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Accuracy and Runtime Improvements with SCALE 6.2

Bradley T. Rearden*, Benjamin R. Betzler, Matthew A. Jessee, William J. Marshall, Ugur Mertyurek, and Mark L. Williams

Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6170, USA
* reardenb@ornl.gov

Abstract - *The SCALE Code System is a widely used modeling and simulation suite for nuclear safety analysis and design that is developed, maintained, tested, and managed by the Reactor and Nuclear Systems Division of Oak Ridge National Laboratory. SCALE provides a comprehensive, verified and validated, user-friendly tool set for criticality safety, reactor physics, radiation shielding, radioactive source-term characterization, and sensitivity and uncertainty analysis. Since 1980, regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design. SCALE 6.2 represents one of the most comprehensive revisions in the history of SCALE, providing several new capabilities and significant improvements in many existing features. This paper provides a review of improved accuracy and runtime performance with SCALE 6.2 for criticality safety and reactor physics applications.*

I. INTRODUCTION

The SCALE Code System is a widely used modeling and simulation suite for nuclear safety analysis and design that is developed, maintained, tested, and managed by the Reactor and Nuclear Systems Division of Oak Ridge National Laboratory (ORNL) [1]. SCALE provides a comprehensive, verified and validated, user-friendly tool set for criticality safety, reactor physics, radiation shielding, radioactive source-term characterization, and sensitivity and uncertainty analysis. Since 1980, regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design. SCALE provides an integrated framework with dozens of computational modules, including three deterministic and three Monte Carlo radiation transport solvers that are selected based on the desired solution strategy. SCALE includes current nuclear data libraries and problem-dependent processing tools for continuous-energy (CE) and multigroup (MG) neutronics and coupled neutron-gamma calculations as well as activation, depletion, and decay calculations. SCALE includes unique capabilities for automated variance reduction for shielding calculations and for sensitivity and uncertainty analysis. SCALE's graphical user interfaces assist with accurate system modeling, visualization of nuclear data, and convenient access to desired results. SCALE 6.2 represents one of the most comprehensive revisions in the history of SCALE, providing several new capabilities and significant improvements in many existing features.

This paper provides a review of improved accuracy and runtime performance with SCALE 6.2 for criticality safety and reactor physics applications.

II. NUCLEAR DATA

The accuracy of all neutronics calculations depends on the availability of accurate nuclear data libraries generated from reliable sources using robust processing tools. ENDF/B-VII.1 nuclear data libraries are introduced in SCALE 6.2. CE data are available for general-purpose neutron, gamma, and coupled neutron/gamma calculations. MG neutron libraries in the 252– and 56-group structure are available, where the 252-group library is for general-purpose applications and the 56-group library is intended for light water reactor (LWR) analysis. Coupled neutron/gamma MG libraries are available in a fine 200-neutron/47-gamma group structure and a broad 28-neutron/19-gamma structure. The AMPX code system was used to generate these libraries [2]. The AMPX code system is available as part of the distribution of SCALE 6.2.

III. CONTINUOUS-ENERGY DATA PROCESSING

Investigations into the CE data generated by the AMPX code system for deployment in SCALE 6.0 and 6.1 revealed a need for improvement in the S(α,β) treatment, especially for forward-peaked kinematics. The SCALE 6.2 ENDF/B-VII.0 and ENDF/B-VII.1 data libraries have been generated using new AMPX processing procedures, and the benchmark testing results with SCALE 6.2 show substantially improved results relative to SCALE 6.1. [3] The calculated to experiment (C/E) ratio for select critical benchmark results for thermal mixed-oxide (MOX) systems from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [4] are provided in Fig. 1, which shows that the bias in the SCALE 6.2 ENDF/B-VII.0 CE results is reduced relative to SCALE 6.1 along with the experimental uncertainty and the calculated uncertainty due to cross-section covariance data. Additional testing has revealed that biases as large as 1000 pcm for burned LWR fuel are resolved with the improved treatment. Additional details and further results are provided in Ref. 5.

