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NCSD Conference Paper #3
7/18/01 11:28 AM

Computational Physics and Engineering Division (10)

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Charlotta E. Sanders and Mark D. DeHart

Oak Ridge National Laboratory,*
P.O. Box 2008,
Oak Ridge, TN 37831-6370

sandersc@ornl.gov (865) 574-5279
dehartmd@ornl.gov (865) 576-3468

Submitted to the
2001 ANS Embedded Topical Meeting on
Practical Implementation of Nuclear Criticality Safety,
November 11–15, 2001,
Reno, Nevada, USA

Organized and Sponsored by the
Nuclear Criticality Safety Division of the American Nuclear Society

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*Managed by UT-Battelle, LLC, under contract DE-AC05-00OR22725 for the U.S. Department of Energy.

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Executive Summary

The concept of burnup credit was introduced in the late 1980s as a mechanism to take credit for the reduced reactivity worth of spent nuclear fuel (SNF) in various potential applications. At present, most research has been directed toward transportation and dry storage applications. Within this realm, Interim Staff Guidance on burnup credit (ISG-8) for pressurized water reactor SNF, issued by the Nuclear Regulatory Commission's Spent Fuel Project Office, recommends an approach based on limited burnup credit based on that available from actinide nuclides only. To take credit for this safety margin, however, ISG-8 also recommends evaluation of the magnitude of the additional reactivity margin associated with nuclides not included in the safety analysis. A computational benchmark has been developed to provide a common reference for evaluation of license submittals. This benchmark provides results of analyses performed with the SAS2H and CSAS25 sequences of the SCALE 4.4a code package. Independent calculations have been performed to verify the original benchmark calculations. This paper presents results of calculations performed with both HELIOS-1.6/KENO V.a codes and HELIOS-1.6/MCNP4B codes. These calculations estimate non-safety-basis reactivity margin based on the benchmark specification. The paper provides comparisons of results that demonstrate that the various code packages produce very similar results, and reinforces the validity of the original analyses.

1. Introduction

Spent fuel storage in dry casks is currently licensed under the requirement that the cask would remain subcritical in an accident scenario even if loaded with fresh fuel. In other words, no credit is taken for the reduction in the fuel reactivity as a result of in-reactor burnup and post-irradiation decay. This approach can be improved by applying burnup credit, i.e., taking credit for some or all of the reactivity decrement associated with burned fuel. Burnup credit allows increased cask loading or loading with higher initial enrichments than would be possible if all fuel were assumed to be fresh. The Interim Staff Guidance [1] on burnup credit (ISG-8) for pressurized water reactor (PWR) spent nuclear fuel (SNF), issued by the Spent Fuel Project Office of the Nuclear Regulatory Commission (NRC), recommends an approach that limits credit for the reactivity reduction associated with burnup to that available from actinide isotopes only. Further, the actinides are limited to those that have been validated (e.g., benchmarks of applicable fuel assay measurements). The NRC does not currently advocate credit for the

reactivity reduction due to fission products. This is because of the greater uncertainties associated with inventory prediction and cross-section data for fission products, due to a lack of sufficient measured data for validation. Hence, an added safety margin exists due to the presence of fission product and actinide nuclides not included in the safety analysis. To take credit for this safety margin, however, ISG-8 recommends evaluation of the magnitude of the additional reactivity by a license applicant.

A computational benchmark has been developed to provide a common reference for evaluation of license submittals [2]. This benchmark specification provides for the estimation of additional reactivity margin by an applicant, using codes, data, and modeling approximations consistent with the applicant's approach. Additionally, a qualified understanding of the additional margin may be a first step toward further burnup credit that uses some, or all, of this margin in safety analyses. The benchmark provides a well-documented reference problem that will help to compare estimates of reactivity margin available from fission products and minor actinides, as a function of initial fuel enrichment, burnup and cooling time for a defined cask design.

