections for use in MOX fuel analysis," J. Nucl. Sci. Technol., Supp.2, p.1057 (2002).*

Further improvement in CBZLIB: current-weight total XS

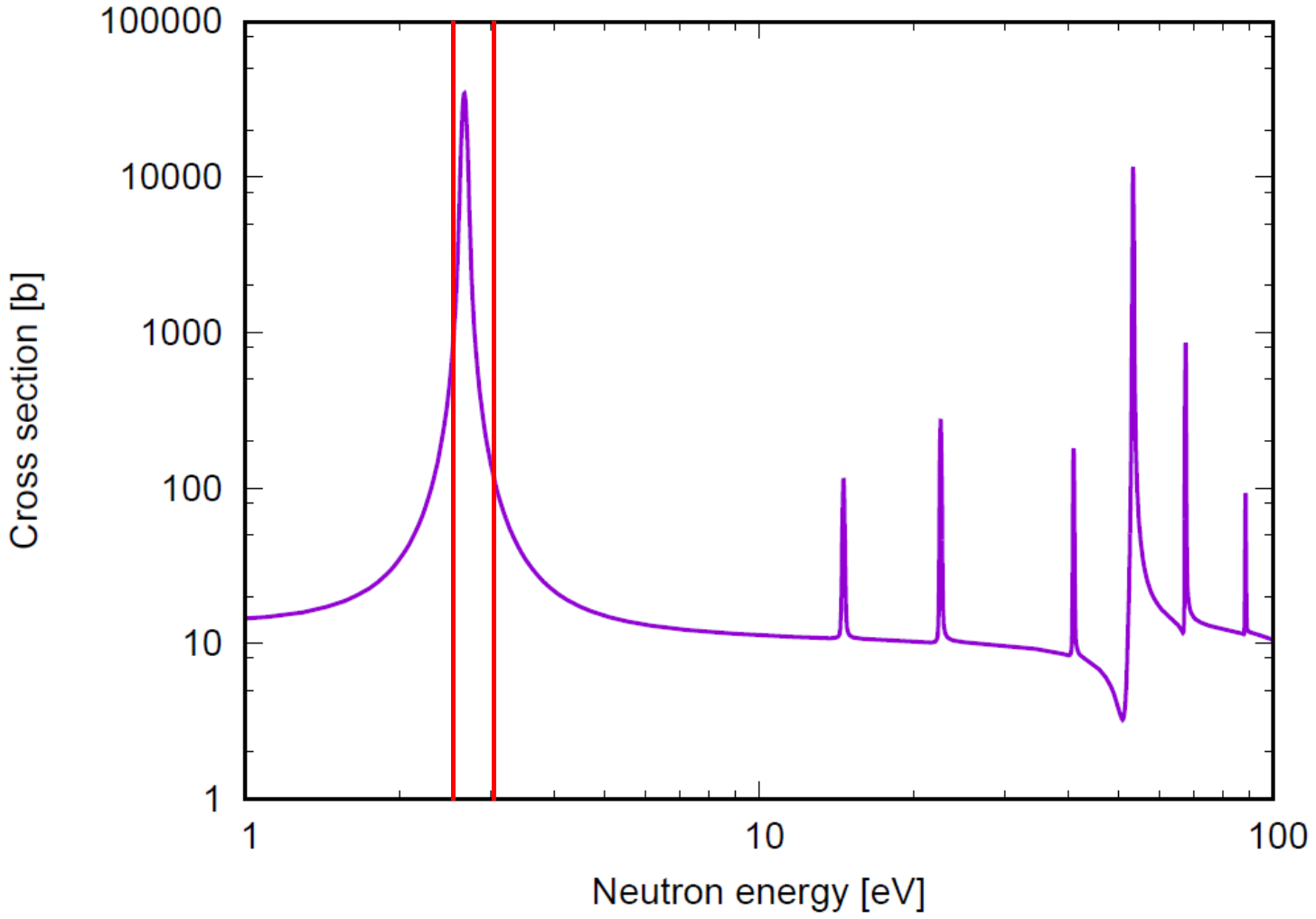
Current-weight total cross sections of U-238 calculated with several different LWR pin-cell models. Error bars show possible ranges.