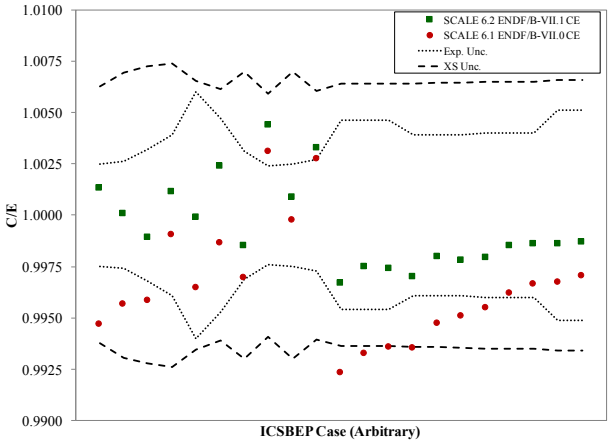

Fig. 1. SCALE C/E results for International Criticality Safety Benchmark Evaluation Project thermal mixed oxide critical systems.

Additionally, the probability tables that provide CE treatment in the unresolved resonance range have been improved, primarily through the inclusion of additional resolution and error correction. Testing with the new probability tables has shown reduced biases for systems that are sensitive to the intermediate energy range [5].

A total of 411 critical experiments from the ICSBEP have been modeled and cataloged in the SCALE Verified, Archived Library of Inputs and Data (VALID). [6] The VALID suite was used throughout the development of SCALE 6.2 to track the effects of incremental changes in the data processing and data libraries. The systems cover a range of fissile nuclides, material forms, and neutron energy spectra, as shown in TABLE I; the individual ICSBEP cases included in VALID are shown in TABLE II. Although the test suite is not exhaustive, it does provide a general indication of code performance across a broad collection of systems routinely modeled in SCALE using both KENO V.a and KENO-VI Monte Carlo Geometry Packages.

TABLE I. Types of Systems Included in the SCALE VALID Suite

Fissile materials
High-enriched uranium (HEU), Intermediate-enriched uranium (IEU) Low-enriched uranium (LEU) Plutonium (Pu) Mixed uranium/plutonium oxides (MIX)
Fuel form
Metal (MET), Fissile solution (SOL) Multi-material composition (e.g. fuel pins – COMP)
Neutron spectra
Fast (FAST) Thermal (THERM)

TABLE II. ICSBEP Cases Available in the SCALE VALID Suite

Sequence / Geometry	**Experiment class**	**ICSBEP case numbers**	**Number of configurations**
CSAS5 / KENO V.a	HEU-MET-FAST (HMF)	15, 16, 17, 18, 19, 20, 21, 25, 30, 38, 40, 65	18
	HEU-SOL-THERM (HST)	1, 13, 14, 16, 28, 29, 30	52
	IEU-MET-FAST (IMF)	2, 3, 4, 5, 6, 7, 8, 9	8
	LEU-COMP-THERM (LCT)	1, 2, 8, 10, 17, 42, 50, 78, 80	140
	LEU-SOL-THERM (LST)	2, 3, 4	19
	MIX-COMP-FAST (MCF)	5, 6	2
	MIX-COMP-THERM (MCT)	1, 2, 4	21
	MIX-SOL-THERM (MST)	2	3
	PU-MET-FAST (PMF)	1, 2, 5, 6, 8, 10, 18, 22, 23, 24	10
	PU-SOL-THERM (PST)	1, 2, 3, 4, 5, 6, 7, 11, 20	81
CSAS6 / KENO-VI	HEU-MET-FAST	5, 8, 9, 10, 11, 13, 24, 80, 86, 92, 93	27
	IEU-MET-FAST	19	2
	MIX-COMP-THERM	8	28

