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Benchmark Calculations for the Doppler Coefficient of Reactivity

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Abstract – *The Doppler coefficient of reactivity is a crucial parameter in the evaluation of several transients in light water reactors (LWRs). It is relatively small in magnitude and cannot be measured directly in operating reactors. Doppler coefficients are presented for slightly idealized pressurized water reactor pin cells. These coefficients were calculated with the MCNP-3A continuous-energy Monte Carlo code using data taken directly from the ENDF/B-V nuclear data library. This combination represents the most rigorous analytical tool and the best nuclear data available. Consequently, these results comprise a set of numerical benchmarks that may be used to evaluate the accuracy of LWR lattice physics codes in predicting Doppler behavior at operating conditions. An example of one such evaluation, using the CELL-2 code, is included.*

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-drop accident in boiling water reactors (BWRs) and the control-rod-ejection and steamline-break accidents in pressurized water reactors (PWRs). 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 ~1%. Furthermore, that reactivity change cannot be measured directly in an operating reactor but instead must be inferred from a combination of other measured parameters.

These factors taken together produce a relatively large uncertainty in the Doppler coefficient. An uncertainty of ~10% in the Doppler coefficient traditionally has been assumed in LWR safety analyses to produce an acceptably conservative model. However, a recent study[1,2] has raised questions about the accuracy and consistency of the Doppler coefficient computed by a variety of LWR lattice physics codes and has suggested that the uncertainty in the Doppler coefficient may be significantly >10%.

This paper addresses that concern by constructing a set of numerical benchmarks for the Doppler

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coefficient of reactivity at conditions characteristic of operating PWRs. These benchmark results have been obtained using the most rigorous analytical tool available, a continuous-energy Monte Carlo code. In addition, the nuclear data used in the analysis were taken directly from the ENDF/B-V data library,[3] the most accurate source of such data currently available for LWR analysis. The intent is to provide a set of reference results that can be used to evaluate the accuracy of LWR lattice physics codes in predicting Doppler coefficients.

The results presented in this paper are an extension of a previous study[4,5] that employed the MCNP-3A Monte Carlo code[6] to establish reference results for PWR pin cells at a variety of thermal-hydraulic conditions. In contrast to that previous study, the present study focuses exclusively on Doppler feedback, and it incorporates a wider range of fuel enrichments.

CASE DESCRIPTION

The pin cells in this study are based on an "optimized" fuel assembly design, which has been used in both initial and reload cycles of several PWRs. In particular, the core of a reactor that was the subject for the study of a natural-circulation transient[7,8] contained assemblies of this design, and the original motivation for the present study was to assess the accuracy of the Electric Power Research Institute's (EPRI's) EPRI-PRESS lattice physics package[9] in predicting a variety of reactivity coefficients for that core. At the same time, this design is sufficiently similar to other PWR assembly designs that judgments made in this study with regard to the Doppler coefficient should be generally valid. Furthermore, since Doppler behavior in BWRs is very similar to that in PWRs, these results should be meaningful as a benchmark for both PWR and BWR lattice physics codes.

The geometry that was studied corresponds to an infinite array of infinitely long PWR pin cells at beginning of life (BOL). This condition was effected in MCNP-3A by applying reflecting boundary conditions at each of the six boundaries of a single pin cell. The dimensions of that pin cell are presented in Table I, and a schematic of the cell is given in Fig. 1. It is assumed to be at a pressure of 2250 psia and a soluble boron concentration of 1400 ppm.

TABLE I

Dimensions for Calculations

Outer radius of fuel pellet (cm)	0.39306
Outer radius of cladding (cm)	0.45802
Pin cell pitch (cm)	1.26209
Equivalent pin cell radius (cm)	0.71206

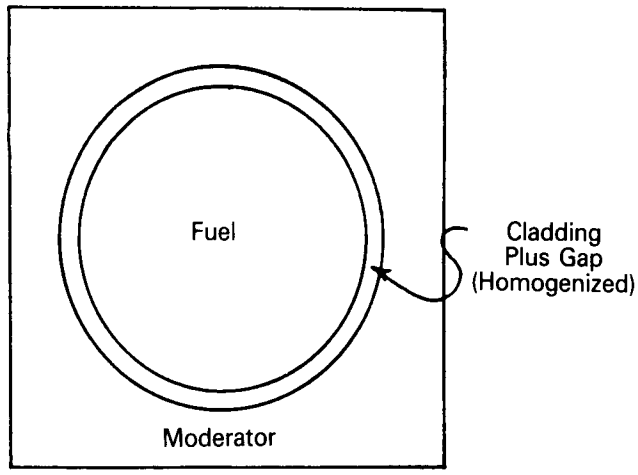

Fig. 1. Pin-cell geometry.