Average values are implemented to CBZLIB as a correction factor. This means that each of CBZLIB has its specific applicable problems.

Further improvement in CBZLIB: current-weight total XS

In addition to U-238, total cross section of Pu-242 in the 61th group (2.38 – 3.06 eV) is also corrected because of its large impact.



Test of CBZLIB against LWR pin-cell problems

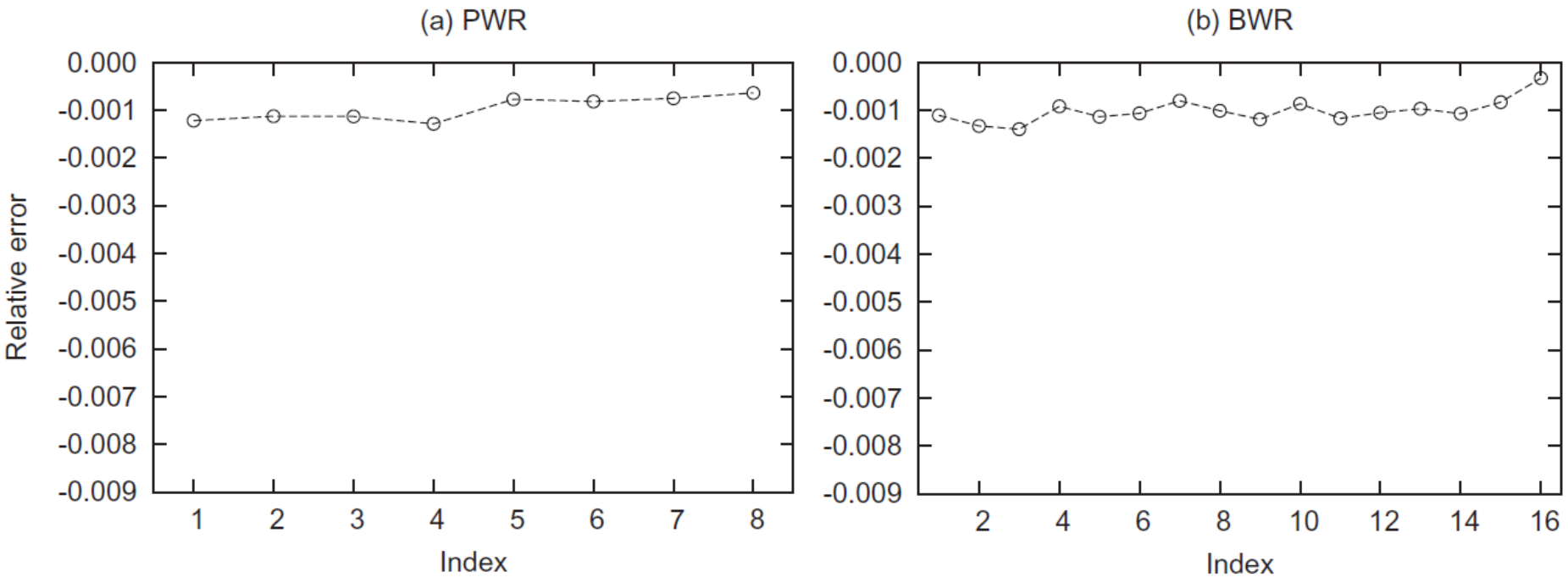
PWR

ID	Fuel type	U-235 enrichment [%]	Pu enrichment [%]	Pu-vector [P8/P9/P0/P1/P2/A1]
1	UO2	3.4		
2	UO2	4.1		
3	UO2	4.7		
4	MOX	0.2	13	4.1/45.4/25.3/9.6/13.0/2.6
5	MOX	0.2	5	2.1/54.5/25.0/9.3/6.4/2.7
6	MOX	0.2	10	2.1/54.5/25.0/9.3/6.4/2.7
7	MOX	0.2	13	2.1/54.5/25.0/9.3/6.4/2.7
8	MOX	0.2	5	0.04/79.24/17.8/2.4/0.4/0.2

