

## **KENO CONTINUOUS-ENERGY CALCULATIONS FOR A SUITE OF COMPUTATIONAL BENCHMARKS FOR THE DOPPLER REACTIVITY DEFECT**

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### **ABSTRACT**

Continuous-energy capabilities have been added to development versions of the KENO V.a and KENO-VI Monte Carlo packages within the SCALE code system. Recently, continuous-energy cross-section data has been added to SCALE based on ENDF/B-VI evaluations for more than 300 nuclides and a range of temperatures. Ongoing analyses have been able to demonstrate the accuracy of the new continuous-energy capabilities. This work describes recently completed calculations for a computational benchmark developed to assess codes and data used to calculate the Doppler coefficient with a range of UO<sub>2</sub> and MOX fuel types. Results are compared to MCNP calculations for the benchmark and are found to be in exceptionally good agreement.

*Key Words:* Continuous energy, KENO, SCALE, Monte Carlo

### **1. INTRODUCTION**

KENO V.a and KENO-VI are Monte Carlo codes that solve the integral form of the neutral-particle Boltzmann transport equation. These codes, which are part of the SCALE [1] code system, are used for performing criticality calculations for systems with fissionable material and are based on a multigroup representation of energy-dependent cross sections. In general, continuous-energy Monte Carlo methods are preferred over multigroup methods because the continuous-energy treatment, based on evaluated data libraries such as ENDF/B-VI, avoids many of the assumptions inherent in a multigroup treatment. However, continuous-energy treatment is much more demanding in terms of computer storage space for data, memory requirements, and calculation execution time.

Continuous-energy versions of both KENO V.a and KENO-VI have been developed at the Oak Ridge National Laboratory (ORNL) and are being extensively tested [2–4]. These codes utilize continuous-energy libraries generated using the latest AMPX [5] cross-section processing system. ENDF/B-VI.7 data for more than 300 nuclides and isotopes have recently been processed through AMPX to generate continuous-energy cross-section data for multiple temperatures. Continuous-energy versions of KENO and these newly generated data have been

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and are continuing to be tested using various problem sets including sample problems from SCALE and critical benchmark cases.

Extension of both versions of KENO to perform in continuous-energy mode has required both the design of a new continuous-energy cross-section format and the development of the appropriate Monte Carlo transport procedures to sample the new cross-section format. The nuclear data within the ENDF system are voluminous in nature and cannot be used directly in radiation transport codes. As a result, a cross-section processing system must be used to process raw ENDF data and generate nuclear data libraries that can be efficiently accessed by radiation transport codes. In order to facilitate the development of independent transport procedures, a new continuous-energy cross-section library structure has been developed for KENO. Several new processing modules have been developed for the AMPX-2000 [5] cross-section processing system at ORNL.

The details of the continuous-energy library format are beyond the scope of this paper; however, the essential components of a continuous-energy KENO cross-section library include the following: (1) average number of neutrons (delayed and prompt) produced by fission,  $\nu(E)$ ; (2) one-dimensional continuous-energy cross sections as a function of temperature,  $\sigma(E, T)$ ; (3) two-dimensional pointwise joint probability distributions that describe the energy and angle of particles emerging from a collision,  $f(E \rightarrow E', \mu)$ ; and (4) probability tables for sampling the cross sections in the unresolved-resonance region.

In this paper, results are presented from calculations performed as part of a computational benchmark for calculating the Doppler coefficient of reactivity for UO<sub>2</sub> and mixed oxide (MOX) fuel pin cells [6]. The benchmark was established to determine the ability of various code systems, using a variety of data sources, to calculate the magnitude of Doppler feedback between hot zero power (HZP) and hot full power (HFP) conditions. In this paper, the benchmark is also being used to assess the performance of the KENO codes and AMPX-processed data relative to MCNP calculations using NJOY-generated cross sections from ENDF/B-VI evaluations.

