Westinghouse Non-Proprietary Class 3

WCAP-17889-NP
Revision 0

June 2014

Validation of SCALE 6.1.2 with 238-Group ENDF/B-VII.0 Cross Section Library for APR1400 Design Certification

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June 2014

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1.0 INTRODUCTION

The purpose of this document is to summarize the validation of the SCALE Version 6.1.2 code system CSAS5 Module (Reference 1) to be used in the APR1400 design certification application to the US NRC.

In order to validate the SCALE Version 6.1.2 code system, the NRC publication "Guide for Validation of Nuclear Criticality Safety Calculational Methodology" (Reference 4) is followed and, as recommended in Reference 4, the "International Handbook of Evaluated Criticality Safety Benchmark Experiments" (Reference 2), has been used as the primary source of critical benchmarks for the validation. References 3, 6 and 7 are also used as sources of critical benchmarks.

This validation is designed to cover fresh and spent fuel storage. It also covers the criticality analysis for any movement of fuel from the spent fuel pool to the core or cask loading and other normal operations in the spent fuel pool. The validation is adequate to cover LWR UO_2 fuel with square-pitched assembly designs.

2.0 CALCULATIONAL METHOD

The analysis methodology employs SCALE Version 6.1.2, as documented in Reference 1, using a 238-group ENDF/B-VII Release 0 (ENDF/B-VII.0) neutron cross-section library.

Standard material compositions are employed in the SCALE analyses consistent with the material descriptions in References 3, 6, 7, and 8.

All calculations are performed on systems with the following hardware and software characteristics:

- SCALE Version 6.1.2
- SUSE Linux 11.0

Correct installation and operation of the SCALE code system is verified by performing test cases on the platform described above.

The results of this validation suite may be used directly in a criticality safety analysis using the same code system, version, cross-section library, and computing platform. If a different code system is used in the analysis, then the validation will be re-performed following the same methodology outlined here. If a different computing platform is used in the analysis, then the appropriate justification should be made to the use of the results of this validation suite.

3.0 VALIDATION METHOD

Validation of SCALE Version 6.1.2 for criticality safety calculations has been performed following methodology described in Reference 4. Validation includes quantification of the difference between calculated and experimental k_{eff}, called the bias. The bias and the uncertainty associated with the bias are used in combination with other biases and uncertainties as well as additional subcritical margin to ensure the regulatory requirements are met. Statistical analysis is performed to determine whether trends exist in the bias. The range of benchmark experiment parameters used in the validation defines the area of applicability (AOA), which establishes the limits of the systems that can be analyzed using the validation presented here.

As described in Reference 4, the basic methodology used in the validation is:

1. Define the range of parameters to be validated
2. Select critical experiment data
3. Model experiments
4. Analyze the data
   a. Test for normality
   b. Determine bias and bias uncertainty
   c. Identify trends in the data

This validation is intended to cover the range of parameters associated with APR1400 spent fuel pool analyses. [

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3.1 TEST FOR NORMAL DISTRIBUTION

The statistical evaluation performed must be appropriate for the distribution of the data. If the data is normally distributed, then a technique such as a one-sided tolerance limit can be used to determine the appropriate bias and bias uncertainty. If the data is found to be non-normally distributed according to the statistical testing procedures utilized herein, a non-parametric treatment may be applied as discussed in Section 3.4. [

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3.2 DETERMINATION OF BIAS AND BIAS UNCERTAINTY

The statistical analysis presented in Section 2.4.1 of Reference 4 is followed here. This approach involves determining a weighted mean that incorporates the uncertainty from both the measurement (σ_{exp}) and the calculation method (σ_{calc}). For the benchmark experiments chosen from References 2, 6, and 7, the experimental uncertainties presented in References 2, 6, and 7 are used. Experimental uncertainty is not presented for the experiments contained in Reference 3 so the average value of experimental uncertainties of similar experiments documented in Reference 2 is used. This is consistent with the recommendation in Reference 4 that engineering judgment be used to approximate typical experimental uncertainties rather than assume no experimental uncertainty.

If the critical experiment being modeled is at a state other than critical (i.e. $k \neq 1.0$), then an adjustment is made to the calculated value of k_{eff}. This adjustment is done by normalizing the calculated eigenvalue to the experimental value. This normalization assumes that the inherent bias in the calculation is not affected by the normalization, which is valid for small differences in k_{eff}. To normalize k_{eff}, the following formula is used:

$$k_{norm} = \frac{k_{calc}}{k_{experiment}} \tag{3.1}$$

The normalized k_{eff} values are used in the subsequent determination of the bias and bias uncertainty, therefore all subsequent instances of k_{eff} should be taken to mean the normalized k_{eff} value.