The average bias for each class of experiments in terms of absolute Δk and their associated standard deviation due primarily to the measurement uncertainty provided in the ICSBEP, including the minimal Monte Carlo stochastic uncertainty, are shown in Fig 2. The results shown in Fig. 2 are only for the CE calculations and illustrate the performance of SCALE 6.2 with the latest ENDF/B-VII.1 library compared with the performance of SCALE 6.1 with the ENDF/B-VII.0, which was the most recent library available when it was released. The lower bias for MOX systems, demonstrated in detail in Fig. 1, is evident in Fig. 2 as well where they are shown as "MCT." The bias for the water-moderated LCT cases is also reduced. The reactivity overprediction for the PST systems is a documented weakness in the ENDF/B‑VII.1 library [7], and the bias increases for HMF and MCF are also due to differences between ENDF/B-VII.0 and ENDF/B-VII.1.

Historically, only neutron CE data libraries with a specific reaction subset of the ENDF libraries have been supported in KENO Monte Carlo criticality safety codes. AMPX capabilities for the generation of CE neutron data have been improved and extended to support CE depletion, sensitivity analysis, and coupled neutron-gamma shielding analysis. Capabilities were added to generate gamma interaction data and to produce gamma yield data from neutron interactions. In addition, wide ranges of neutron reactions not needed for criticality calculations were also added to provide desired responses in the SCALE Monaco fixed-source Monte Carlo code [3].

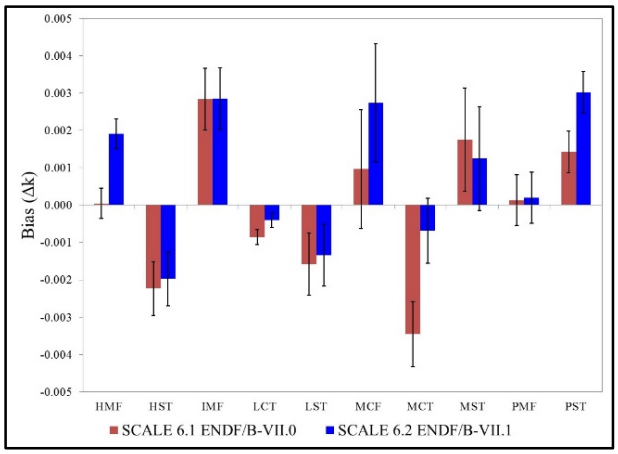

Fig. 2. Comparison of SCALE 6.1 and SCALE 6.2 CE results for a range of different types of systems.

The improved CE data have been comprehensively reviewed, verified, and validated with approximately 5,000 infinite medium eigenvalue tests, 6,300 fixed-source transmission tests, and more than 400 criticality and shielding benchmark experiments to ensure robust and accurate calculations.

IV. MULTIGROUP DATA PROCESSING

For MG analyses, ORNL has performed detailed comparisons between SCALE CE and MG results, and historically a bias of 200 to 500 pcm has been observed where the 238-group library is applied to LWR systems. The new 252-group structure for SCALE 6.2 provides a more detailed representation of the ^{238}U resonance structure. AMPX has been used to develop new 56– and 252-energy-group ENDF/B-VII.1 neutron cross-section libraries. In addition to the new group structures, the libraries have been generated using a new weighting spectrum with improved resonance self-shielding parameters. Specifically, for actinides and hydrogen in H_2O, a temperature-dependent CE flux spectrum has been generated with the CE CENTRM module for a pressurized water reactor (PWR) pin cell, and the CE flux spectrum has been used as a weighting function for library generation. Intermediate resonance parameters (lambdas) for all isotopes, which are included in the library provide a capability for improved self-shielding with the Bondarenko method. Bondarenko shielding factors, as a function of background cross section and temperature, were computed for all actinides (except ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu) using CE spectra calculated by CENTRM for homogeneous mixtures of the resonance material and hydrogen, corresponding to the respective background cross section. For the nuclides ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, and ^{241}Pu, the Bondarenko factors are based on CENTRM CE calculations for heterogeneous pin cell models that span the range of anticipated self-shielding conditions. The thermal cutoff for moderators and the free-gas approximation has been raised from 3 eV to 5 eV. The new library has been tested by analyzing a wide variety of critical benchmark experiments and by comparing results with CE Monte Carlo results. The 252-group results presented in Fig. 1 demonstrate consistent performance with the SCALE 6.2 CE results for the thermal MOX critical benchmark experiments. Based on additional studies with the 252-group library, computational benchmark comparisons with CE results at room temperature and elevated temperatures show agreement within 100 pcm in most cases.

