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A Deterministic Study of the Deficiency of the Wigner-Seitz Approximation for Pu/MOX Fuel Pins

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Abstract

The Wigner-Seitz pin-cell approximation has long been applied as a modeling approximation in analysis of UO_2 lattice fuel cells. In the past, this approximation has been appropriate for such fuel. However, with increasing attention drawn to mixed-oxide (MOX) fuels with significant plutonium content, it is important to understand the implications of the approximation in a uranium-plutonium matrix. The special geometric capabilities of the deterministic NEWT computer code have been used to assess the adequacy of the Wigner-Seitz cell in such an environment, as part of a larger study of computational aspects of MOX fuel modeling. Results of calculations using various approximations and boundary conditions are presented, and are validated by comparison to results obtained using KENO V.a and XSDRNPM.

1 Introduction

Under the auspices of the Nuclear Energy Agency (NEA) of the Organization for Economic Cooperation and Development (OECD), an international Working Group was formed in 1991 for the study of computational phenomena related to burnup credit. Studies involve intercode comparisons for various burnup credit consideration, using a wide variety of codes, methods, and data. Such comparisons serve to highlight potential limitations or deficiencies in the various code systems, data, or modeling methods. The Phase IV-A benchmark specification (Bowden, 1998), distributed to the working group in March 1998, describes calculations to be performed for the analysis of mixed-oxide (MOX) fuel pins in a two-dimensional, infinite lattice configuration.

The MOX computational benchmark included studies of three fuel types: (a) reference (first-generation) MOX derived from LWR UO_2 recycle, (b) MOX enrichment based on disposition of weapons-grade Pu, and (c) later-generation MOX that would result from MOX recycling. For each fuel type, calculations were performed for specific isotopic compositions predicted for various burnup states and cooling times, with different sets of nuclides present. Hence, the benchmark consisted of a total of 63 criticality calculations.

Benchmark calculations based on this specification were performed at the Oak Ridge National Laboratory (ORNL) using three different computer codes: XSDRNPM (Greene, 1995) (1-D discrete ordinates), NEWT (DeHart, 1998) (2-D discrete ordinates with flexible geometry capabilities), and KENO V.a (Petrie, 1995) (3-D Monte Carlo). In addition, calculations were performed using each code with both the 238-group (Greene, 1994) and 44-group (DeHart, 1994) versions of ENDF/B-V data available within the SCALE code system (SCALE, 1995).

It was noted (Santamarina, 1998) at the 1998 meeting of the Burnup Credit Working Group that the Wigner-Seitz approximation for a pin cell in MOX fuel can produce erroneous results. The Wigner-Seitz approximation uses a cylindrical outer boundary and white boundary conditions to replace the square moderator boundary associated with a pin in a square lattice (Lewis, 1984). The exact geometry is depicted in Figure 1(a); the Wigner-Seitz approximation is shown in Figure 1(b). In the Wigner-Seitz equivalent cell, a radius is used such that the volume of the moderator is precisely the same as in the exact cell. White boundary conditions are applied in the approximate model because of computational difficulties associated with reflective boundary conditions on a cylindrical outer boundary. Because the approximation reduces a two-dimensional (2-D) cell to a simpler one-dimensional (1-D) form, it becomes more computational efficient. In the past, this approximation has been found to be acceptable for UO_2 fuel pin-cell modeling.

