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Title: Computational Benchmarks for the Doppler Reactivity Defect

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Submitted to:

COMPUTATIONAL BENCHMARKS FOR THE DOPPLER REACTIVITY DEFECT

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1. INTRODUCTION

The Doppler coefficient of reactivity is a crucial parameter in the evaluation of several transients for light water reactors (LWRs), including the control-rod-ejection and steamline-break accidents in pressurized water reactors (PWRs). However, it is relatively small in magnitude: Doppler feedback in going from hot zero power (HZP) to hot full power (HFP) in an LWR produces a reactivity change of only about 1000 pcm. Furthermore, that reactivity change cannot be measured directly in an operating reactor but instead must be inferred from a combination of other parameters.

Taken together, these factors produce a relatively large uncertainty in the Doppler coefficient of reactivity. An uncertainty of approximately 10% in the Doppler coefficient traditionally has been assumed in LWR safety analyses to produce an acceptably conservative model. That concern has been compounded by the contributions from plutonium isotopes, both in mixed-oxide fuel and in high-burnup UO_2 fuel.

This document addresses that concern by constructing a set of computational benchmarks for the Doppler reactivity defect and thereby for the Doppler coefficient of reactivity. The benchmarks are relatively simple but retain all of the important contributors to Doppler reactivity feedback. They are based on previous benchmark studies[1,2] but extend them to higher enrichments and MOX concentrations and to weapons-grade MOX configurations.

Analysts who perform calculations for some or all of these benchmarks are invited to contribute their results for eventual inclusion in this or a companion document. The specific information requested is identified in the appendix, along with an address to which that information may be sent.

2. OVERVIEW OF THE BENCHMARKS

The geometry for these benchmarks corresponds to an infinite array of identical, infinitely long PWR fuel pin cells. Such an array can be modeled as a single rectangular pin cell with reflecting boundary conditions on the top, bottom, and four sides.

The pin cells are based on an "optimized" fuel assembly design that has been used in both initial and reload cycles of several PWRs. However, this design is sufficiently similar to other PWR assembly designs that results from these benchmarks should be relevant for them as well.

The objective of these benchmarks is to calculate the Doppler defect between hot full power (HFP) and hot zero power (HZP) conditions. For the purposes of these calculations, the temperatures of the moderator and the cladding are assumed to remain at 600 K for both conditions. The temperature of the fuel is assumed to rise from 600 K at HZP to a uniform 900 K at HFP. A pressure of 2250 psi is assumed for both conditions. The moderator is borated water and contains 1400 PPM of boron for all calculations. These temperatures and the soluble boron content are the same as in the previous studies.[1,2]

Benchmark specifications are provided for three types of fuel: conventional UO_2, reactor-recycle mixed-oxide (MOX), and weapons-grade MOX. As Tables 2-1 and 2-2 indicate, the UO_2 cases span the range from normal uranium to 5 wt.% enriched, while the MOX cases cover the range from 1 wt.% PuO_2 to 6 wt.% (weapons-grade) and 8 wt.% (reactor-recycle).

The pin cells have been idealized in a number of ways to simplify the calculations. None of the idealizations have any significant impact on Doppler behavior. First, the fuel is assumed to be pure UO_2 or MOX, with no impurities or fission products present. Second, the enriched uranium is assumed to contain only ^{234}U, ^{235}U, and ^{238}U, with the ^{234}U content proportional to the ^{235}U concentration. Similarly, the MOX fuel is assumed to contain only pure PuO_2 and UO_2, with the Pu containing only the four principal isotopes of plutonium and the uranium being normal uranium. Third, the cladding is taken to be pure zirconium, with no minor constituents of Zircaloy present. Finally, the presence of any structural materials (e.g., spacers) has been ignored. A schematic of the benchmark geometry is given in Fig. 2-1.

The constituents of the plutonium fuel are given in Table 2-3. The composition of the reactor-recycle plutonium is the same as that used in an earlier study,[2] while the composition of the of the weapons-grade plutonium is taken from a recent paper.[3]

Table 2-1. Fuel Enrichments for UO_2 Benchmarks.

Case	Enrichment (wt.%)
1	0.711
2	1.6
3	2.4
4	3.1
5	3.9
6	4.5
7	5.0

Table 2-2. PuO_2 Content of Fuel for MOX Benchmarks (wt.%).