Detailed results are shown in Fig. 3 with the C/E ratios for a suite of 123 low-enriched uranium systems moderated with water. The results for both the SCALE 6.1 238-group library based on ENDF/B-VII.0 and the SCALE 6.2 252-group library based on ENDF/B-VII.1 are shown. Both combinations slightly under-predict k_{eff}, but the magnitude of the bias is reduced slightly from -0.00185 Δk to -0.00148 Δk. The bias for the 56-group library based on ENDF/B-VII.1 is only 0.00062 Δk; for the sake of clarity, the detailed results are not shown in Fig. 3. These results demonstrate the improvements resulting from the optimized group structures available in SCALE 6.2.

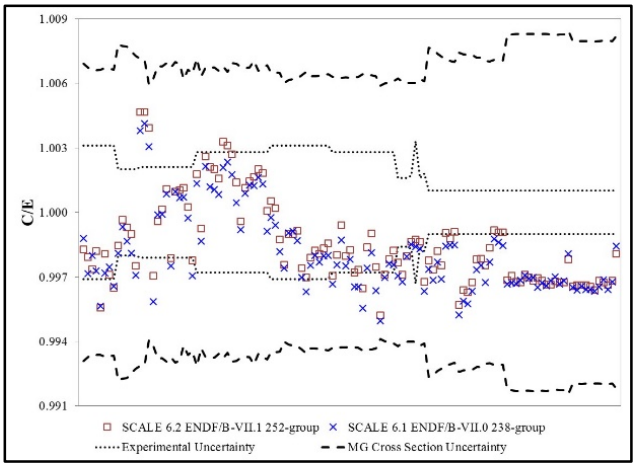

Fig. 3. Comparison of SCALE 6.1 and SCALE 6.2 MG results for 123 LCT benchmarks.

V. MODERNIZED RESONANCE SELF-SHIELDING

Most SCALE sequences have been updated to perform resonance self-shielding of MG cross sections and one-dimensional neutron transport calculations using the modern XSProc module. [8] XSProc provides the capabilities of BONAMI, CENTRM, PMC, WORKER, and XSDRN and has been demonstrated to produce equivalent results to the prior independent codes. XSProc runtime and memory requirements are substantially improved, especially when calculations with many unit cells are being performed. Generally, speedups in self-shielding of about 3× are realized, but in an extreme test case using an as-loaded spent nuclear fuel storage package with hundreds of unique materials, the cross-section processing and cell homogenization time was reduced from 5 days to 3.7 minutes while still obtaining equivalent results. This substantial speedup is due primarily to the modernized internal data structures of XSProc the minimize the need for disk access during a calculation.

XSProc provides for infinite homogeneous medium, lattice cell, multiregion, and double heterogeneous cell types. For all but the double heterogeneous cells, a new capability is implemented for accelerated self-shielding using intermediate resonance (IR) approximation Bondarenko treatment for the full energy range (PARM=BONAMI) as well as the more rigorous option of CE treatment in the resolved resonance range (PARM=CENTRM), with default treatment set as CE. Only the CENTRM path is available for double heterogeneous cell types.

XSProc provides capabilities for

- resonance self-shielding of microscopic data,
- macroscopic cross sections for mixtures,
- one-dimension MG transport calculations to calculate eigenvalues and flux-weighting functions,
- group collapsing of cross sections using flux spectra from the one-dimensional eigenvalue calculation or user input fixed source spectra, and
- spatial homogenization of cross sections across material zones.