Although these results are obtained only at BOL, they are significant for any point in the fuel cycle. Uranium isotopes, primarily ^{238}U, account for the predominant portion of Doppler feedback throughout the lifetime of the fuel.

The pin cell is idealized in three further respects: (a) the cladding is taken to be natural zirconium rather than an alloy, (b) the gap between the fuel pellet and the cladding is homogenized with the cladding to form a single region, and (c) the uranium in the fuel pellet is assumed to contain only ^{235}U and ^{238}U. These three idealizations substantially reduce the complexity of the problem without significantly altering the Doppler feedback. (For example, homogenizing the cladding with the gap has a negligible effect on reactivity, since zirconium has little impact on either neutron moderation or neutron absorption.)

The cases studied include fuel pins of five different enrichments at each of two thermal-hydraulic conditions. The five enrichments span the range from natural uranium (0.711 wt% ^{235}U) to 3.9 wt% enriched uranium. Natural uranium is used as an axial blanket at the top and/or bottom of some PWR assembly designs, while 3.9 wt% is typical of the enrichment of reload fuel assemblies for extended cycles. The two thermal-hydraulic conditions are characteristic of PWRs at HZP and HFP, respectively, and differ only in the temperature of the fuel pellet. The HZP is assumed to correspond to a uniform temperature of 600 K, while HFP corresponds to a uniform fuel temperature of 900 K but is otherwise identical to HZP. The contents and temperatures of each of the three regions are summarized in Tables II, III, and IV.

MONTE CARLO RESULTS

The MCNP-3A calculations with a million neutron histories were run for each of the ten cases, and the

TABLE II

Isotopic Concentrations in the Fuel

Fuel Temperature (K)	Fuel Enrichment (wt%)	Number Density (atom/b·cm)		
		^{16}O	^{235}U	^{238}U
600 (HZP)	0.711	0.0461309	0.000166078	0.0228994
	1.6	0.0461355	0.000373729	0.0226940
	2.4	0.0461397	0.000560588	0.0225093
	3.1	0.0461433	0.000724086	0.0223476
	3.9	0.0461475	0.000910933	0.0221163
900 (HFP)	0.711	0.0457561	0.000164729	0.0227133
	1.6	0.0457607	0.000370693	0.0225096
	2.4	0.0457648	0.000556033	0.0223264
	3.1	0.0457684	0.000718202	0.0221660
	3.9	0.0457725	0.000903532	0.0219827

TABLE III

Isotopic Concentrations in the Cladding

Cladding Temperature (K)	Isotope	Number Density (atom/b·cm)
600[a]	Zirconium (natural)	0.0383243
600[b]	Zirconium (natural)	0.0389087

[a]Fuel temperature at 600 K.
[b]Fuel temperature at 900 K.

TABLE IV

Isotopic Concentrations in the Moderator

Moderator Temperature (K)	Number Density (atom/b·cm)		
	^{1}H	^{10}B	^{16}O
600	0.0442326	0.0000102133	0.0221163

Doppler defect from HZP to HFP then was computed as

$$\Delta\rho_{Dop} \equiv \frac{k_{HFP} - k_{HZP}}{k_{HFP}\,k_{HZP}} \quad . \tag{1}$$

This number of neutron histories produces standard deviations of no more than 0.0007 in the eigenvalue, and the corresponding standard deviations in the Doppler defect are on the order of 10% of the defect itself. The eigenvalues and Doppler defects from these calculations are summarized in Tables V and VI, respectively. The latter table also contains the average Doppler coefficient of reactivity for the range from HZP to HFP based on the computed Doppler defect.

