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Validation of SCALE-4 for a Reference Problem Set

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FOR THE UNITED STATES
DEPARTMENT OF ENERGY

ORNL/M--1332

DE91 016050

VALIDATION OF SCALE-4 FOR A REFERENCE PROBLEM SET*

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July 1991

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Prepared under the direction of
Sandia National Laboratories
under subcontract 66-0162 with Oak Ridge National Laboratory

MARTIN MARIETTA ENERGY SYSTEMS, INC.
managing the
Oak Ridge National Laboratory Oak Ridge Y-12 Plant
Oak Ridge Gaseous Diffusion Plant Paducah Gaseous Diffusion Plant
for the
U.S. DEPARTMENT OF ENERGY
under contract DE-AC05-84OR21400

This report presents the results of criticality calculations performed to validate the recently released SCALE-4 modular code system[1] for light water reactor (LWR) fuel for a proposed reference problem set of critical experiments[2] which model various conditions typical of transportation and storage casks. In order to validate SCALE-4, the CSAS4 control module was used to calculate the effective neutron multiplication factor (k_{eff}) via the BONAMI,[3] NITAWL-II,[4] and KENO V.a[5] codes. Calculations were performed with both SCALE-4 and SCALE-3. The cross-section libraries used were the 27-group ENDF/B-IV library (27GROUPNDF4) and the 27-group ENDF/B-IV burnup library (27BURNUPLIB). The 27BURNUPLIB library is an extension of the 27GROUPNDF4 library to include fission product nuclides which are necessary for depleted fuel analyses. The added fission product cross sections were obtained from ENDF/B-V data.

Sixteen experiments from eight references were modeled in order to examine eight different aspects of criticality related to fuel storage in transportation and storage casks:

(1) neutron interaction between fuel assemblies,

(2) effectiveness of neutron flux traps between fuel assemblies to reduce reactivity,

(3) effect of voiding on the effectiveness of neutron flux traps,

(4) effectiveness of neutron absorber plates and rods to reduce interaction between fuel assemblies,

(5) reactivity effect of commonly used biological shielding materials,

(6) neutron spectra shift or relative neutron moderation caused by dissolved boron,

(7) plutonium buildup and uranium depletion, and

(8) subcritical neutron multiplication in a cask configuration, including neutron poison baskets.

Table 1 lists the experiments modeled, their distinctive characteristics as related to the aspects of criticality listed above, and the calculated k_{eff} values. The calculations were performed with 600 neutrons per batch and a minimum of 120,000 histories. All experiments were water moderated and

Table 1. Experiment descriptions and calculated results

Reference/Experiment	Characteristics	SCALE-4 27GROUP	SCALE-4 27BURNUP	SCALE-3 27GROUP
5 / 214R	Flux traps	.9894±.0022	.9933±.0022	.9891±.0024
5 / 214V3	Flux traps with voids	.9971±.0022	.9918±.0020	.9990±.0023
Mean k_{eff}		.9932	.9926	.9941
6 / 005	No plates	.9950±.0021	.9912±.0021	.9950±.0022
6 / 017	Boral™ plates	.9970±.0022	.9915±.0020	.9894±.0020
6 / 024	Aluminum plates	.9943±.0020	.9956±.0017	.9972±.0022
6 / 028	SS304 plates	.9890±.0029	.9952±.0019	.9923±.0021
Mean k_{eff}		.9938	.9934	.9935
7 / N/A	Depleted uranium walls	.9971±.0020	.9991±.0018	.9972±.0022
7 / N/A	Lead walls	1.0046±.0024	.9980±.0024	.9994±.0021
8 / N/A	Steel walls	.9979±.0023	.9981±.0021	1.0002±.0022
Mean k_{eff}		.9999	.9984	.9989
9 / 173	No boron, wide pitch	.9920±.0024	.9918±.0022	.9950±.0021
9 / 177	2.55 g/l boron, wide pitch	.9925±.0016	.9957±.0020	.9969±.0020
9 / 178	No boron, narrow pitch	.9903±.0023	.9930±.0024	.9966±.0019
9 / 181	2.55 g/l boron, narrow pitch	.9870±.0015	.9897±.0019	.9916±.0020
Mean k_{eff}		.9904	.9925	.9950
10 / 2282	B_4C rods between assemblies	.9893±.0022	.9862±.0020	.9886±.0020
11 / 196	Ass'y of mixed oxide & UO_2 rods arranged in an uniform pattern to approximate 20,000 MWD/MTU burnup	.9840±.0020	.9801±.0018	.9843±.0017
12 / TTC-5	7 assemblies encased in AlB_2 alloy sleeves arranged in a subcritical shipping cask geometry (k_{eff}=0.92)	.9051±.0020	.9032±.0024	.9001±.0024