The computational benchmark of Ref. [2] presents results of analyses performed with the SAS2H (depletion) and CSAS25 (criticality) sequences of the SCALE 4.4a code package. Independent calculations have been performed to verify the original benchmark calculations. This paper presents results of calculations performed with both HELIOS-1.6 (depletion)/KENO V.a (criticality) codes and HELIOS-1.6/MCNP4B (criticality) codes. As per the benchmark specification, these calculations estimate additional (non-safety-basis) reactivity margin as a function of burnup and cooling time for 4 wt % enriched fuel. This paper provides a brief description of the various code packages, comparisons of the results between the various code packages and a discussion of the differences observed between the different codes and data.

2. Background

Criticality safety analyses for commercial spent fuel storage and transport canisters have in the past assumed that the spent fuel is unirradiated (fresh) with uniform isotopic compositions. The assumption of fresh fuel simplifies the safety analysis because fuel-operating history does not have to be considered. However, because this assumption neglects the reactivity decrease resulting from irradiation, severe limits are imposed on the SNF capacity for a given package volume.

To date, the typical approach for validation of depletion calculations has been to quantify calculated isotopic predictions through comparison against radiochemical assay measurements from spent nuclear fuel samples. Consequently, utilization of nuclides in a safety analysis process has been primarily limited by the availability of measured assay data. In particular, there is very little available assay data for fission products and therefore many criticality analyses include only a limited set of actinide isotopes.

The use of a subset of actinides in burnup credit calculations is commonly referred to as "actinide-only" burnup credit. The nuclides used in this paper for actinide-only calculations are consistent with those specified in the DOE Topical Report on Burnup Credit [3], with the exception that ^{236}U and ^{237}Np are also included. The use of a subset of possible actinides and

fission products will be referred to herein as "actinide + fission product" burnup credit. The nuclides used in this work for actinide + fission product calculations are consistent with those identified in Table 2 of Ref. [4] as being the most important for burnup credit criticality calculations. Table 1 lists the nuclides included for the two classifications of burnup credit for this study. These "classes" of burnup credit and the nuclides included within each are defined here for the purposes of discussion; other terminology and specific sets of nuclides have been defined and used elsewhere in the literature.

Table 1. Nuclides Associated with the Various Classifications of Burnup Credit.

Actinide-Only Burnup Credit Nuclides (12 total)									
^{234}U	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{237}Np
^{241}Am	O[†]								
Actinide + Fission Product Burnup Credit Nuclides (29 total)									
^{234}U	^{235}U	^{236}U	^{238}U	^{238}Pu	^{239}Pu	^{240}Pu	^{241}Pu	^{242}Pu	^{241}Am
^{243}Am	^{237}Np	^{95}Mo	^{99}Tc	^{101}Ru	^{103}Rh	^{109}Ag	^{133}Cs	^{147}Sm	^{149}Sm
^{150}Sm	^{151}Sm	^{152}Sm	^{143}Nd	^{145}Nd	^{151}Eu	^{153}Eu	^{155}Gd	O[†]	

3. Code Description

As mentioned earlier, Ref. [2] provides results of analyses performed with the SAS2H and CSAS25 sequences of the SCALE 4.4a code package. The calculations described herein have been performed independently with other code packages. All depletion calculations for independent evaluation were performed using the HELIOS-1.6 code package [5]. HELIOS is a two-dimensional, generalized-geometry transport theory code based on the method of collision probabilities with current coupling. All calculations described herein are for an infinite array of fuel assemblies and utilize the 45-group neutron cross-section library, based on ENDF/B-VI that is distributed with the HELIOS-1.6 code package. The various structures within each of the assembly models were coupled using angular current discretization (interface currents).