BWR

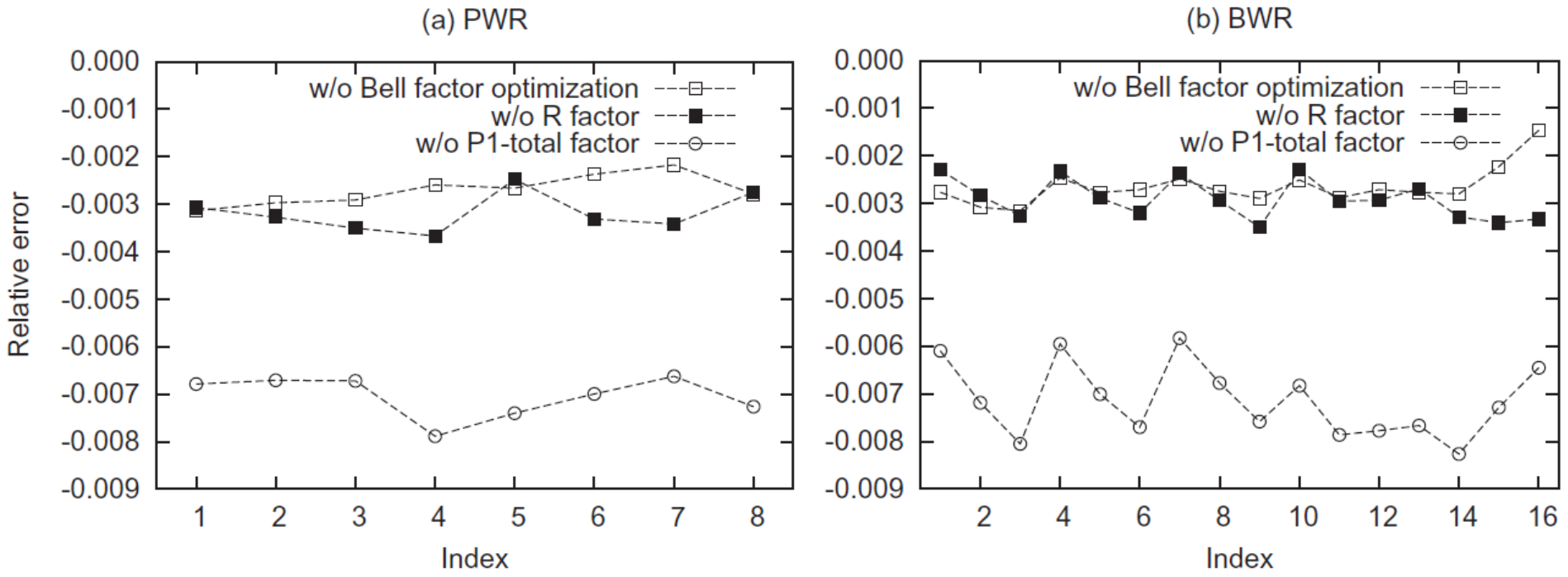
ID	Fuel type	Step	Void ratio [%]	U-235 enrichment [%]	Pu enrichment [%]	Pu-vector [P8/P9/P0/P1/P2/A1]
1	UO2	I	0	3.0		
2	UO2	I	40	3.0		
3	UO2	I	70	3.0		
4	UO2	II	0	3.8		
5	UO2	II	40	3.8		
6	UO2	II	70	3.8		
7	UO2	III	0	4.1		
8	UO2	III	40	4.1		
9	UO2	III	70	4.1		
10	MOX	II	0	0.2	4	1.5/58.7/26.6/8.3/4.0/0.8
11	MOX	II	40	0.2	4	1.5/58.7/26.6/8.3/4.0/0.8
12	MOX	II	40	0.2	4	1.7/53.4/29.7/8.7/5.6/0.9
13	MOX	II	40	0.2	4	0.8/67.8/21.8/6.9/2.1/0.7
14	MOX	II	70	0.2	4	1.5/58.7/26.6/8.3/4.0/0.8
15	MOX	II	70	0.2	8	1.5/58.7/26.6/8.3/4.0/0.8
16	MOX	II	70	0.2	13	1.5/58.7/26.6/8.3/4.0/0.8