## 2. CALCULATIONS

The computational benchmark used in this work sought to determine the Doppler coefficient of reactivity based on eigenvalue calculations performed with fuel temperatures of 600 K (HZP) and 900 K (HFP). Clad, gap, and moderator temperatures were fixed at 600 K for both states for the purpose of this benchmark. The pin cell configuration consisted of a simple infinite-lattice pin-cell with a void-filled gas gap, zirconium cladding, and borated water as the moderator. Three different fuel mixtures were evaluated to assess the impact of plutonium content in MOX fuels relative to UO<sub>2</sub>. For the UO<sub>2</sub> pin cell, calculations were performed for <sup>235</sup>U enrichments ranging from natural uranium (0.71 wt %) to 5 wt %. Two MOX configurations were also evaluated, for different plutonium vectors. The first set consisted of natural uranium blended with a plutonium vector characteristic of weapons-grade fuel, with plutonium mass fractions varying from 1 to 8 wt %. The second set of MOX fuels was based on a conceptual UO<sub>2</sub> recycle plutonium vector, with 1 to 6 wt % plutonium mixed with natural uranium.

Calculations were performed with both KENO V.a and KENO-VI in continuous-energy mode, for all benchmark fuel specifications, at both HZP and HFP conditions. Doppler coefficients were calculated from the HZP and HFP eigenvalues as

$$C_{Doppler} = \frac{\left( \frac{1}{k_{eff,HZP}} - \frac{1}{k_{eff,HFP}} \right)}{\Delta T_{fuel}}. \quad (1)$$

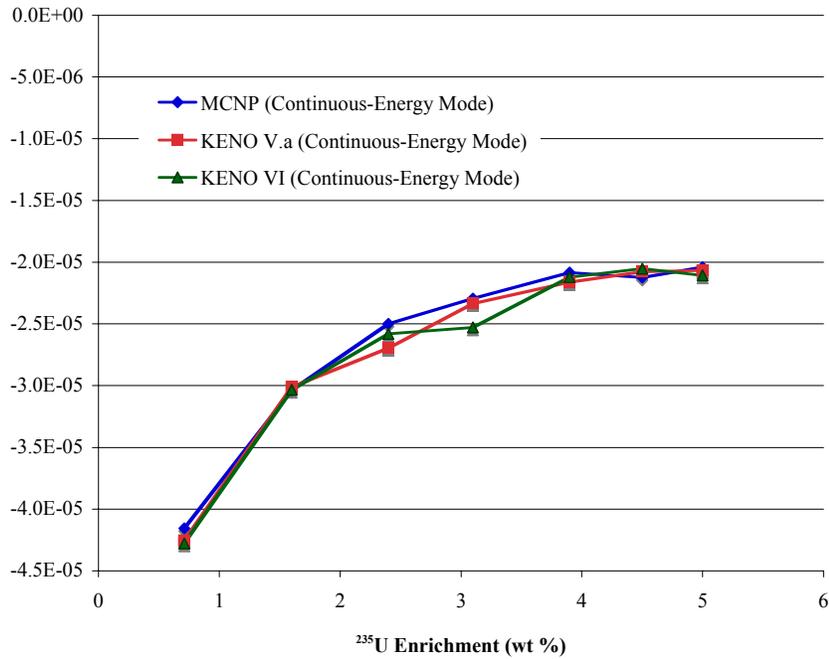
For all cases,  $\Delta T_{fuel}$  was 300 K. All calculations were run with 1100 generations, with 10,000 neutrons per generation and the first 100 generations skipped.