Criticality calculations were performed with both the KENO V.a module of the SCALE system [6] and the Monte Carlo N-Particle (MCNP) code [7]. KENO V.a is a multigroup Monte Carlo criticality program employed to calculate the neutron multiplication factor, k_{eff}, for a three-dimensional (3-D) system. The KENO V.a criticality calculations used the SCALE 238-group cross-sections based on ENDF/B-V. MCNP is a 3-D, continuous-energy, Monte Carlo code that uses pointwise cross section data. The MCNP criticality calculations presented in this paper also used ENDF/B-V data.

[†] Oxygen is neither an actinide nor a significant fission product, but is included in this list because it is an integral and important part of PWR fuel, and is included in all calculations.

4. Results and Discussion

A generic 32 PWR-assembly burnup credit cask design (GBC-32) was developed according to the specifications given in the benchmark report [2] for KENO V.a and MCNP. The fuel assembly design used in the cask is a Westinghouse 17×17 fuel assembly with an initial fuel enrichment of 4 wt % ^{235}U. The fuel specifications are given in Ref. [2]. Depletion calculations were performed assuming that the fuel pellet outside diameter has expanded to the cladding inner diameter (i.e., the gas gap is homogenized with the fuel). Consequently, the fuel density was reduced to account for the increased volume. All depletion calculations were performed using the operational parameters given in Table 2 that ensure a conservative prediction of k_{eff} [4]. A cross-sectional view of the cask model is shown in Figure 1.

Table 2. Summary of parameters used for the depletion calculations

Parameter	Value used in analyses
Moderator temperature (K)	600
Fuel temperature (K)	1000
Fuel density (g/cm^3)	10.1102 (UO_2)
Clad temperature (K)	620
Clad density (g/cm^3)	2.699 (Zr)
Power density (MW/MTU)	60
Moderator boron concentration (ppm)	650 (assumed constant over cycle)

Uniform Axial Burnup Distribution

The active fuel length in the criticality model is divided into 18 equal-length axial regions to allow accurate modeling of the variations in the axial burnup distribution. The first set of calculations assumed a uniform axial burnup at an initial fuel enrichment of 4.0 wt % ^{235}U. Table 3 lists k_{eff} values as a function of burnup and 0 year cooling time as well as the differences between the k_{eff} values produced by the different code systems. The k_{eff} values are given for two different nuclide sets: actinide-only and actinide + fission products (according to Table 1). The column labeled *Benchmark* provides the results listed in Ref. [2]. It can be seen that the Δk values (i.e., differences of k_{eff} between the various codes) are increasing with burnup for the actinide-only calculations while there are no such apparent trend for the actinide + fission product calculations. Further, Δk values are primarily negative for the actinide only comparisons while the Δk values are mostly positive for the actinide + fission products comparisons. SAS2H is known to underestimate ^{235}U and overestimate fission products (due to limitations in the 1-D SAS2D model), which may explain why the actinide-only differences are negative and the actinide + fission product results are positive. The differences in k_{eff} with burnup between the independent calculations and the benchmark lie within an acceptable 1%. Interestingly, the

difference is largest at 40 GWd/MTU, and decreases in going to 60 GWd/MTU. The magnitudes of Δk for KENO - MCNP results are generally lower than the other comparisons. This is due to the fact that HELIOS performed the depletion part of the calculation for both the KENO and MCNP results. In addition, the differences between the codes seem to increase with burnup for the actinide-only cases but decrease with burnup for the actinide + fission product errors. It is likely that errors associated with fission product cross-sections appear to offset errors associated with actinide cross-sections.