TABLE V

Eigenvalues from MCNP-3A

Fuel Enrichment (wt%)	Fuel Temperature (K)	Cladding and Moderator Temperature (K)	Eigenvalue
0.711	600	600	0.6638 ± 0.0006
	900	600	0.6567 ± 0.0008
1.6	600	600	0.9581 ± 0.0006
	900	600	0.9484 ± 0.0006
2.4	600	600	1.0961 ± 0.0007
	900	600	1.0864 ± 0.0007
3.1	600	600	1.1747 ± 0.0007
	900	600	1.1641 ± 0.0006
3.9	600	600	1.2379 ± 0.0006
	900	600	1.2271 ± 0.0006

The MCNP-3A results are generally well behaved and correspond to the expected physical behavior. The eigenvalues and Doppler defects both can be fitted to smooth curves as a function of fuel enrichment, as shown in Figs. 2 and 3, respectively. In addition, the average number of collisions per particle produces a smooth but monotonically decreasing curve as a function of fuel enrichment, as shown in Fig. 4. A large

TABLE VI

Doppler Defects and Coefficients from MCNP-3A

Fuel Enrichment (wt%)	$\Delta\rho_{Dop}$	Doppler Coefficient (pcm/K)
0.711	−0.0163 + 0.0023	−5.4 ± 0.8
1.6	−0.0108 + 0.0009	−3.6 ± 0.3
2.4	−0.0081 + 0.0008	−2.7 ± 0.3
3.1	−0.0078 + 0.0007	−2.6 ± 0.2
3.9	−0.0071 + 0.0006	−2.4 ± 0.2

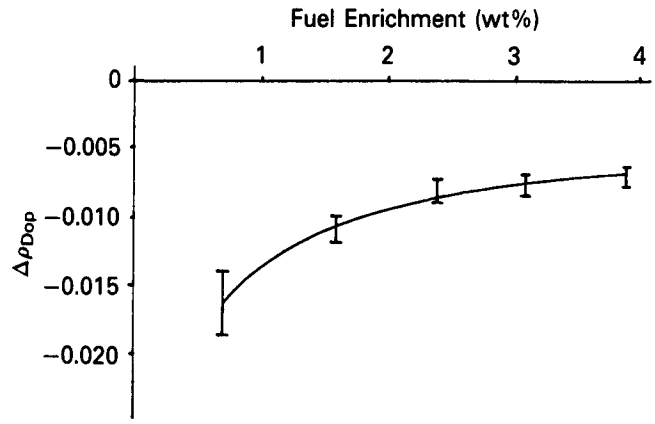

Fig. 3. Doppler defect as a function of fuel enrichment.

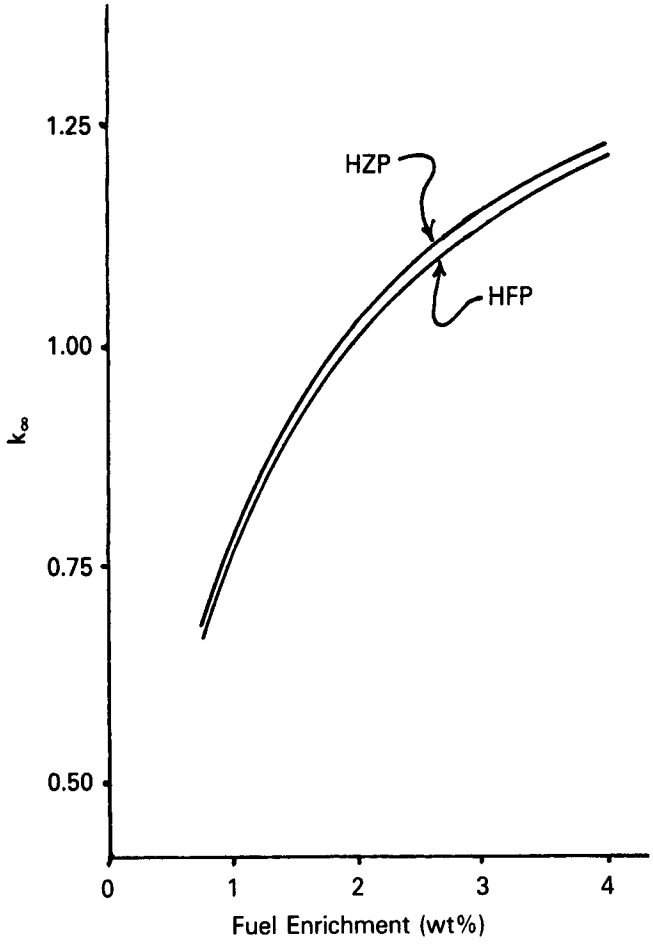

Fig. 2. Eigenvalue behavior as a function of fuel enrichment.