Case	Reactor-Recycle	Weapons-Grade
1	1.0	1.0
2	2.0	2.0
3	4.0	4.0
4	6.0	6.0
5	8.0	—

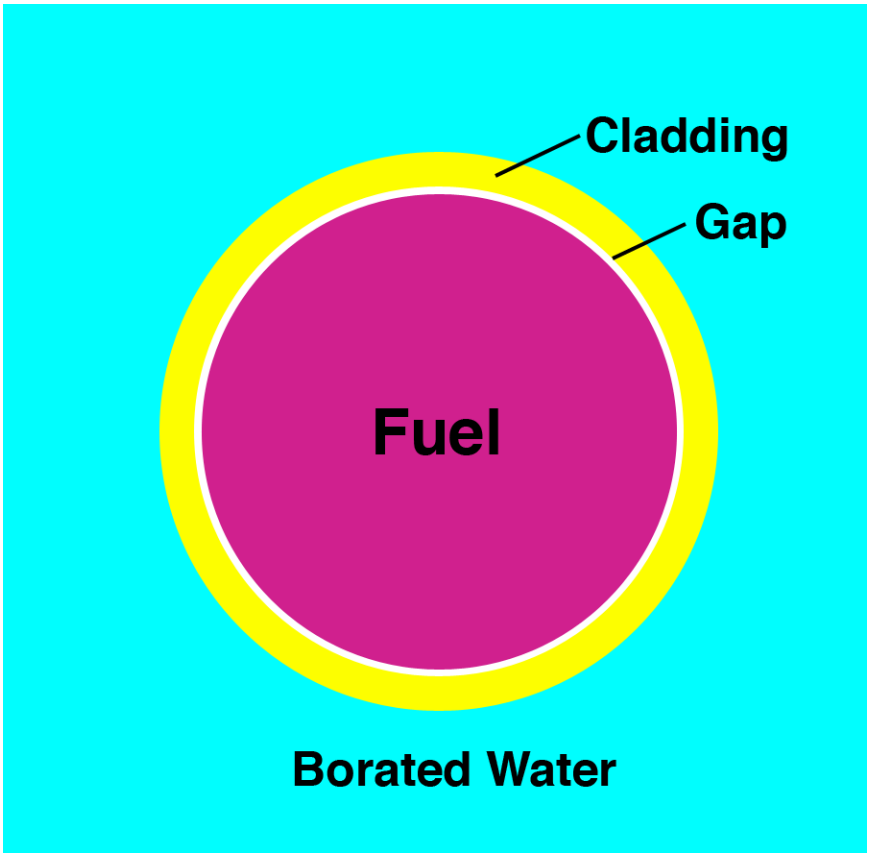

Figure 2-1. Schematic of the Geometry for the Benchmarks.

Table 2-3. Isotopic Content of Plutonium (at.%).

Isotope	Reactor-Recycle	Weapons-Grade
^{239}Pu	45.0	93.6
^{240}Pu	30.0	5.9
^{241}Pu	15.0	0.4
^{242} Pu	10.0	0.1

3. BENCHMARK SPECIFICATIONS

The specific information needed to construct the various benchmarks is given in the following sections.

3.1. Pin Cell Dimensions

Dimensions for the fuel, cladding, and pitch at the temperatures of interest are provided in Table 3-1. The room-temperature dimensions are the same as those used in the previous studies.[1,2]

Table 3-1. Radii and Pitch.

Parameter	300 K	600 K	900 K / 600K
Outer Radius of Fuel (cm)	0.39306	0.39398	0.39433
Inner Radius of Cladding (cm)	0.40077	0.40226	0.40226
Outer Radius of Cladding (cm)	0.45802	0.45972	0.45972
Pitch (cm)	1.26209	1.26678	1.26678

3.2 Cladding

At room temperature, the nominal density of Zircaloy density is 6.56 g/cm^3. Removal of materials other than zirconium (Sn, Cr, Fe, Ni) reduce that density by approximately 1.5% to 6.4616 g/cm^3. At 600 K, the density is reduced further to 6.3902 g/cm^3 by thermal expansion.

Atomic densities can be obtained from the general formula

$$N = \frac{0.60221 \cdot w_f \cdot d}{W} \qquad (1)$$

where N is the atomic number density in atoms/b-cm, w_f is the weight fraction of the element or isotope of interest in the material, d is the mass density of the material, and W is the atomic weight of that element or isotope. This formula, in conjunction with the density of 6.3902 g/cm^3, produces a number density of 0.0421838 atoms/b-cm for zirconium in the cladding.