reflected, unless otherwise noted. The labels "27GROUP" and "27BURNUP" denote the 27GROUPNDF4 and the 27BURNUPLIB libraries, respectively.

The first set of experiments[6] listed in Table 1 consisted of four fuel assemblies of 4.31 weight percent (wt %) UO_2 rods in a 1.891-cm square lattice pitch arranged in a 2 x 2 array. The assemblies were separated by a 3.73-cm-wide neutron flux trap created by 0.673-cm-thick Boral™ plates. Voids were created in the flux trap region of experiment # 214V3 by inserting three 0.63-cm-thick aluminum plates. This resulted in voiding of 51% and decreased the critical size of the experiment by approximately 9.5%. This configuration is illustrated in Fig. 1.

The second experimental set[7] consisted of three fuel assemblies of 2.35 wt % UO_2 rods in a 2.032-cm square lattice pitch arranged in a row. Plates of Boral™, aluminum, or stainless steel were inserted between the fuel assemblies (0.645 cm from the center assembly) to determine the effect on the critical separation between the fuel assemblies.

The third set[8,9] consisted of three fuel assemblies of 4.31 wt % UO_2 rods in a 1.892-cm square lattice pitch arranged in a row, similar to the setup of the second set. Reflecting walls of depleted uranium, lead, or steel were positioned on both sides of the fuel assemblies, 1.956 cm from the cell boundary of the assemblies.

The fourth set[10] examined the effects of adding soluble boron to the water moderator. These experiments used a single array of 4.31 wt % UO_2 rods at two different lattice pitches, 1.890 cm and 1.715 cm, in order to study the effect of water-to-fuel volume ratios on highly borated systems. Although the wide-pitched assembly required less rods (357) to achieve criticality than the narrow pitched one (509) with no boron in the system, the opposite was true for the borated cases (1237 versus 1192 rods, respectively). With no boron, the wide-pitched assembly has greater moderation than the narrow-pitched assembly and is, therefore, more reactive. For the borated cases, the greater moderation of the wide-pitched assembly results in greater boron worth and lower reactivity compared to the narrow-pitched experiment.