### 3. RESULTS

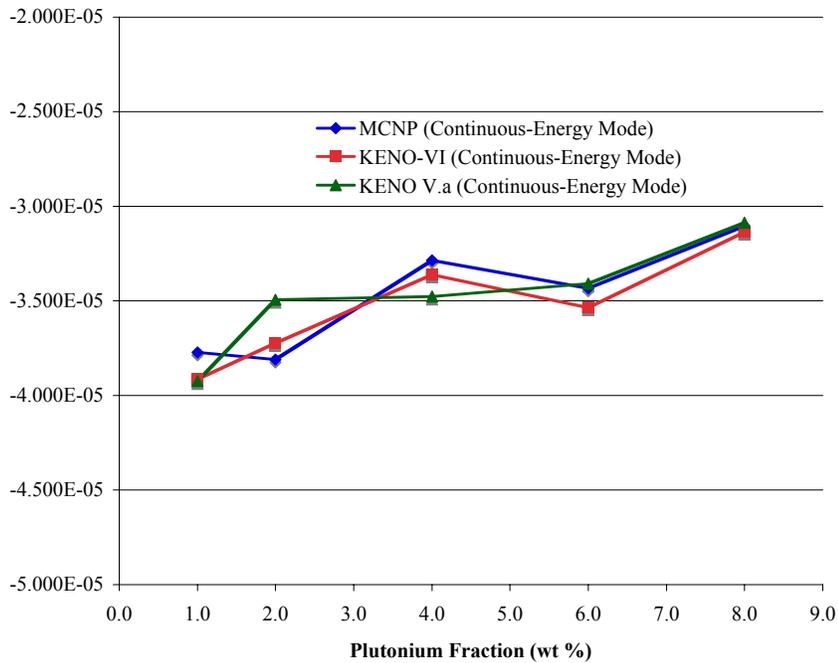
Eigenvalue results for KENO V.a and KENO-VI calculations were found to be statistically identical. The average difference in  $k_{eff}$  results was 0.012% between the two codes, which is less than the standard deviation resulting from statistical uncertainties. Doppler coefficients show some variability; however, those variations are due to the stochastic uncertainty in the eigenvalues. The behavior of the Doppler coefficient should in fact be a smoothly varying trend.

As an independent check, results were compared to MCNP calculations for the same benchmark [7]. All calculations were performed using ENDF/B-VI data. Figures 1–3 compare the results of the three codes, plotting the Doppler coefficient as a function of  $^{235}\text{U}$  enrichment (Fig. 1) and plutonium content (Figs. 2 and 3). Error bars are not plotted, but statistical errors were typically in the range of 3–8%. The results illustrated in the figures show exceptional agreement between the three methods. A comparison of the differences between the MCNP and KENO-VI was made to try to discern any trends in results. Tables I–III show the differences between the two eigenvalues predicted by the two codes. All eigenvalues were computed with a standard deviation uncertainty of less than or equal to 0.00025. It can be seen from Table I that MCNP overpredicts  $k_{inf}$  for  $\text{UO}_2$  relative to KENO-VI by on the order of 0.2%, with perhaps an increasing bias with increasing enrichment. Table II, which shows results for MOX with a reactor-recycle plutonium vector, indicates that MCNP underpredicted the fuel eigenvalue relative to KENO-VI; a clearer trend of an increasing bias with increasing  $\text{PuO}_2$  content is shown. Finally, Table III shows an initially positive bias that becomes more negative with increasing  $\text{PuO}_2$  content. Differences between HFP and HZP states are seen but are on the order of the Monte Carlo uncertainties, and no conclusions are justified.

It is unclear whether the  $k_{inf}$  differences result from differences between codes or between data. The KENO calculations were performed using ENDF/B-VI data processed by AMPX-2000; the MCNP calculations were based on ENDF/B-VI data processed by NJOY.