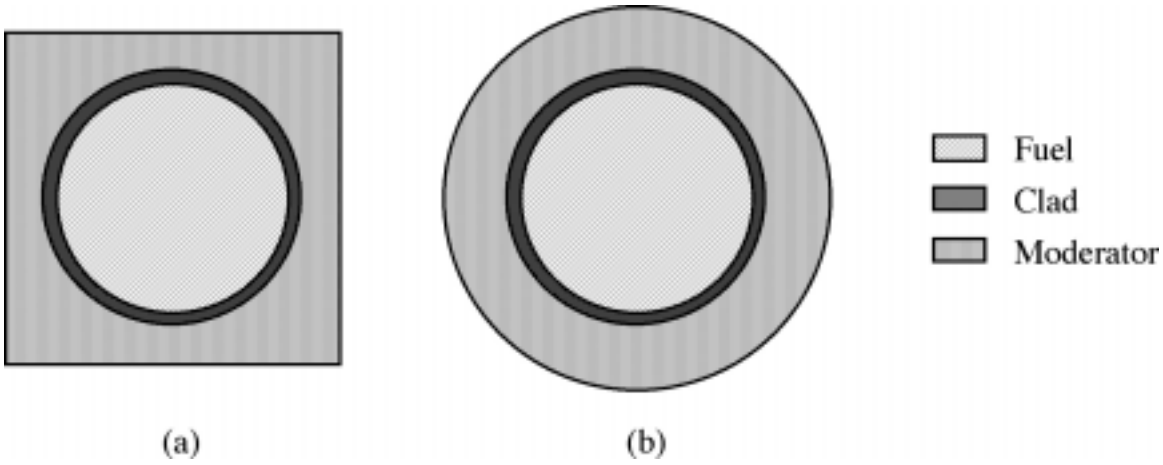

Figure 1. Exact and Wigner-Seitz representations of a pin cell.

To confirm the response of the Wigner-Seitz cell approximation for MOX fuel, and to try to understand the physics of the matter, ORNL volunteered to use various transport solutions available within the SCALE system to study this effect.

2 Approach

ORNL has the unique capability to study the behavior of the pin-cell model based on discrete-ordinates theory, using 1-D XSDRNPM calculations and 2-D NEWT calculations, using identical cross-section data and processing techniques. The 1-D nature of XSDRNPM requires the use of the Wigner-Seitz equivalent cell. In general, this approximation is also necessary in multidimensional discrete-ordinates methods because of the constraints of orthogonal meshing schemes. However, the NEWT transport code allows a flexible, unstructured grid layout, such that the cylindrical fuel/clad region can be very closely approximated within an exact square pin-cell boundary. Figure 2 illustrates a NEWT model for a fuel/clad/moderator pin cell. All computational cells within this model are polygons; irregular (nonrectangular) cells are used to closely approximate curved surfaces. In practice, symmetry would be used to reduce this problem to a 1/4 cell representation of a single quadrant. After NEWT and XSDRNPM calculations were completed, significant discrepancies were noted between results, especially for the SCALE 238-group library. Hence, KENO V.a calculations were performed to assess which method was giving the largest error.

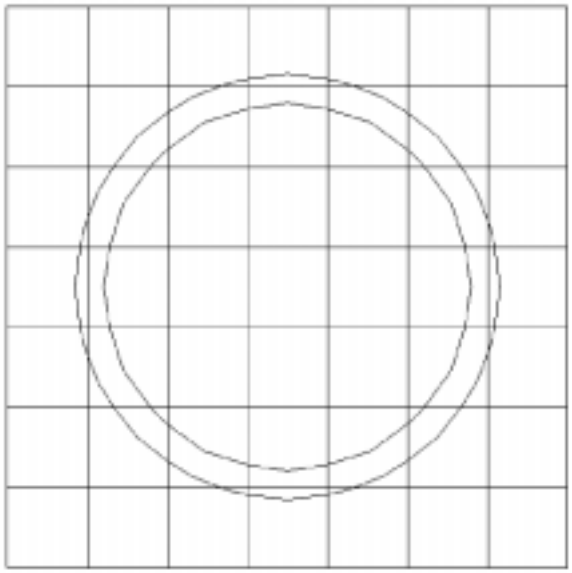

Figure 2. NEWT grid structure for a pin cell.

Results of Benchmark Calculations

Results of the six sets of calculations are listed in Table 1. The discrete-ordinates solutions were performed using S_8 quadrature and P_3 scattering, with convergence criteria of 0.0001; KENO V.a calculations also used P_3 scattering, and were based on 2×10^6 neutron histories. Overall, results show good agreement between NEWT and KENO V.a for each of the two cross-section libraries. Differences between these results for each code and cross-section library are illustrated in Figure 3, which shows the error of each solution relative to the KENO V.a solution for each case. One-sigma error bars are shown for each of the KENO V.a calculations; deterministic calculations have an error term on the order of ±0.0001.

4 Discussion

Figure 3 illustrates significant differences between solutions for the various codes. Because there is no absolute solution, all calculations are compared with 238-group KENO V.a results. This is not meant to imply that KENO provides the best solution; it is simply used as a reference solution for comparison of relative error terms.