With this modernized tool, sequence-specific control is available for the generation of on-disk or in-memory data libraries for microscopic or macroscopic data containing selected reaction cross sections and scattering data.

VI. ENHANCED RESONANCE SELF-SHIELDING METHODS

A new two-dimensional CENTRM option is available to explicitly treat the boundary of square-pitched and triangular-pitched LWR fuel pins with a Method-of-Characteristics (MoC) CE transport option, resulting in approximately 100 pcm reduction in bias between MG and CE calculations. However, the runtime is increase by a factor of approximately two when using this option. To enable this option, the user sets *NPXS=6* in the *centrm data* section of *celldata*.

New options are available in CENTRM/PMC to address the effects of resonance self-shielding on scattering matrices using the *N2D=* option in *centrm data* in *celldata*: *N2D=2* performs self-shielding corrections on the 0^{th} order scattering data (like default the *N2D=- 1* method) but also corrects the higher-order Legendre moments with corresponding higher-order fluxes; and *N2D=- 2* similarly treats the higher-order Legendre moments and explicitly treats within-group elastic scattering removal.

BONAMI has been rewritten as part of the overall SCALE modernization effort. BONAMI now implements IR approximation theory as well as the previous narrow resonance approximation. The IR approximation allows for improved accuracy for systems with overlapping resonances and provides a rapid self-shielding option using only full-range Bondarenko factors. This technique produces accurate results and provides up to a 10× speedup relative to CE treatment with CENTRM. IR theory is described in the updated BONAMI chapter of the SCALE manual. To enable this option, the user sets *PARM=BONAMI* on the sequence specification record (e.g. *=t-depl PARM=BONAMI*) and *IROPT=1* in the *more data* section of *celldata*.

VII. POLARIS—NEW ADVANCED LATTICE PHYSICS MODULE

Polaris is a new two-dimensional lattice physics code for SCALE that utilizes a new MG self-shielding method, called the Embedded Self-Shielding Method (ESSM) [9], and a new MoC transport solver. Polaris provides substantially simplified input requirements and improved runtime performance compared to TRITON.

The ESSM approach computes MG self-shielded cross sections using Bondarenko interpolation. The background cross section utilized in the interpolation is determined by a series of two-dimensional MoC fixed-source calculations, similar to the subgroup method that does not require explicit *celldata* input. Additionally, heterogeneous lattices are explicitly treated without the need to externally compute Dancoff factors. Additional details on ESSM are provided in Ref. 9.

Polaris currently employs ESSM with either the 252-group or 56-group ENDF/B-VII.1 libraries. Each library contains cross sections, IR parameters, and full-range Bondarenko factors for all nuclides.

Polaris utilizes the self-shielded cross sections within a MG two-dimensional eigenvalue calculation using the new MoC transport solver. The MoC solver has been developed within Denovo, which was originally developed for parallel three-dimensional Cartesian mesh MG discrete ordinates (S_N) calculations [10]. Polaris also provides a critical spectrum calculation for correcting the flux distribution for computing both few-group homogenized cross-section edits and depletion reaction rates.

Polaris is integrated with ORIGEN for depletion calculations. The depletion of each pin, or radial subregion of the pin, is based on the local normalized flux distribution. Cross sections in the ORIGEN transition matrix are updated from the MG self-shielded cross sections and the MG flux distribution for each depletion region. The critical-spectrum correction to the flux distribution for depletion is controlled by an input user option. The cross-section updates are performed in-memory as compared to the file-based approach utilized in the TRITON lattice physics sequence. Polaris supports branch calculations for the generation of few-group constants for reactor core simulators.