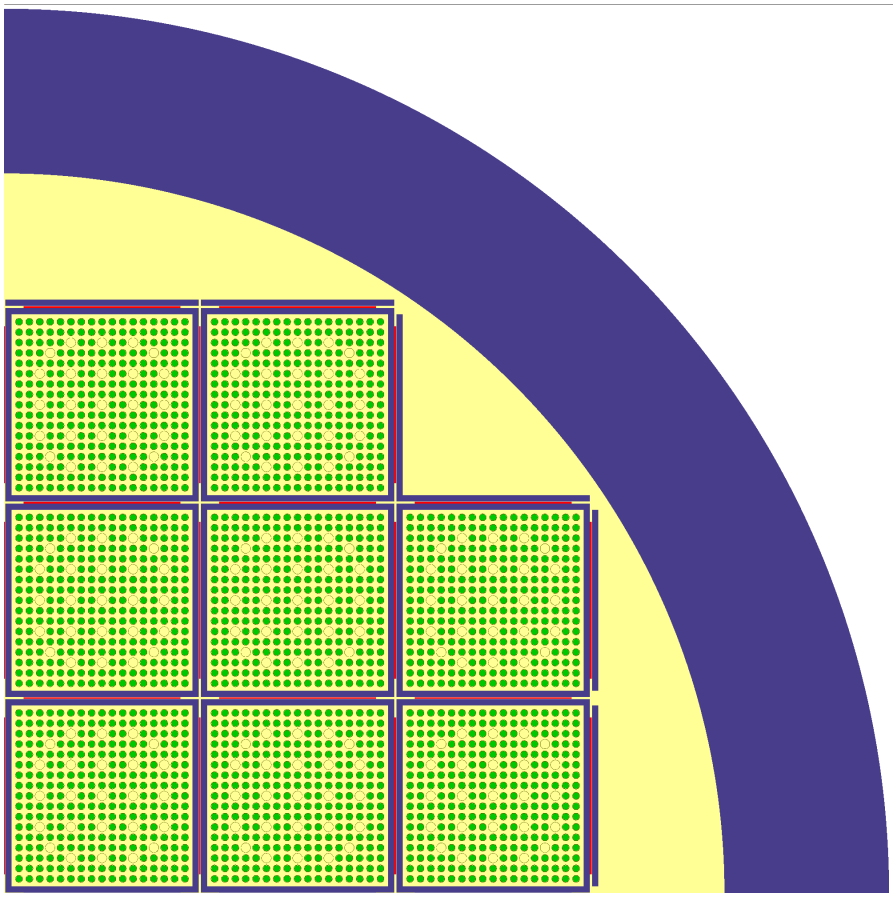

Figure 1. Radial cross section of ¼ of the GBC-32 cask .

Table 3. k_{eff} values with uniform axial burnup for the cask as a function of burnup. The results correspond to an initial fuel enrichment of 4.0 wt % ^{235}U and zero cooling time.

Actinide only						
Burnup (GWd/MTU)	k_{eff} (KENO)	k_{eff} (Benchmark)	k_{eff} (MCNP)	Δk (KENO-Benchmark)	Δk (MCNP-Benchmark)	Δk (KENO-MCNP)
0	1.1398[a]	1.13983[b]	1.13990[c]	-0.00003	0.00007	-0.0001
20	1.0399	1.04253	1.03924	-0.00263	-0.00329	0.00066
30	0.9897	0.99331	0.99300	-0.00361	-0.00031	-0.0033
40	0.9427	0.94777	0.94543	-0.00507	-0.00234	-0.00273
60	0.8559	0.86753	0.86279	-0.01163	-0.00474	-0.00689
Actinide + Fission products						
0	1.1398	1.13983	1.13990	-0.00003	0.00007	-0.0001
20	0.9932	0.98755	0.98993	0.00565	0.00238	0.00327
30	0.9306	0.92337	0.92955	0.00723	0.00618	0.00105
40	0.8711	0.86140	0.86834	0.00970	0.00694	0.00276
60	0.7670	0.76200	0.76534	0.00500	0.00334	0.00166

[a] Standard deviations for the KENO results are all < 0.0006.
[b] Standard deviations for the benchmark results are all < 0.0007.
[c] Standard deviations for the MCNP results are all < 0.0005.