The following numerous features are observed in the data of Table 1 and the plots of Figure 3:

- Both NEWT and KENO V.a are in good agreement. On the average, NEWT is 0.098% higher than KENO with the 238-group library. The agreement is improved with the 44-group library, with NEWT being 0.026% higher on the average.
- All calculations show the best agreement for Case B (weapons Pu) fuel. Agreement is not as good for Case A (first-generation recycle), and is worst for Case C (later-generation recycle). The trend mirrors relative concentrations of ^{238}Pu, ^{240}Pu, and ^{242}Pu in the fuels, which are lowest for Case B, higher in Case A, and highest in Case C.
- The change in bias with fuel type relative to the KENO/238-g solution is in a positive direction for all codes and data, with the exception of the 238-g XSDRNPM solution, which is in a negative direction.

- There are definite group structure effects: 44-group calculations show more variation with burnup than 238-group calculations, relative to KENO 238-group calculations. The relative error increases with increasing burnup.
- The largest variation between 238-group and 44-group results is seen for cases with no fission products and *all* actinides. The error is significantly larger than for cases with no fission products and *major* actinides. This group structure effect must therefore be due to treatment of curium nuclides.
- The XSDRNPM 238-group calculations are on the average 0.47% lower than corresponding 44-group XSDRNPM calculations and 0.48% lower than KENO 238-group calculations. The 44-group XSDRNPM solutions average 0.22% less than average 44-group KENO solutions.

Differences between 44-group and 238-group libraries are most likely the result of differences between the group structures in the SCALE libraries. Although the broad-group structure of the 44-group library retains much of the thermal range structure of its parent 238-group library, lower energy resonances in plutonium may not be properly captured. In addition, the 44-group library was collapsed from the 238-group library, assuming a fresh-fuel UO_2 pin spectrum. This collapsing spectrum may be inadequate to capture the effects of high concentrations of plutonium in MOX fuels.

Table 1. ORNL Phase IV-A results submitted to OECD Burnup Credit Working Group

Case No.	XSDRNPM 44-group	NEWT 44-group	KENO V.a 44-group	XSDRNPM 238-group	NEWT 238-group	KENO V.a 238-group
1	1.2947	1.2980	1.2979(4)*	1.2916	1.2989	1.2978(5)
2	1.1779	1.1807	1.1802(4)	1.1741	1.1807	1.1795(4)
3	1.1081	1.1107	1.1108(4)	1.1041	1.1103	1.1093(4)
4	1.0523	1.0546	1.0543(4)	1.0480	1.0538	1.0527(4)
5	1.2385	1.2415	1.2413(4)	1.2342	1.2412	1.2406(4)
6	1.2013	1.2039	1.2041(4)	1.1961	1.2028	1.2017(4)
7	1.1728	1.1751	1.1755(4)	1.1669	1.1732	1.1724(4)
8	1.2386	1.2416	1.2416(4)	1.2340	1.2411	1.2407(4)
9	1.2033	1.2060	1.2053(4)	1.1975	1.2042	1.2027(4)
10	1.1795	1.1819	1.1812(4)	1.1724	1.1788	1.1778(4)
11	1.1317	1.1345	1.1345(4)	1.1278	1.1343	1.1333(4)
12	1.0519	1.0544	1.0542(4)	1.0480	1.0539	1.0539(4)
13	0.9882	0.9903	0.9908(3)	0.9843	0.9896	0.9891(4)
14	1.1955	1.1987	1.1985(4)	1.1908	1.1978	1.1957(4)
15	1.1514	1.1541	1.1537(4)	1.1461	1.1527	1.1516(4)
16	1.1196	1.1220	1.1217(4)	1.1138	1.1199	1.1196(4)
17	1.1957	1.1989	1.1983(4)	1.1908	1.1979	1.1968(4)
18	1.1538	1.1566	1.1563(4)	1.1480	1.1547	1.1539(4)
19	1.1274	1.1299	1.1301(4)	1.1206	1.1269	1.1259(4)
20	1.4162	1.4180	1.4182(4)	1.4102	1.4154	1.4146(4)
21	1.2221	1.2239	1.2242(4)	1.2189	1.2243	1.2239(4)
22	1.1106	1.1123	1.1122(3)	1.1078	1.1129	1.1129(4)
23	1.0322	1.0337	1.0341(4)	1.0290	1.0337	1.0322(4)
24	1.2918	1.2937	1.2934(4)	1.2884	1.2942	1.2934(5)