3.3 Moderator

At 2250 psia and 600 K, the density of unborated water is approximately 0.66163 g/cm^3. Retaining that density and adding 1400 PPM of boron (and assuming negligible displacement of water) produces, in conjunction with Eq. (1), the atomic densities given in Table 3-2. The presence of trace isotopes of oxygen (^{17}O, ^{18}O) is ignored.

Table 3-2. Atomic Densities for Water at 600 K with 1400 PPM of Boron.

Isotope	Number Density (atoms/b-cm)
^{1}H	4.42326 x 10^{-2}
^{10}B	1.02133 x 10^{-5}
^{11}B	4.11098 x 10^{-5}
^{16}O	2.21163 x 10^{-2}

3.4 UO_2 Fuel

The fuel is assumed to be at 95% of theoretical density (10.96 g/cm^3 at room temperature). The resulting densities at the temperatures of interest are given in Table 3-3.

The fuel is further assumed to be pure UO_2, with no ^{236}U present. The composition for each enrichment is given in Tables 3-4 and 3-5. The concentrations are derived using Eq. (1) and the mass densities in Table 3-3.

Table 3-3. Density of UO_2 Fuel.

Temperature (K)	Density (g/cm^3)
293	10.412
600	10.339
900	10.312

Table 3-4. UO_2 Fuel Composition at 600 K (atoms/b-cm).

Enrichment (wt.%)	^{16}O	^{234}U	^{235}U	^{238}U
0.711	4.61171×10^{-2}	0	1.66029×10^{-4}	2.28925×10^{-2}
1.6	4.61218×10^{-2}	3.00175×10^{-6}	3.73618×10^{-4}	2.26843×10^{-2}
2.4	4.61260×10^{-2}	4.50257×10^{-6}	5.60420×10^{-4}	2.24981×10^{-2}
3.1	4.61297×10^{-2}	5.81576×10^{-6}	7.23867×10^{-4}	2.23352×10^{-2}
3.9	4.61339×10^{-2}	7.31651×10^{-6}	9.10661×10^{-4}	2.21490×10^{-2}
4.5	4.61371×10^{-2}	8.44205×10^{-6}	1.05075×10^{-3}	2.20093×10^{-2}
5.0	4.61397×10^{-2}	9.37998×10^{-6}	1.16749×10^{-3}	2.18930×10^{-2}

3.5 Reactor-Recycle MOX Fuel

The reactor-recycle MOX fuel is presumed to have the same density and the same coefficient of thermal expansion as the UO_2 fuel. The composition for each MOX concentration is given in Tables 3-6 and 3-7. The values are derived using Eq. (1), the mass densities in Table 3-3, and the plutonium isotopics from Table 2-3.

Table 3-5. UO_2 Fuel Composition at 900 K (atoms/b-cm).

Enrichment (wt.%)	^{16}O	^{234}U	^{235}U	^{238}U
0.711	4.59967×10^{-2}	0	1.65595×10^{-4}	2.28328×10^{-2}
1.6	4.60014×10^{-2}	2.99391×10^{-6}	3.72642×10^{-4}	2.26251×10^{-2}
2.4	4.60056×10^{-2}	4.49081×10^{-6}	5.58956×10^{-4}	2.24393×10^{-2}
3.1	4.60093×10^{-2}	5.80057×10^{-6}	7.21977×10^{-4}	2.22768×10^{-2}
3.9	4.60134×10^{-2}	7.29740×10^{-6}	9.08283×10^{-4}	2.20911×10^{-2}
4.5	4.60166×10^{-2}	8.42000×10^{-6}	1.04801×10^{-3}	2.19519×10^{-2}
5.0	4.60192×10^{-2}	9.35548×10^{-6}	1.16445×10^{-3}	2.18358×10^{-2}

3.6 Weapons-Grade MOX Fuel

The weapons-grade MOX fuel also is presumed to have the same density and the same coefficient of thermal expansion as the UO_2 fuel. The composition for each MOX concentration is given in Tables 3-8 and 3-9. The concentrations are derived using Eq. (1), the mass densities in Table 3-3, and the plutonium isotopics from Table 2-3.

Table 3-6, Part 1. Reactor-Recycle MOX Fuel Composition at 600 K (atoms/b-cm).

MOX Composition (wt.%)	^{16}O	^{235}U	^{238}U
1.0	4.61140×10^{-2}	1.64368×10^{-4}	2.26636×10^{-2}
2.0	4.61108×10^{-2}	1.62708×10^{-4}	2.24347×10^{-2}
4.0	4.61042×10^{-2}	1.59387×10^{-4}	2.19768×10^{-2}
6.0	4.60977×10^{-2}	1.56067×10^{-4}	2.15190×10^{-2}
8.0	4.60912×10^{-2}	1.52746×10^{-4}	2.10611×10^{-2}

Table 3-6, Part 2. Reactor-Recycle MOX Fuel Composition at 600 K (atoms/b-cm).