Test of CBZLIB against LWR pin-cell problems



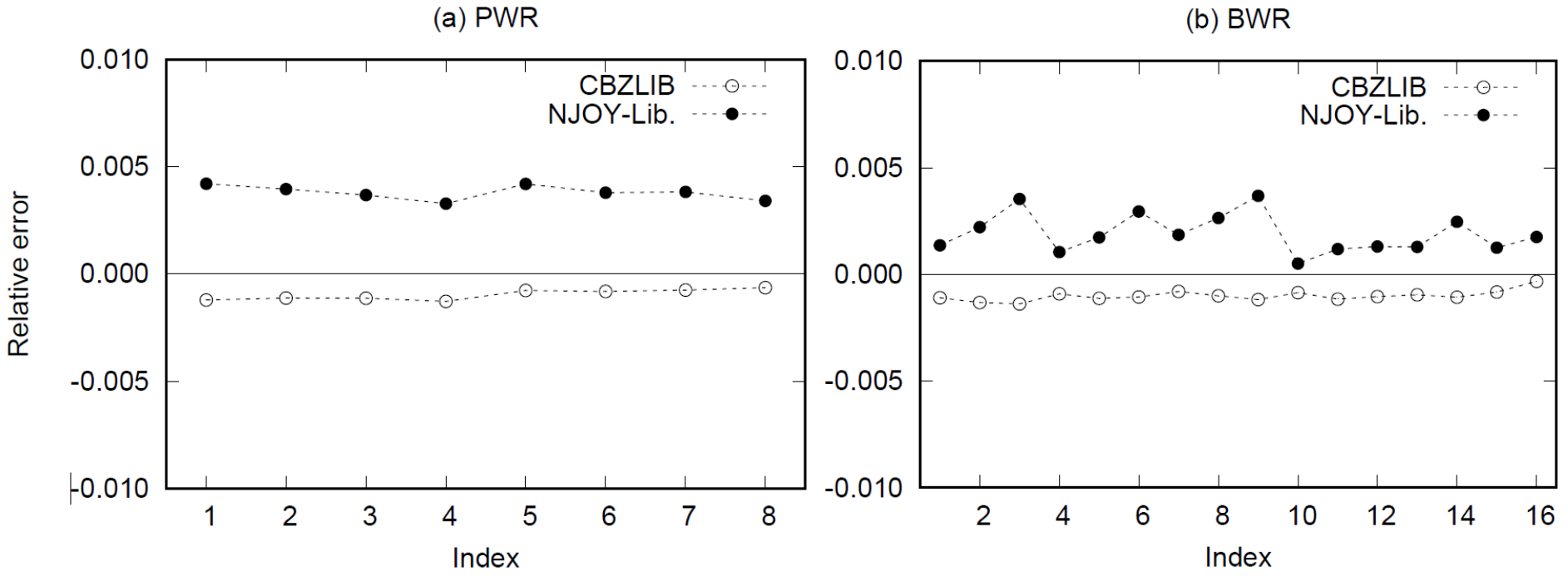
Good agreement with continuous-energy Monte Carlo results is observed in a wide range of LWR pin-cell problems.