Table 4 lists k_{eff} values for a burnup of 60 GWd/MTU and 5-year cooling time. Upon comparing the Δk values with the corresponding ones from the calculations with zero cooling time, it can be seen that, in general, the differences have increased with a 5-year cooling time. The increase can be attributed to the build up of fission products with large cross-section uncertainties. The differences between the various codes still lie within 1%.

Table 4. k_{eff} values with uniform axial burnup for the cask at 60 GWd/MTU burnup. The results correspond to an initial fuel enrichment of 4.0 wt % ^{235}U and a cooling time of 5 years.

Actinide only						
Burnup (GWd/MTU)	k_{eff} (KENO)	k_{eff} (Benchmark)	k_{eff} (MCNP)	Δk (KENO-benchmark)	Δk (MCNP-benchmark)	Δk (KENO-MCNP)
60	0.8296[a]	0.84129[b]	0.84009[c]	–0.01169	–0.00120	–0.01049
Actinide + Fission products						
60	0.7246	0.71732	0.72744	0.00728	0.01012	–0.00284

[a] Standard deviations for the KENO results are all < 0.0005.
[b] Standard deviations for the benchmark results are all < 0.0004.
[c] Standard deviations for the MCNP results are all < 0.0004.

Table 5 lists k_{eff} values corresponding to a burnup of 60 GWd/MTU and a 20-year cooling time. The Δk values at 60 GWd/MTU of the 5-year cooling time and 20 year cooling are fairly similar. Consequently, the additionally increase in cooling time did not affect the differences between the

codes significantly. It is interesting to note that Δk is fairly constant, or slightly decreasing, with cooling time for the actinide-only calculations, but is increasing with cooling time for the actinide + fission product calculations. Differences in both actinides and fission product concentrations are attributed to the depletion model. However, because of the shorter half-lives of fission products versus actinides, differences are more manifest for fission products in the 5-20 year cooling time frame. For example, the strong absorber ^{155}Gd is beginning to buildup after about 5 year of cooling time due to decay of its parent, ^{155}Eu ($\tau_{½}$=4.75 years). The small differences that can be noted for the actinide only cases are primarily due to the change in the concentration of the ^{241}Pu isotope ($\tau_{½}$=14.4 years).

Table 5. k_{eff} values with uniform axial burnup for the cask at 60 GWd/MTU burnup. The results correspond to an initial fuel enrichment of 4.0 wt % ^{235}U and a cooling time of 20 year.

Actinides only						
Burnup (GWd/MTU)	k_{eff} (KENO)	k_{eff} (Benchmark)	k_{eff} (MCNP)	Δk (KENO-benchmark)	Δk (MCNP-benchmark)	Δk (KENO-MCNP)
60	0.7733 [a]	0.78298 [b]	0.78150 [c]	–0.00968	–0.00148	–0.00820
Actinide + Fission products						
60	0.6669	0.65852	0.67223	0.00838	0.01371	–0.00533

[a] Standard deviations for the KENO results are all < 0.0004.
[b] Standard deviations for the benchmark results are all < 0.0005.
[c] Standard deviations for the MCNP results are all < 0.0004.

Axially Varying Burnup Distribution

The second set of calculations used a non-uniform axial burnup (the active fuel length in the criticality model divided into 18 equal-length axial regions) at an initial fuel enrichment of 4.0 wt % ^{235}U. The axial burnup profile used corresponds to the bounding profile suggested by Ref. [3] for PWR fuel with average assembly discharge burnup greater than 30 GWd/MTU. Table 6 lists k_{eff} values as a function of burnup and 0 year cooling time as well as the differences between the k_{eff} values produced by the different code systems. As before, the k_{eff} values are given for two different nuclide sets: actinide-only and actinide + fission products. The column labeled *Benchmark* refers to the results listed in the benchmark report. It is interesting to note that while the actinide-only Δk values are increasing with increasing burnup, the Δk values for actinide + fission products are actually decreasing. The k_{eff} values are higher for the non-uniform axial burnup calculations than for the uniform burnup calculations. The increase in reactivity is due to the under-burned (with respect to the assembly-average burnup) regions near the fuel ends. The Δk values of the uniform axial model and the non-uniform axial model are essentially unaffected for both the actinide-only and actinide + fission cases. The differences in k_{eff} with burnup between the independent calculations and the benchmark lie within 1.1 % for the high burnup 60 GWd/MTU cases.