**Figure 1. Doppler coefficients calculated for UO<sub>2</sub> fuel.**



**Figure 2. Doppler coefficients calculated for weapons-grade MOX fuel.**

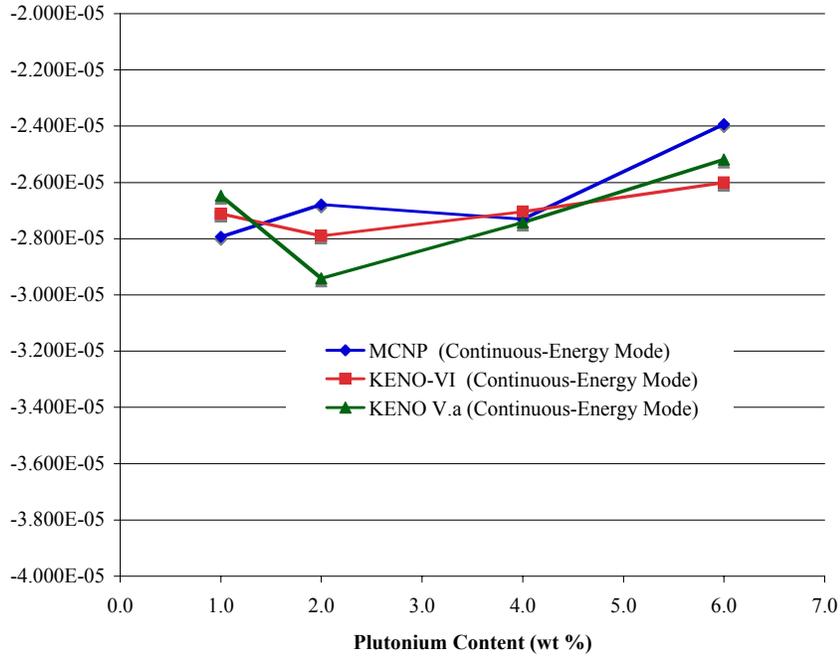


Figure 3. Doppler coefficients calculated for recycle-grade MOX fuel.

Table I. Differences between KENO-VI and MCNP eigenvalues for UO<sub>2</sub> fuel

Enrichment (wt % <sup>235</sup> U)	$\Delta k_{inf}$ (MCNP – KENO-VI)	
	HFP	HZP
0.711	0.001840	0.001430
1.6	0.002060	0.002030
2.4	0.002240	0.001760
3.1	0.002800	0.002010
3.9	0.002960	0.002400
4.5	0.002660	0.002610
5.0	0.002480	0.002350

**Table II. Differences between KENO-VI and MCNP eigenvalues for reactor-recycle-grade MOX fuel**

Enrichment (wt % PuO <sub>2</sub> )	$\Delta k_{inf}$ (MCNP – KENO-VI)	
	HFP	HZP
1.0	0.00149	0.001890
2.0	0.004420	0.003670
4.0	0.005610	0.006480
6.0	0.007580	0.007740
8.0	0.008420	0.009110

**Table III. Differences between KENO-VI and MCNP eigenvalues for weapons-grade MOX fuel**

Enrichment (wt % PuO <sub>2</sub> )	$\Delta k_{inf}$ (MCNP – KENO-VI)	
	HFP	HZP
1.0	0.001300	0.002060
2.0	0.000020	-0.000350
4.0	-0.002380	-0.002460
6.0	-0.002900	-0.003880
1.0	0.001300	0.002060

#### 4. CONCLUSIONS

Although still under development, both KENO V.a and KENO-VI appear to perform well relative to MCNP for this benchmark suite when run in continuous-energy mode. Earlier studies have shown similar behavior for other benchmarks and critical experiments. Completion and publication of the entire set of benchmark results will provide a wider range of results for comparison, from which additional conclusions may be drawn. Although not described in this paper, benchmark results were also submitted for calculations performed by both KENO V.a and KENO-VI in multigroup mode, as well as deterministic results from NEWT calculations, all based on ENDF/B-VI data.

Although the Doppler coefficients showed excellent agreement, a bias in the eigenvalue was observed between the MCNP and KENO results. These differences were not investigated in detail and are possibly the result of the different cross-section processing methodology (NJOY vs AMPX). A direct comparison between MCNP and KENO results using cross sections

processed from the same original ENDF data using AMPX (which can create MCNP-format continuous-energy data) would perhaps confirm that differences seen result from differences in cross-section processing.

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