Table 1 (continued)

Case No.	XSDRNPM 44-group	NEWT 44-group	KENO V.a 44-group	XSDRNPM 238-group	NEWT 238-group	KENO V.a 238-group
25	1.2160	1.2176	1.2180(4)	1.2129	1.2182	1.2172(4)
26	1.1667	1.1678	1.1676(4)	1.1623	1.1674	1.1675(4)
27	1.2918	1.2937	1.2937(4)	1.2884	1.2941	1.2933(4)
28	1.2164	1.2180	1.2170(4)	1.2131	1.2184	1.2176(4)
29	1.1694	1.1705	1.1700(4)	1.1645	1.1696	1.1688(4)
30	1.1958	1.1975	1.1971(4)	1.1924	1.1976	1.1972(4)
31	1.0623	1.0639	1.0641(3)	1.0595	1.0643	1.0639(4)
32	0.9706	0.9719	0.9722(3)	0.9676	0.9719	0.9715(4)
33	1.2699	1.2719	1.2725(4)	1.2662	1.2719	1.2720(4)
34	1.1766	1.1784	1.1780(4)	1.1733	1.1785	1.1777(4)
35	1.1192	1.1203	1.1195(3)	1.1147	1.1197	1.1188(4)
36	1.2699	1.2720	1.2718(4)	1.2662	1.2719	1.2703(4)
37	1.1771	1.1789	1.1785(4)	1.1736	1.1788	1.1781(4)
38	1.1222	1.1234	1.1235(4)	1.1173	1.1223	1.1217(4)
39	1.1887	1.1927	1.1911(4)	1.1866	1.1948	1.1931(4)
40	1.1063	1.1101	1.1091(4)	1.1013	1.1090	1.1070(4)
41	1.0633	1.0669	1.0665(4)	1.0574	1.0646	1.0628(4)
42	1.0271	1.0304	1.0299(4)	1.0208	1.0277	1.0261(4)
43	1.1067	1.1105	1.1096(4)	1.1013	1.1090	1.1080(4)
44	1.0683	1.0720	1.0713(4)	1.0613	1.0687	1.0675(5)
45	1.0407	1.0443	1.0440(4)	1.0329	1.0401	1.0383(4)
46	1.1590	1.1630	1.1627(4)	1.1531	1.1613	1.1591(5)
47	1.1448	1.1485	1.1477(4)	1.1372	1.1450	1.1437(4)
48	1.1335	1.1368	1.1364(4)	1.1249	1.1324	1.1306(4)
49	1.1594	1.1634	1.1625(4)	1.1530	1.1611	1.1593(4)
50	1.1496	1.1535	1.1526(4)	1.1407	1.1487	1.1471(4)
51	1.1470	1.1506	1.1497(4)	1.1364	1.1442	1.1423(4)
52	1.0530	1.0567	1.0569(4)	1.0482	1.0556	1.0539(4)
53	1.0035	1.0069	1.0067(4)	0.99802	1.0050	1.0039(4)
54	0.9622	0.9653	0.9656(3)	0.9565	0.9630	0.9617(4)
55	1.0536	1.0574	1.0575(4)	1.0485	1.0560	1.0546(4)
56	1.0093	1.0129	1.0118(4)	1.0029	1.0100	1.0085(4)
57	0.9772	0.9806	0.9799(3)	0.9702	0.9770	0.9759(4)
58	1.1080	1.1120	1.1114(4)	1.1021	1.1102	1.1087(4)
59	1.0896	1.0934	1.0930(4)	1.0822	1.0900	1.0890(4)
60	1.0766	1.0800	1.0794(4)	1.0683	1.0757	1.0739(4)
61	1.1086	1.1127	1.1125(4)	1.1023	1.1104	1.1090(4)
62	1.0953	1.0993	1.0991(4)	1.0868	1.0947	1.0935(4)
63	1.0918	1.0955	1.0950(4)	1.0818	1.0895	1.0875(4)

*1.2979(4) is read as 1.2979 ± 0.0004.