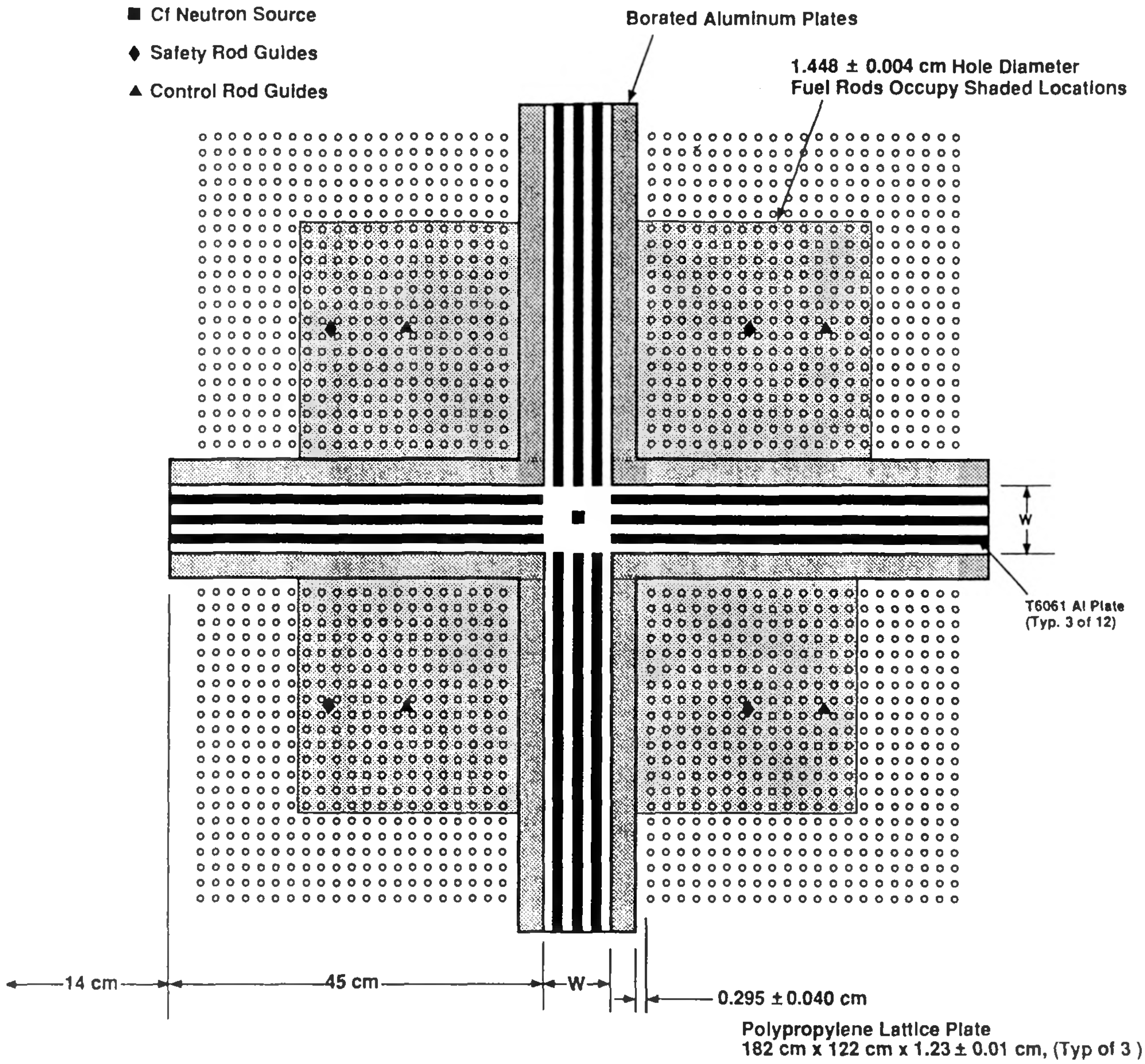

Fig. 1. Configuration for critical experiment no. 214V3.

The next experiment[11] consisted of nine fuel assemblies of 2.46 wt % UO_2 in a 1.636 square lattice pitch arranged in a 3 x 3 array. The assemblies were separated by a water gap containing 84 equally spaced B_4C rods.

The experiment from Ref. 12 had 583 mixed oxide pins (2 wt % PuO_2, 98 wt % natural UO_2) and 1174 4.31 wt % UO_2 rods distributed uniformly in a close-packed triangular pitch of 1.598 cm to obtain a Pu/^{235}U ratio approximating that of 20,000 MWD/MTU burnup.

The final experiment[13] consisted of seven assemblies of 4.31 wt % UO_2 rods encased in AlB_2 alloy sleeves arranged in a subcritical shipping cask geometry. The measured k_{eff} of this experiment was 0.92 $\pm$ 0.005. This was determined using the Garelis-Russell method of analysis. The Gozani method was also used to analyze the measured data and yielded a k_{eff} of 0.91. Reference 13 concludes "even if the measurement data contains some harmonic contamination, k_{eff} for the assembly lies somewhere between 0.91 and 0.92 since the Gozani and the Garelis-Russell methods of analyses have a bracketing effect with respect to harmonics."