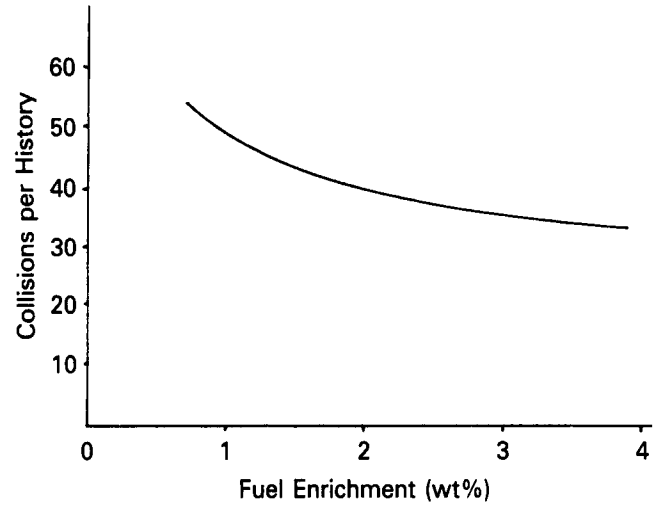

Fig. 4. Average collisions per history as a function of fuel enrichment.

fraction of the collisions occurs after the neutron is thermalized, and the probability of absorption for a thermal neutron increases as the concentration of ^{235}U increases. (Strictly speaking, of course, a neutron history in MCNP-3A is terminated not by absorption but by sufficiently small statistical weight; however, a collision with a strong absorber reduces that weight much more than a collision with a weak absorber.) Finally, the statistical convergence of the MCNP-3A calculations generally is well behaved, and the sample mean exhibited only relatively small variations throughout the sequence of calculations. The sample mean and its associated standard deviation for the cases at 2.4 wt% are shown in Fig. 5 in increments of 100 000 neutron histories.

EVALUATION OF CELL-2

The CELL-2 code of EPRI's EPRI-PRESS reactor physics package[9] performs pin-cell spectrum calculations. It is compatible with both its own "production" library and with a library[10] derived directly from ENDF/B-V. The CELL-2 results presented in this paper are obtained using the latter library. Consequently, any differences observed in the CELL-2 results relative

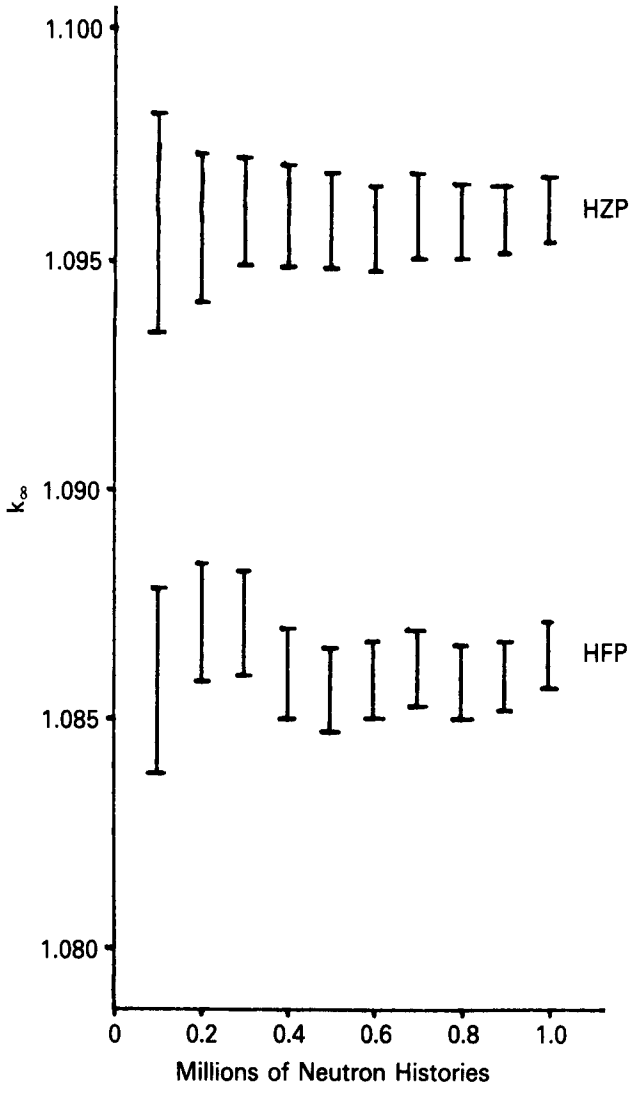

Fig. 5. The MCNP-3A convergence behavior for cases with 2.4 wt% fuel enrichment.

to those from MCNP-3A can be attributed to approximations inherent in the CELL-2 methodology.