The Monte Carlo and experimental uncertainties are root-sum-squared to create a combined uncertainty for each experiment:

$$\sigma_t = \sqrt{\sigma_{calc}^2 + \sigma_{experiment}^2} \tag{3.2}$$

A weighted mean k_{eff} ($\bar{k}_{eff}$) is calculated by using the weighting factor $1/\sigma_t^2$. The use of this factor reduces the "weight" of the data with high uncertainty. Within a set of data, the "i^{th}" member of that set is shown with a subscript "i." Henceforth, unless otherwise specified, the uncertainty for an "i^{th}" k_{eff} is shown as σ_t and is taken to mean the combined calculational and experimental uncertainty, shown above as σ_t. The weighted equation variables for the single-sided lower tolerance limit are presented below:

Variance about the mean:

$$s^2 = \frac{\left(\frac{1}{n-1}\right)\sum \frac{1}{\sigma_i^2}\left(k_{eff_i} - \bar{k}_{eff}\right)^2}{\frac{1}{n}\sum \frac{1}{\sigma_i^2}} \tag{3.3}$$

Average total uncertainty:

$$\bar{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} \tag{3.4}$$

The weighted mean k_{eff} value:

$$\bar{k}_{eff} = \frac{\sum \frac{1}{\sigma_i^2} k_{eff_i}}{\sum \frac{1}{\sigma_i^2}} \tag{3.5}$$

The square root of the pooled variance:

$$S_P = \sqrt{s^2 + \bar{\sigma}^2} \tag{3.6}$$

Where:

s^2 = variance about the mean

n = number of critical experiments used in the validation

$\bar{\sigma}$ = average total uncertainty

Bias is determined by the relation:

$$Bias = \begin{matrix} \bar{k}_{eff} - 1.0 & if\ \bar{k}_{eff} < 1.0 \\ 0.0 & if\ \bar{k}_{eff} \geq 1.0 \end{matrix} \tag{3.7}$$

3.3 IDENTIFY TRENDS IN THE DATA

Trends are determined using regression fits to the calculated results. Based on a visual inspection of the data plots, it is determined that a linear fit is sufficient to determine a trend in the bias. The data plots are shown in Section 4.2. In the equations below, "*x*" is the independent variable representing some parameter (e.g., enrichment). The variable "*y*" represents keff. Variables "*a*" and "*b*" are coefficients for the function where "*b*" is the slope and "*a*" is the intercept.

Per Reference 4, the equations used to produce a weighted fit of a straight line to the data are given below.

$$Y(x) = a + bx$$

$$a = \frac{1}{\Delta}\left[\sum \frac{x_i^2}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{yx_i}{\sigma_i^2}\right]$$

$$b = \frac{1}{\Delta}\left[\sum \frac{1}{\sigma_i^2} \sum \frac{yx_i}{\sigma_i^2} - \sum \frac{x_i}{\sigma_i^2} \sum \frac{y_i}{\sigma_i^2}\right] \tag{3.8}$$

$$\Delta = \sum \frac{1}{\sigma_i^2} \sum \frac{x_i^2}{\sigma_i^2} - \left(\sum \frac{x_i}{\sigma_i^2}\right)^2$$

Once the data has been fit to a line, a determination as to the "goodness of fit" must be made. Per Reference 4, two steps should be employed when determining the goodness of fit. The first step is to plot the data against the independent variable which allows for a visual evaluation on the effectiveness of the regression fit. The resulting plots are shown in Section 4.2.

The second step is to numerically determine a goodness of fit after the linear relations are fit to the data. This adds a useful measure because visual inspection of the data plot will not necessarily reveal just how good the fit is to the data. Per Reference 4, the linear correlation coefficient is one standard method used to numerically measure the goodness of fit.

The linear-correlation coefficient is a quantitative measure of the degree to which a linear relationship exists between two variables. For weighted data, the linear correlation coefficient is:

$$r = \frac{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum \frac{1}{\sigma_i^2} (x_i - \bar{x})^2} \sqrt{\sum \frac{1}{\sigma_i^2} (y_i - \bar{y})^2}} \quad (3.9)$$

Where the weighted mean for the independent parameter is:

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} \quad (3.10)$$

The weighted mean for the dependent parameter ($\bar{y}$) is $\bar{k}_{eff}$, as shown in Equation 3.5.

The value of r^2 is the coefficient of determination. It can be interpreted as the percentage of variance of one variable that is predictable from the other variable. The closer r^2 approaches the value of 1, the better the fit of the data to the linear equation.

In addition to the linear correlation coefficient, the Student t-test is used to determine if the linear fit of the data is statistically significant. A trend is statistically significant when the slope of the linear regression fit (b) is equal to some specified value (b_0). For the purposes of this validation suite, the null hypothesis, H_0: $\rho = 0$ is that no statistically significant trend exists (slope is zero), i.e. b_0 is set to zero with an alternative hypothesis of H_1: $\rho \neq 0$, at a significance level of $\alpha = 0.05$.