VIII.CONTINUOUS-ENERGY MONTE CARLO DEPLETION

SCALE 6.1 provided MG Monte Carlo depletion that coupled SCALE MG cross-section processing capabilities with KENO and ORIGEN. A new CE-based KENO/ORIGEN Monte Carlo depletion capability has been developed and can be utilized by simply changing the input library specification. CE depletion is especially useful for models with complex geometry that present difficulties in obtaining accurate resonance self-shielded MG data, and for models with many depletion regions where run-time to generate and store the resonance self-shielded cross-section data for each material is prohibitive.

The methodology implemented in this initial release of CE Monte Carlo depletion is the most robust, using reaction rate tallies for each cross section of each nuclide. However, it is intended as a reference calculation, not for routine production use. Subsequent updates to this capability are planned for accelerated performance.

KENO has also been updated for improved reproducibility across computer platforms, but these gains in reliability have resulted in slower MG calculations in SCALE 6.2 than were available in SCALE 6.1.

IX. TRITON RUN-TIME IMPROVEMENTS

Two-dimensional lattice physics calculations with TRITON will realize substantial speedups due to the use of XSProc for resonance self-shielding as well as numerous optimizations within the NEWT code. Speedups of 2× to 6× faster calculations are common, and some models have realized speedups of 30× relative to previous versions of NEWT. Calculation times for 1,470 TRITON calculations used to generate the ORIGEN reactor libraries for SCALE 6.1.3 and SCALE 6.2 are shown in Fig. 4. For the calculation, the average calculation time was reduced by a factor of 4.

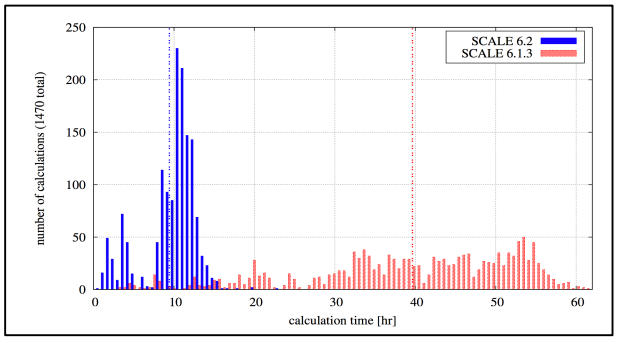

Fig. 4. Comparison of calculation times for 1,470 TRITON calculations.

X. LATTICE PHYSICS ACCURACY

In addition to the criticality safety benchmark assessments described above, approximately 400 numeric LWR lattice benchmarks were developed to compare k_{eff} and pin-by-pin fission rate distributions between CE-KENO, TRITON/NEWT, and the newly developed Polaris lattice physics code. The numeric benchmarks spanned a wide range of lattice designs and system parameters such as fuel temperature, soluble boron concentration, moderator density, control rod and control blade design and composition, and burnable absorber design and composition.

Fig. 5 provides a pin-by-pin fission rate comparison for a 17×17 PWR lattice at nominal conditions. The reference solution was generated with CE-KENO using

150 million particle histories such that the pin fission rate statistical uncertainty is less than 0.01%. The top number represents the percentage difference for the NEWT calculation; the bottom number is the Polaris pin fission rate difference. Fig. 5 displays excellent consistency for both TRITON/NEWT and Polaris with reference CE Monte Carlo calculation, with pin fission rate root mean square (RMS) of 0.09% and 0.07%, respectively.

Comparisons are given in Fig. 6 for a boiling water reactor (BWR) 10×10 lattice at 40% void fraction. Pin fission rate errors are generally higher for BWR lattices than for PWR lattices due to the more heterogeneous design. Pin fission rate differences of 0.9% are shown in the northwest corner pin, where the neutron moderation from the wide bypass region is most significant. BWR lattice modeling with TRITON/NEWT presents modeling challenges such as performing prior calculations with the SCALE MCDANCOFF code to compute pin-by-pin Dancoff factors for the self-shielding calculations with XSProc. The Polaris self-shielding calculation is performed with ESSM, which explicitly accounts for nonuniform self-shielding effects without user setup of the unit cell calculations or Dancoff factor calculations. The RMS and maximum pin fission rate differences for Polaris with CE-KENO are 0.23% and 0.84%, respectively. The TRITON/NEWT pin fission rate RMS and maximum pin fission rate differences are 0.5% and 0.90%, respectively.