It must be emphasized that CELL-2, in contrast to MCNP-3A, is designed to be used on a regular and frequent basis for PWR physics calculations. For example, the MCNP-3A calculations in this study were performed on a MicroVAX-II and consumed ~10 days each. (The same calculations on a Cray-1 would take ~8 h each.) In contrast, each CELL-2 calculation requires at most a few minutes of mainframe computer time. Monte Carlo codes such as MCNP-3A are designed to incorporate as few approximations as possible, while spectrum codes such as CELL-2 are designed as a compromise between accuracy and computational speed.

The CELL-2 code makes two approximations to the pin-cell geometry described in Table I. First, the calculation for the 62 energy groups above 1.855 eV completely homogenizes the pin cell, although it does

TABLE VII

Eigenvalues from CELL-2

Fuel Enrichment (wt%)	Fuel Temperature (K)	Cladding and Moderator Temperature (K)	Eigenvalue
0.711	600	600	0.6652
	900	600	0.6578
1.6	600	600	0.9605
	900	600	0.9507
2.4	600	600	1.0989
	900	600	1.0883
3.1	600	600	1.1773
	900	600	1.1663
3.9	600	600	1.2404
	900	600	1.2291

make an allowance that accounts for the heterogeneous nature of fast fission. Second, while the calculation for the 35 energy groups below 1.855 eV retains separate spatial regions, it replaces the square outer boundary of the cell and its reflecting boundary condition by a circular boundary (that preserves the area of the cell) and an analytic boundary condition that corresponds to isotropic reflection.

A preliminary analysis was carried out to demonstrate the equivalence of those two representations for thermal spectrum calculations, as first suggested by Honeck.[11] The CELL-2 pin-cell cases with circular outer boundaries were run with a reflecting boundary condition and with the isotropically reflecting boundary condition. The difference in eigenvalues between these two cases was ~0.01 Δk. The MCNP-3A cases were run for the same pin cell with a square outer boundary and with a circular outer boundary. The difference in eigenvalues from the MCNP-3A cases was essentially the same as that from the CELL-2 cases. In addition, once a bias was accounted for (see below), the CELL-2 eigenvalue for the case with normal reflection was in excellent agreement with the MCNP-3A eigenvalue for the case with the circular boundary, while the CELL-2 eigenvalue for the case with isotropic reflection was in excellent agreement with the MCNP-3A case with the square boundary.

The eigenvalues computed by CELL-2 for the 10 pin-cell cases are shown in Table VII. These eigenvalues have a nearly constant bias relative to the sample mean from the corresponding MCNP-3A calculation. In particular,

$$k_\infty^{C2} = (\bar{k}_\infty^{MCNP} + 0.0021) \pm 0.0005 \ , \qquad (2)$$

TABLE VIII

Doppler Defects and Coefficients from CELL-2

Fuel Enrichment (wt%)	$\Delta\rho_{Dop}$	Doppler Coefficient (pcm/K)
0.711	−0.0168	−5.6
1.6	−0.0107	−3.6
2.4	−0.0089	−3.0
3.1	−0.0080	−2.7
3.9	−0.0071	−2.4

where k_∞^{C2} is the eigenvalue from CELL-2 and $\bar{k}_\infty^{MCNP}$ is the corresponding sample mean from MCNP-3A. Note that the standard deviation associated with this relationship is smaller than the standard deviations from the MCNP-3A calculations. Furthermore, once the bias of 0.0021 is accounted for, eight of the ten CELL-2 eigenvalues differ from the MCNP-3A sample mean by no more than the standard deviation associated with that sample mean, and the two others are barely outside that range.

The Doppler defects predicted by CELL-2, calculated according to Eq. (1), are presented in Table VIII. Those Doppler defects are in excellent agreement with the MCNP-3A results presented in Table VI, as is to be expected given the essentially constant difference in the eigenvalues from the two codes. All five Doppler defects from CELL-2 fall within a single standard deviation of the corresponding Doppler defect from MCNP-3A. The consistency between them is illustrated in Fig. 6.