MOX Composition (wt.%)	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	1.03031×10^{-4}	6.86872×10^{-5}	3.43436×10^{-5}	2.28957×10^{-5}
2.0	2.06062×10^{-4}	1.37374×10^{-4}	6.86872×10^{-5}	4.57915×10^{-5}
4.0	4.12123×10^{-4}	2.74749×10^{-4}	1.37374×10^{-4}	9.15830×10^{-5}
6.0	6.18185×10^{-4}	4.12123×10^{-4}	2.06062×10^{-4}	1.37374×10^{-4}
8.0	8.24247×10^{-4}	5.49498×10^{-4}	2.74749×10^{-4}	1.83166×10^{-4}

Table 3-7, Part 1. Reactor-Recycle MOX Fuel Composition at 900 K (atoms/b-cm).

MOX Composition (wt.%)	^{16}O	^{235}U	^{238}U
1.0	4.59936×10^{-2}	1.63939×10^{-4}	2.26044×10^{-2}
2.0	4.59904×10^{-2}	1.62283×10^{-4}	2.23761×10^{-2}
4.0	4.59838×10^{-2}	1.58971×10^{-4}	2.19194×10^{-2}
6.0	4.59773×10^{-2}	1.55659×10^{-4}	2.14628×10^{-2}
8.0	4.59708×10^{-2}	1.52347×10^{-4}	2.10061×10^{-2}

Table 3-7, Part 2. Reactor-Recycle MOX Fuel Composition at 900 K (atoms/b-cm).

MOX Composition (wt.%)	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	1.02762×10^{-4}	6.85079×10^{-5}	3.42539×10^{-5}	2.28360×10^{-5}
2.0	2.05524×10^{-4}	1.37016×10^{-4}	6.85079×10^{-5}	4.56719×10^{-5}
4.0	4.11047×10^{-4}	2.74031×10^{-4}	1.37016×10^{-4}	9.13438×10^{-5}
6.0	6.16571×10^{-4}	4.11047×10^{-4}	2.05524×10^{-4}	1.37016×10^{-4}
8.0	8.22094×10^{-4}	5.48063×10^{-4}	2.74031×10^{-4}	1.82688×10^{-4}

Table 3-8, Part 1. Weapons-Grade MOX Fuel Composition at 600 K (atoms/b-cm).

MOX Composition (wt.%)	^{16}O	^{235}U	^{238}U
1.0	4.61154×10^{-2}	1.64368×10^{-4}	2.26636×10^{-2}
2.0	4.61136×10^{-2}	1.62708×10^{-4}	2.24347×10^{-2}
4.0	4.61099×10^{-2}	1.59387×10^{-4}	2.19768×10^{-2}
6.0	4.61061×10^{-2}	1.56067×10^{-4}	2.15190×10^{-2}

Table 3-8, Part 2. Weapons-Grade MOX Fuel Composition at 600 K (atoms/b-cm).

MOX Composition (wt.%)	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	2.14958×10^{-4}	1.35497×10^{-5}	9.18623×10^{-7}	2.29656×10^{-7}
2.0	4.29916×10^{-4}	2.70994×10^{-5}	1.83725×10^{-6}	4.59312×10^{-7}
4.0	8.59831×10^{-4}	5.41988×10^{-5}	3.67449×10^{-6}	9.18623×10^{-7}
6.0	1.28975×10^{-3}	8.12982×10^{-5}	5.51174×10^{-6}	1.37794×10^{-6}

Table 3-9, Part 1. Weapons-Grade MOX Fuel Composition at 900 K (atoms/b-cm).

MOX Composition (wt.%)	^{16}O	^{235}U	^{238}U
1.0	4.59950×10^{-2}	1.63939×10^{-4}	2.26044×10^{-2}
2.0	4.59932×10^{-2}	1.62283×10^{-4}	2.23761×10^{-2}
4.0	4.59895×10^{-2}	1.58971×10^{-4}	2.19194×10^{-2}
6.0	4.59857×10^{-2}	1.55659×10^{-4}	2.14628×10^{-2}

Table 3-9, Part 2. Weapons-Grade MOX Fuel Composition at 900 K (atoms/b-cm).