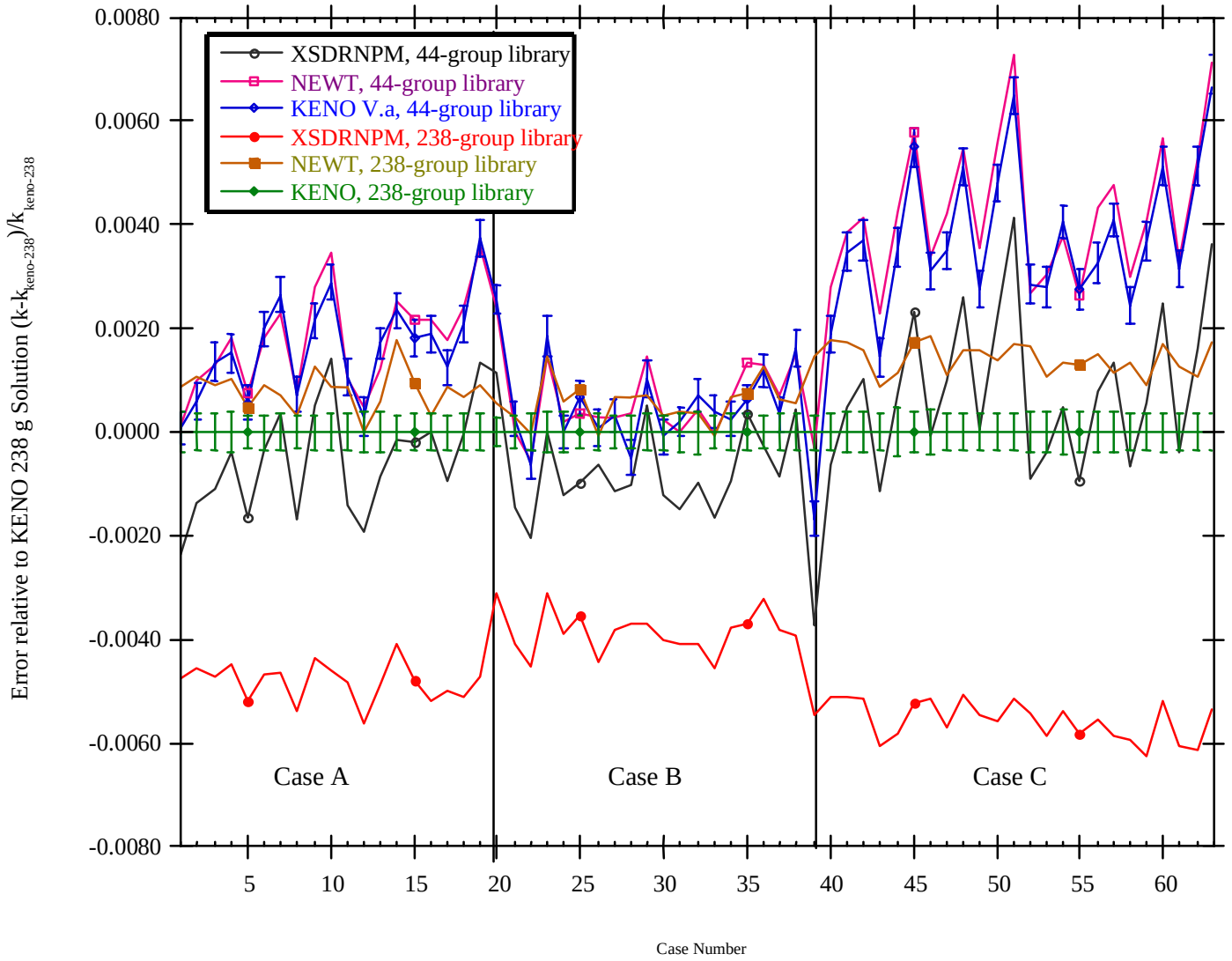

Figure 3. Difference between k_{eff} calculated by KENO V.a/238 g and other solutions.