Table 6. k_{eff} values with non-uniform axial burnup for the cask as a function of burnup. The results correspond to an initial fuel enrichment of 4.0 wt % ^{235}U and zero cooling time.

Actinide only						
Burnup (GWd/MTU)	k_{eff} (KENO)	k_{eff} (Benchmark)	k_{eff} (MCNP)	Δk (KENO-Benchmark)	Δk (MCNP-Benchmark)	Δk (KENO-MCNP)
30	0.9911[a]	0.99512[b]	0.98675[c]	–0.00402	–0.00837	0.00435
60	0.8851	0.89627	0.88834	–0.01117	–0.00793	–0.00324
Actinide + Fission products						
30	0.9418	0.93577	0.94277	0.00603	–0.00700	–0.00097
60	0.8210	0.81741	0.81926	0.00359	0.00185	0.00174

[a] Standard deviations for the KENO results are all < 0.0006.
[b] Standard deviations for the benchmark results are all < 0.0006.
[c] Standard deviations for the MCNP results are all < 0.0004.

5. Conclusion

This paper has presented the results of a computational benchmark and independent calculations to verify the benchmark calculations for the estimation of the additional reactivity margin available from fission products and minor actinides in a PWR burnup credit storage/transport environment. The calculations were based on a generic 32 PWR-assembly cask. The differences between the independent calculations and the benchmark lie within 1% for the uniform axial burnup distribution, which is acceptable. The Δk for KENO - MCNP results are generally lower than the other Δk values, due to the fact that HELIOS performed the depletion part of the calculation for both the KENO and MCNP results. The differences between the independent calculations and the benchmark for the non-uniform axial burnup distribution were within 1.1 %.

References

1. *Spent Fuel Project Office Interim Staff Guidance – 8, Rev. 1 – Limited Burnup Credit*, U.S. Nuclear Regulatory Commission, July 30, 1999.

2. J. C. WAGNER, *Computational Benchmark for Estimation of Reactivity Margin from Fission Products and Minor Actinides in PWR Burnup Credit*, ORNL/TM-2000/306, in preparation.

3. *Topical Report on Actinide-Only Burnup Credit for PWR Spent Nuclear Fuel Packages*, DOE/RW-0472, Rev. 2, U.S. Department of Energy, Office of Civilian Radioactive Waste Management, September 1998.

4. C. V. PARKS, M. D. DeHART and J. C. WAGNER, *Review and Prioritization of Technical Issues Related to Burnup Credit for LWR Fuel*, NUREG/CR-6665 (ORNL/TM-1999/303), U.S. Nuclear Regulatory Commission, Oak Ridge National Laboratory, February 2000.

5. J. J. CASAL, R. J. J. STAMM'LER, E. A. VILLARINO, and A. A. FERRI, "HELIOS: Geometric Capabilities of a New Fuel-Assembly Program," Vol. 2, p. 10.2.1 113, *Intl Topical Meeting on Advances in Mathematics, Computations, and Reactor Physics,* Pittsburgh, Pennsylvania, April 28–May 2, 1991.

6. *SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation*, NUREG/CR-0200, Rev. 6 ORNL/NUREG/CSD-2/R6), May 2000. Available from Radiation Safety Information Computational Center at Oak Ridge National Laboratory as CCC-545.

7. J. F. BRIESMEISTER, *MCNP -- A General Monte Carlo N-Particle Transport Code, Version 4C*, Los Alamos National Laboratory, LA-13079-M (2000).