MOX Composition (wt.%)	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu
1.0	2.14397×10^{-4}	1.35143×10^{-5}	9.16224×10^{-7}	2.29056×10^{-7}
2.0	4.28793×10^{-4}	2.70286×10^{-5}	1.83245×10^{-6}	4.58112×10^{-7}
4.0	8.57586×10^{-4}	5.40572×10^{-5}	3.66490×10^{-6}	9.16224×10^{-7}
6.0	1.28638×10^{-3}	8.10859×10^{-5}	5.49735×10^{-6}	1.37434×10^{-6}

4. MODELING INSTRUCTIONS AND DESIRED RESULTS

4.1 Guidance for Calculations

Two approximations frequently are employed in pin-cell calculations. One homogenizes the cladding with the gap between it and the fuel. The other replaces the square sides of the pin cell with an outer radius and changes the associated boundary condition from pure reflection to white (reflective but isotropic).

Homogenizing the gap with the cladding is expected to have little impact on reactivity and is considered acceptable for this benchmark. It is requested, however, that analysts who employ that approximation note it in the appropriate section of their responses.

Changing the outer boundary from a square to a circle is more problematic. Although that approximation has been shown to be acceptable for UO_2 cases (see Ref. 1, for example), it can produce significant changes in reactivity for MOX pin cells. Consequently, it is recommended that it not be employed for these benchmarks. It is requested, however, that analysts who do choose to employ it state in the appropriate section of their responses that they have done so.

4.2 Information to Be Provided

A description of the methods and models employed is required for a useful comparison of results. The following information should be provided:

- Origin of the cross-section library and its name and version (also identify any *ad hoc* data modifications)
- Cross-section processing code name(s) and version(s)
- Calculational methodology (include code name(s) and version(s))
- Representation of energy dependence: number of energy groups employed and energy group structure, or continuous-energy
- Any assumptions, approximations, or differences from the benchmark specifications

4.3 Format for Submission of Results

Please submit the results in the format indicated in the Appendix. Both hard copies and electronic files in a widely used format (Adobe PDF, Open Document, MS Word, or WordPerfect) are acceptable.

5. REFERENCES

1. R. D. Mosteller, L. D. Eisenhart, R. C. Little, W. J. Eich, and J. Chao, "Benchmark Calculations for the Doppler Coefficient of Reactivity," *Nucl. Sci. Eng.*, **107**, pp. 265-271 (March 1991).

2. R. D. Mosteller, J. T. Holly, and L. A. Mott, "Benchmark Calculations for the Doppler Coefficient of Reactivity in Mixed-Oxide Fuel," *Proceedings of the International Topical Meeting on Advances in Mathematics, Computations, and Reactor Physics*, CONF-910414, pp. 9.2 1-1–9.2 1-12, Pittsburgh, Pennsylvania (April 1991).

3. Gray S. Chang and Robert C. Pedersen, "Burnup-Dependent Rim-Effect Comparison of WG-MOX Fuel Pellet in ATR and PWR," *Trans. Am. Nucl. Soc.*, **90**, 555 (June 2004).

APPENDIX

Computational Benchmarks for the Doppler Reactivity Defect

Please submit results to:

Russell D. Mosteller
Los Alamos National Laboratory
MS F663
Los Alamos, NM 87545

Phone: (505) 665-4879
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Name: _____

Organization: _____

Address: _____

_____

Phone: _____

FAX: _____

E-mail: _____

Please submit the results on the following forms or in a similar format. Include additional pages if necessary. Submission of partial results is acceptable, as is the submission of revised results.

Description and Origin of Cross Sections:

Calculation Methodology:

Deviations from Benchmark Specifications:

Results

UO_2 Fuel

Enrichment (wt.%)	HFP k_{eff}	HZP k_{eff}	Doppler Defect ($\Delta\rho$)	Doppler Coefficient ($\Delta\rho/\Delta T$)
0.711				
1.6				
2.4				
3.1				
3.9				
4.5				
5.0				

Reactor-Recycle MOX Fuel

MOX Content (wt.%)	HFP k_{eff}	HZP k_{eff}	Doppler Defect ($\Delta\rho$)	Doppler Coefficient ($\Delta\rho/\Delta T$)
1.0				
2.0				
4. 0				
6.0				
8.0				

Results
(Continued)

Weapons-Grade MOX Fuel

MOX Content (wt.%)	HFP k_{eff}	HZP k_{eff}	Doppler Defect ($\Delta\rho$)	Doppler Coefficient ($\Delta\rho/\Delta T$)
1.0				
2.0				
4. 0				
6.0				