The behavior of the XSDRNPM solutions relative to KENO and NEWT solutions is believed to be a result of the Wigner-Seitz approximation. This approximation has two components: (1) a cylindrical moderator region in place of the actual square region, and (2) a white boundary condition rather than a more realistic reflective boundary. If the discrepancy between Wigner-Seitz and an exact model is due solely to item 1, then the behavior most likely results from different moderating mechanisms between the two different moderator regions. If the differences result from the application of a white boundary condition, then intercell streaming effects are important; intercell streaming would not occur with a white boundary condition. To investigate these phenomena further, additional NEWT calculations were performed to simulate these effects. To test the effect of a white boundary condition, the NEWT calculations performed earlier were modified by replacing the reflective boundary conditions on the moderator boundaries with white boundary conditions. Results (relative to 238-group KENO V.a calculations) are illustrated in Figure 4, and show that the white boundary condition has very little effect on the calculation of k_{eff} for the MOX benchmarks.

Next, calculations were performed to simulate the Wigner-Seitz approximation within NEWT. This approximation cannot be implemented directly within NEWT, since NEWT is a 2-D code based on a Cartesian coordinate system. However, the cylindrical cell was approximated by using a cylindrical moderator region surrounded by a white media and white boundary conditions, as depicted in Figure 5. The white media is a fictitious material with a total and within-group scattering cross section of 1 barn. In the NEWT solution, this has the effect of isotropically distributing neutrons within each energy group, which would look like a boundary condition beyond the moderator boundary. Figure 6 shows the results plotted in Figure 4, with the addition of the NEWT calculated using a simulated Wigner-Seitz cell. The NEWT calculations with the simulated Wigner-Seitz approximation are in close agreement with 1-D XSDRNPM calculations. These results seem to indicate that the underestimate of k_{eff} by XSDRNPM is the result of the cylindrical approximation of the moderator region.

Incidentally, Figure 6 also shows closest agreement between XSDRNPM and NEWT for Case C fuel. This is inconsistent with other calculations, for which the closest agreement is always seen with Case B. It is suspected that the close agreement for Case C is coincidental; it is more likely that there is a general 0.1% bias between XSDRNPM and NEWT, which offsets the bias between the two results for Case C. Such a bias could result from the simulated Wigner-Seitz cell in NEWT, or from angular redistribution error in the XSDRNPM cylindrical solution. However, no effort was made to determine if such a bias was present; the goal was to demonstrate the similarity of error in the cylindrical approximation for two independent computer codes.

It can be shown that the average moderator thickness for a cylindrical cell (moderator radius - fuel radius) is always less than that of a square cell (average moderator radius - fuel radius). Thus, even though the Wigner-Seitz approximation provides equivalent moderator volumes, the effective moderator thickness seen by a neutron leaving the fuel region is larger. This may result in increased moderation in the square cell relative to the cylindrical approximation. Because uranium is relatively insensitive to small spectral changes, the effect of the cylindrical approximation would be small. However, in MOX fuel, because of the ~0.3 eV resonances in ^{239}Pu and ^{241}Pu (primarily the former), and the 1.1 eV resonance in ^{240}Pu, plutonium fuels are more sensitive to spectral changes. It appears that because the broad-group structure of the SCALE 44-group library smears low-resonance-energy cross sections of its parent 238-group library, the 44-group library is not as sensitive to the spectral effects of the cell approximation.