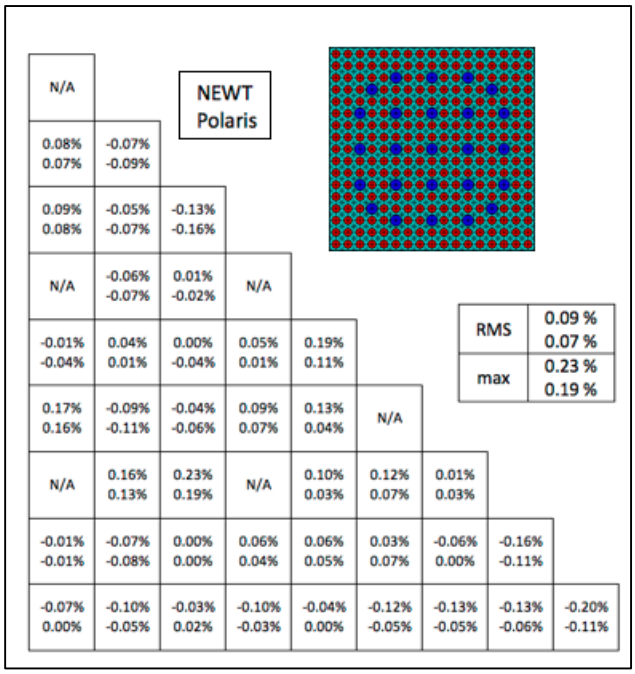

Fig. 5. 17×17 PWR lattice pin fission rate differences at nominal conditions for NEWT and Polaris.

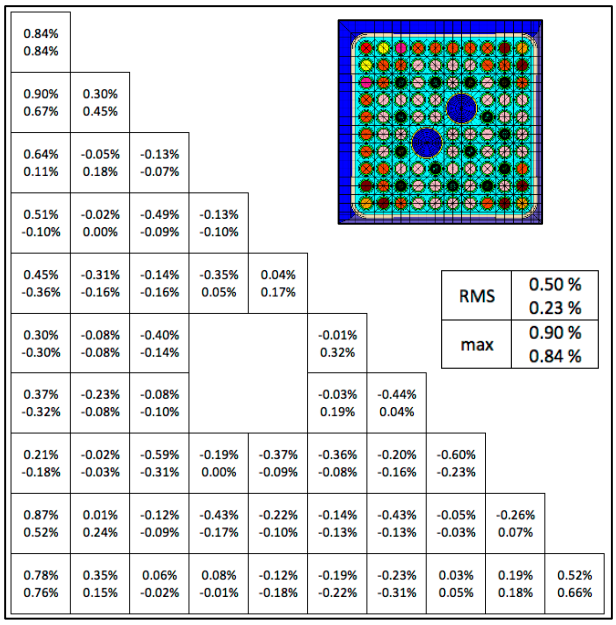

Fig. 6. 10×10 BWR lattice dominant zone pin power differences at 40% void fraction for NEWT and Polaris.