A careful inspection of the results shown in Tables VI and VIII demonstrates that the imposition of a semiarbitrary uncertainty of 10% on the Doppler coefficients from CELL-2 still produces good agreement

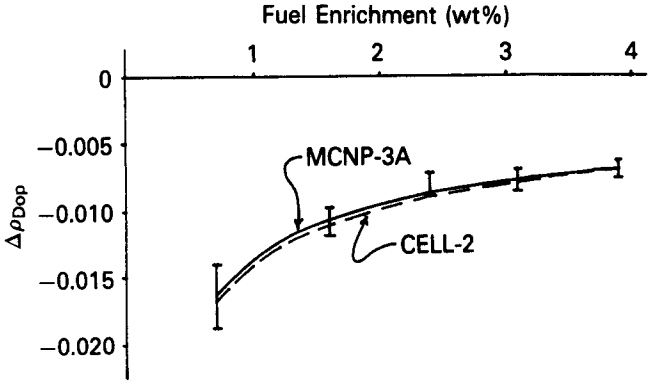

Fig. 6. Comparison of Doppler defects from MCNP-3A and CELL-2.

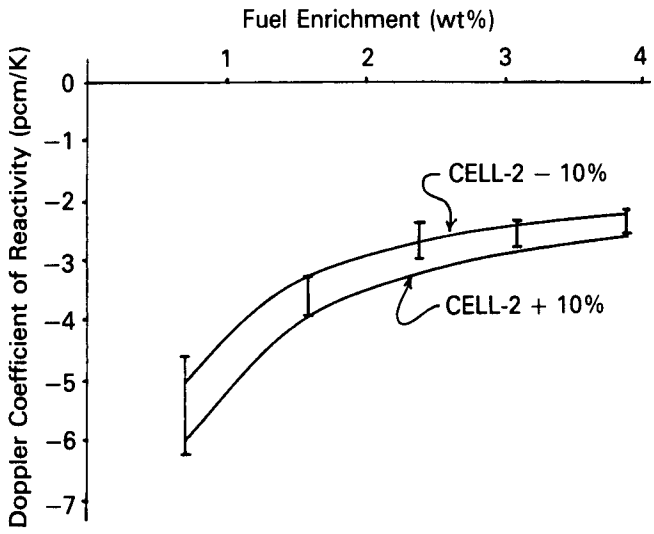

Fig. 7. The CELL-2 Doppler coefficients with 10% uncertainty.

with the Doppler coefficients from MCNP-3A. As shown in Fig. 7, the range of CELL-2 Doppler coefficients associated with an uncertainty of 10% generally falls within the standard deviation associated with the corresponding Doppler coefficient from MCNP-3A.

CONCLUSIONS

This study has defined a set of numerical benchmarks against which the accuracy of lattice physics codes in predicting Doppler feedback can be assessed. These benchmark results were obtained using the Monte Carlo code MCNP-3A and a continuous-energy nuclear data library derived from ENDF/B-V. This combination constitutes the most rigorous analytical tool and the best source of nuclear data currently available for LWR analysis. Furthermore, this study represents the first application of such a combination to conditions characteristic of operating LWRs.

In addition, the ability of the CELL-2 physics code to predict accurate Doppler coefficients has been evaluated against the set of benchmarks. Three significant conclusions can be drawn from that evaluation.

First, CELL-2 consistently overpredicts the eigenvalue for these problems by ~0.002 Δk. Errors of this magnitude, especially when they are consistent from case to case, are well within the range of acceptability for PWR spectrum codes. In fact, errors of this size often are effectively subsumed or even canceled by reactivity biases arising from other engineering approximations in such codes.

Second, CELL-2 predicts Doppler behavior that is in excellent agreement with that calculated by MCNP-3A. Even though the standard deviations associated with the Doppler coefficients from MCNP-3A are very

small, all five CELL-2 Doppler coefficients fall within a single standard deviation of the corresponding sample mean from MCNP-3A.

Third, the imposition of an uncertainty of 10% on the Doppler coefficient from CELL-2 still produces good agreement with the results from MCNP-3A. This result strongly suggests that the application of the traditional 10% uncertainty to the Doppler coefficients calculated by the EPRI-PRESS package provides an acceptably conservative margin for safety and licensing analyses.

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