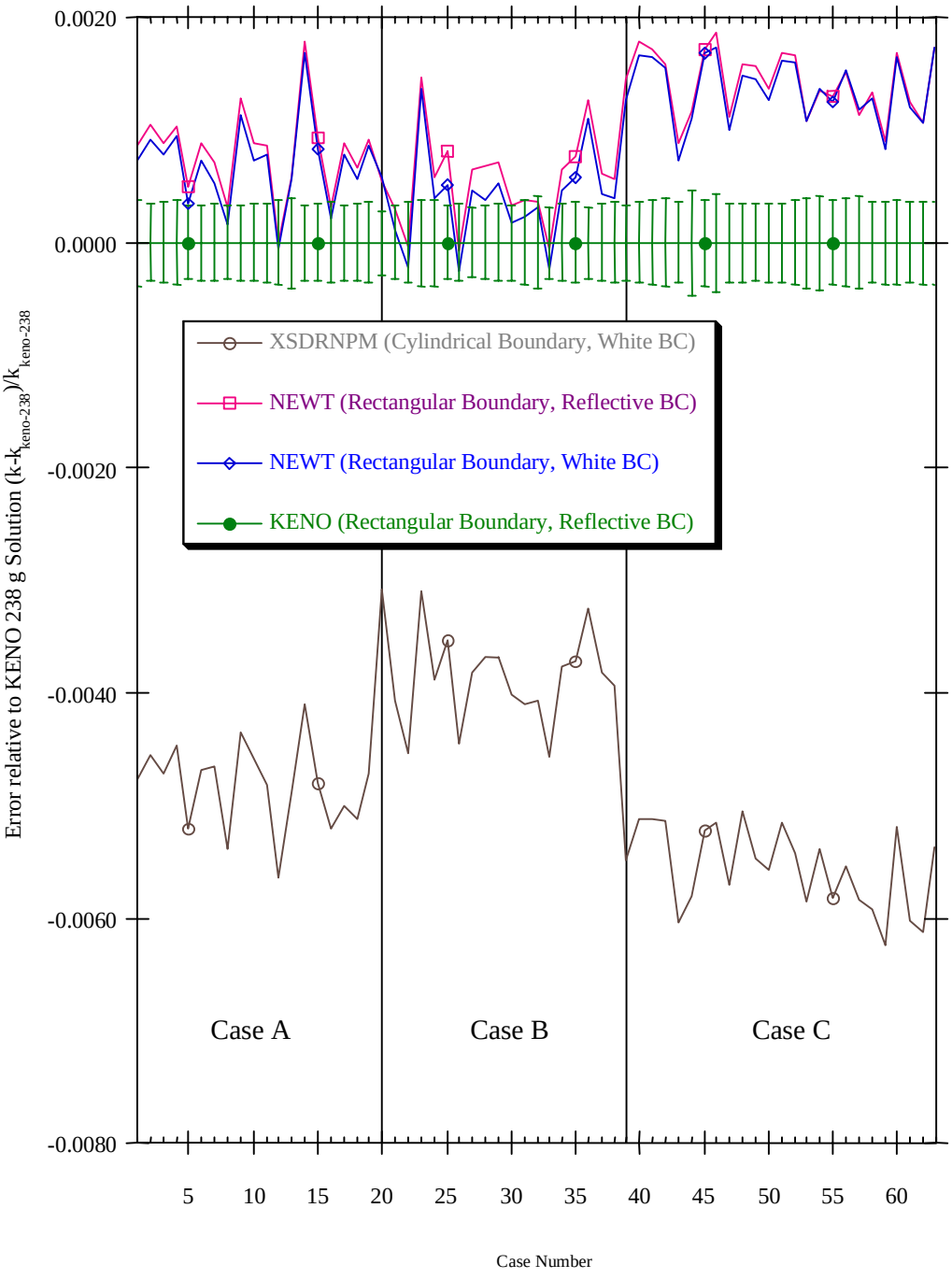

Figure 4. Effect of white boundary conditions in NEWT calculations.

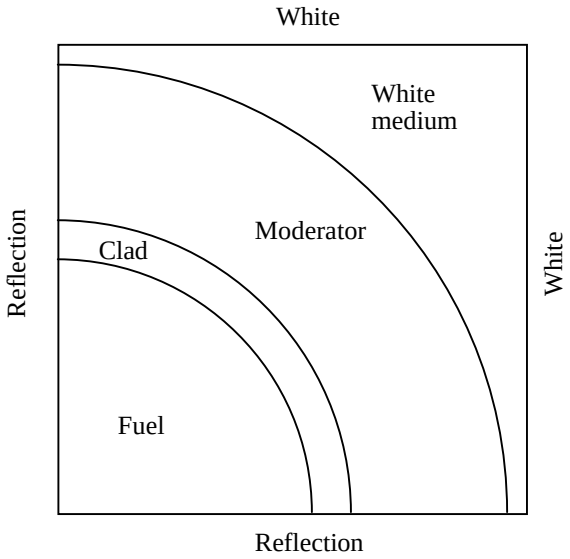

Figure 5. Wigner-Seitz cell representation using NEWT.

5 Conclusions

The purpose of the OECD suite of benchmarks is to obtain a better understanding of computer code and data behavior with respect to well-defined burnup credit problems. The MOX (Phase IV-A) benchmark provides a new twist on burnup credit analyses, with significant amounts of plutonium present. The low-energy resonances in plutonium nuclides create special computational problems that are not seen in uranium fuels. Specifically, group structure effects in multigroup methods may be more pronounced, especially for broad-group libraries not tailored for MOX systems. Furthermore, because of the sensitivity of k_{eff} to the thermal spectrum in MOX fuel, the 1-D Wigner-Seitz cell approximation may be inadequate for MOX fuel pin cells. The error has been found to be as large as ~0.5% $\Delta k/k$ in this study; therefore, it is an important consideration in the analysis of MOX fuel.