XI. BIAS REDUCTION FOR DEPLETION

Historical SCALE biases have been mitigated because of the numerous enhancements included in SCALE 6.2. Fig. 7 shows the results for a reference PWR pin cell burnup calculation using SCALE 6.1 and SCALE 6.2. The SCALE 6.2 CE results are the reference, and the SCALE 6.1 CE results are simply eigenvalue statepoints using the isotopics provide by the SCALE 6.2 results. The large discrepancy between SCALE 6.1 and 6.2 CE results is due primarily to the previously discussed issue with thermal scattering data in SCALE 6.1. The SCALE 6.1 TRITON 238–group results use the default settings from SCALE 6.1. The TRITON 252–group results apply the improved nuclear data library, the CENTRM MoC solver, and the enhanced within-group treatment for CENTRM/PMC, *N2D=-2*. The SCALE 6.2 Polaris results apply the default settings in Polaris applying the ESSM methodology with the IR factors on the library. These calculations demonstrate the impact of improvements in both the MG libraries and resonance self-shielding techniques as well as the improvements in the CE treatments from SCALE 6.1 to SCALE 6.2.

XII. CONCLUSIONS

SCALE 6.2 provides many improvements in accuracy and runtime, especially for reactor physics calculations. CE Monte Carlo biases for MOX or burned-fuel calculations have been minimized with numerous revisions to the CE data and physics implementation in the codes. Historical biases in MG LWR calculations have reduced from 400 to 500 pcm from earlier versions of SCALE to approximately 100 pcm with SCALE 6.2 through many improvements in

the nuclear data, group structures, and resonance self-shielding techniques. Runtimes for lattice physics calculations are greatly improved with the availability of the new Polaris tool as well as numerous enhancements in XSProc and NEWT as applied in TRITON.

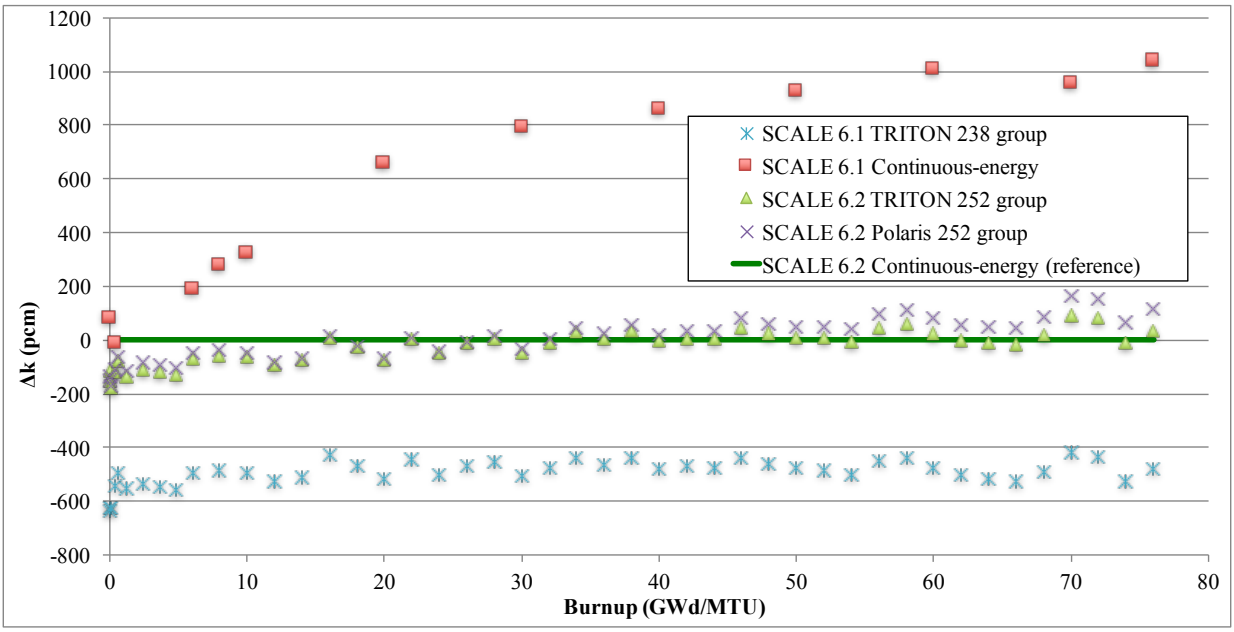

Fig. 7. Comparison of computational biases as a function of burnup.

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