Test of CBZLIB against LWR pin-cell problems



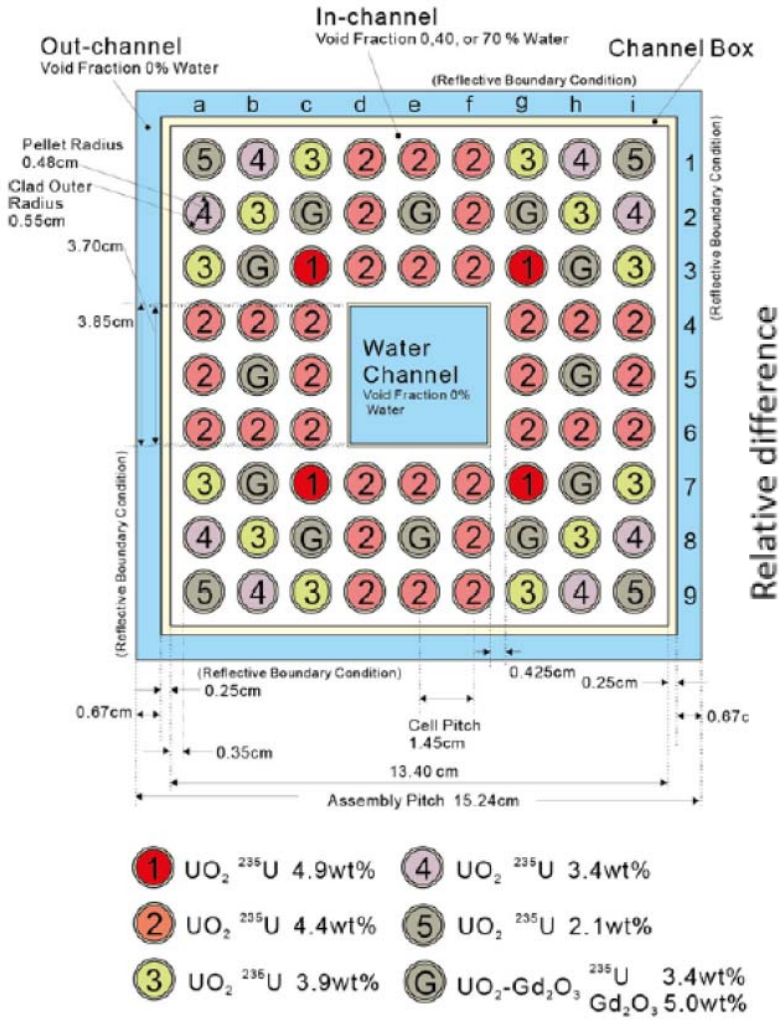
Each of the already-mentioned three techniques has large influence, and current-weight total correction has the most significant impact.

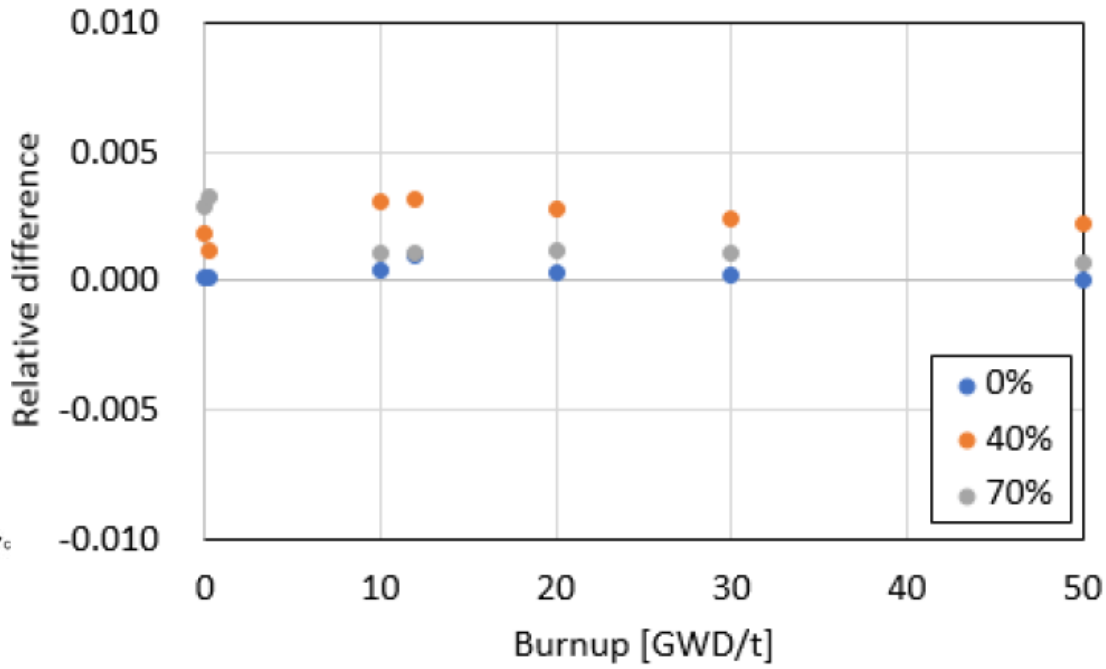
Test of CBZLIB against LWR pin-cell problems



Please be careful that multi-group library generated by NJOY with the NR approximation gives not-bad results as the above.

Test of CBZLIB against BWR assembly problem





Good agreement with MVP-BURN result is obtained in BWR assembly burnup problem.