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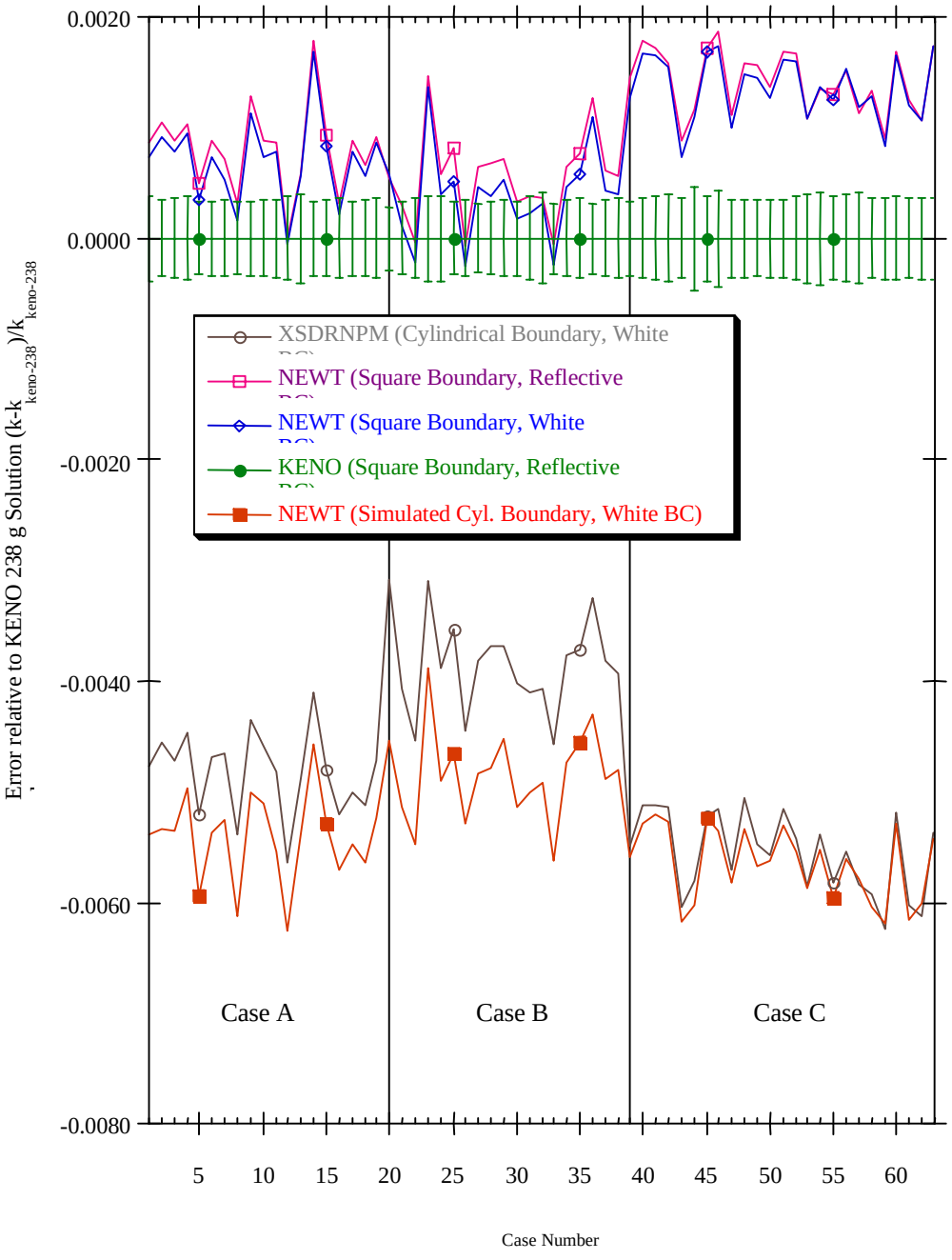

Figure 6. NEWT calculations with simulated Wigner-Seitz boundary.