A summary of the results is presented in Table 2. The mean k_{eff} is given for various categories of experiments to help identify trends in predicting k_{eff}. SCALE-4 underpredicts k_{eff} by approximately 0.7% $\Delta k/k$ for all the critical experiments combined. The 11 water-reflected UO_2 cases have a mean k_{eff} of approximately 0.992 for both SCALE-4 cross-section libraries, while the 3 UO_2 cases with reflecting walls have a mean k_{eff} of almost 1.000. The mixed oxide case is underpredicted by 1.6% to 2.0% $\Delta k/k$, which is a greater underprediction than that seen for any of the individual UO_2 criticals. The subcritical case underpredicts the measured k_{eff} by 1.6 to 2.2% $\Delta k/k$. The trend to underpredict k_{eff} with the 27-group ENDF/B-IV cross-section libraries may generally be attributed to two reasons. First, there is no unresolved resonance shielding for ^{238}U. This is worth approximately 0.5% Δk. Second, the difference in the resolved parameters between ENDF/B-IV and ENDF/B-V is also worth approximately 0.5% Δk. These worths will vary some with parameters which affect the neutron flux spectrum, such as lattice pitch and enrichment.

Table 2. Summary of results - mean k_{eff} by category

Categories	(No. of experiments)	SCALE-4 27GROUP	SCALE-4 27BURNUP	SCALE-3 27GROUP
All critical experiments	(15)	.9931	.9927	.9941
UO_2 criticals reflected by water	(11)	.9921	.9923	.9937
UO_2 criticals reflected by metal	(3)	.9999	.9984	.9989
Mixed oxide criticals	(1)	.9840	.9801	.9843
Subcritical experiments	(1)	.9051	.9032	.9001

This reference problem set covers a large scope of typical transportation and storage cask conditions. SCALE-4 with the 27GROUPNDF4 and the 27BURNUPLIB cross-section libraries produces satisfactory results for unirradiated LWR fuel stored in cask conditions and gives statistically consistent results compared to SCALE-3. Analysis of additional mixed oxide critical experiments is recommended in order to substantiate the trend observed for the mixed oxide case in this study.

In addition to the reference problem set, another set of experiments[14] was modeled to examine the ability of SCALE-4 and the 27-group ENDF/B-IV burnup library to predict gadolinium absorption in LWR fuel. Gadolinium is a strong neutron absorber and a significant fission product with respect to reactivity in burned LWR fuel. These experiments contained a small number of UO_2-Gd_2O_3 fuel rods inserted in selected patterns among fresh UO_2 fuel rods. The UO_2-Gd_2O_3 fuel rods contained 4 wt % Gd_2O_3 and 96 wt % UO_2 (1.944 wt % ^{235}U). The cores simulated a 15 x 15 lattice PWR checkerboard loading of assemblies containing the gadolinium fuel rods. The central zone contained 4.02 wt % UO_2 fuel rods, and the outer zone contained 2.46 wt % UO_2 fuel rods. The strength of the gadolinium absorption is evidenced by the change in the boron concentration between the no-gadolinium case (Core 12) and the 12-Gd-rod assembly configuration (Core 14), which had a total loading of 28 Gd fuel rods. Based on a boron worth calculation of Core 14, this boron change is worth approximately 3.1% $\Delta k/k$. Core 16 was a 16-Gd-rod assembly configuration containing a total rod assembly configuration containing a total of 36 Gd fuel rods. The results are presented in Table 3. The results are statistically consistent with the water-reflected UO_2 criticals in Table 2. These calculations indicate that SCALE-4 can accurately predict the reactivity effect of gadolinium absorption in LWR fuel.

Table 3. Calculated results of gadolinium critical experiments

Reference/Experiment	Description	Boron (ppm)	SCALE-4 27BURNUP
13 / 12	0 Gd rod configuration	1899	.9919±.0015
13 / 14	12 Gd rod configuration	1654	.9939±.0011
13 / 16	16 Gd rod configuration	1579	.9911±.0011
Mean k_{eff}			.9923

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