In order to determine if the null hypothesis is supported, t_{score} is calculated and compared to the Student t-distribution ($t_{\alpha/2,n-2}$). The t_{score} for the slope of a regression line is given by:

$$t_{score} = \frac{(b - b_0)\sqrt{n-2}}{\sqrt{\frac{SSE}{\sum (x_i - \bar{x})^2}}} \quad (3.11)$$

where SSE is the sum of the squares of the residuals:

$$SSE = \sum [k_{eff_i} - (a + bx_i)]^2 \quad (3.12)$$

The null hypothesis is rejected if $|t_{score}| > t_{\alpha/2,n-2}$.

Per Reference 4, when a relationship between a calculated k_{eff} and an independent variable can be determined, a one-sided lower tolerance band may be used. This conservative method provides a fitted curve above which the true population of k_{eff} is expected to lie. The equation for the one-sided lower tolerance band is:

$$K_L = K_{fit}(x) - S_{P_{fit}} \left\{ \sqrt{2F_a^{(2,n-2)} \left[\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi^2_{1-\gamma,n-2}}} \right\} \tag{3.13}$$

$K_{fit}(x)$ is the function derived in the trend analysis described above. Because a positive bias may not be conservative, the equation below must be used for all values of x where $K_{fit}(x) > 1$:

$$K_L = 1 - S_{P_{fit}} \left\{ \sqrt{2F_a^{(2,n-2)} \left[\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi^2_{1-\gamma,n-2}}} \right\} \tag{3.14}$$

where:

p	=	The desired confidence level (0.95)
$F_a^{(fit,n-2)}$	=	The F distribution percentile with degree of fit, n-2 degrees of freedom. The degree of fit is 2 for a linear fit.
n	=	The number of critical experiment k_{eff} values
x	=	The independent fit variable
x_i	=	The independent parameter in the data set corresponding to the i^{th} k_{eff} value
$\bar{x}$	=	The weighted mean of the independent variables
z_{2P-1}	=	The symmetric percentile of the normal distribution that contains the P fraction
γ	=	$\frac{1-p}{2}$
$\chi^2_{1-\gamma,n-2}$	=	The upper Chi-square percentile

For a weighted analysis:

$$\sum (x_i - \bar{x})^2 = \frac{\sum \frac{1}{\sigma_i^2}(x_i - \bar{x})^2}{\frac{1}{n}\sum \frac{1}{\sigma_i^2}} \tag{3.15}$$

$$\bar{x} = \frac{\sum \frac{1}{\sigma_i^2} x_i}{\sum \frac{1}{\sigma_i^2}} \tag{3.16}$$

$$S_{P_{fit}} = \sqrt{s_{fit}^2 + \bar{\sigma}^2} \tag{3.17}$$

$$\bar{\sigma}^2 = \frac{n}{\sum \frac{1}{\sigma_i^2}} \quad (3.18)$$

$$s_{fit}^2 = \frac{\left(\frac{1}{n-2}\right) \sum \left\{ \frac{1}{\sigma_i^2} \left[k_{eff_i} - K_{fit}(x_i) \right]^2 \right\}}{\frac{1}{n} \sum \frac{1}{\sigma_i^2}} \quad (3.19)$$

Within the equation for K_L:

$$Bias = \begin{matrix} K_{fit} - 1.0 & if\ K_{fit} < 1.0 \\ 0.0 & if\ K_{fit} \geq 1.0 \end{matrix} \quad (3.20)$$

And the uncertainty in the bias is:

$$Bias\ Uncertainty = S_{P_{fit}} \left\{ \sqrt{2F_a^{(2,n-2)} \left[\frac{1}{n} + \frac{(x-\bar{x})^2}{\sum (x_i - \bar{x})^2} \right]} + z_{2P-1} \sqrt{\frac{(n-2)}{\chi^2_{1-\gamma,n-2}}} \right\} \quad (3.21)$$

3.4 NON-PARAMETRIC TREATMENT

If the data fails the test for normality, a non-parametric treatment of the data will be necessary. Per Reference 4, the determination of K_L, the lower limit of the 95/95 tolerance interval is as follows:

$$K^L = k_{eff}^{min} - uncertainty\ for\ k_{eff}^{min} - NPM \quad (3.22)$$

where:

k_{eff}^{min} is the minimum normalized k_{eff},

$uncertainty\ for\ k_{eff}^{min}$ is the pooled Monte Carlo and experimental uncertainty, and

NPM is the non-parametric margin, which is added to account for small sample size.

The analysis results in a determination of the degree of confidence that a fraction of the true population of data lies above the smallest observed value. For a population fraction of 95% with a rank order of 1 (the smallest data sample) the equation to determine the percent confidence that a fraction of the population is above the lowest observed value:

$$\beta = 1 - q^n \quad (3.23)$$

For example, for a set that includes 50 experiments, the confidence that 95% of the true population will be above the k_{eff}^{min} is 92.3% ($1 - 0.95^{50}$). Although 59 experiments would be required even for a rank index of 1 to reach a 95/95 tolerance limit as stated in Reference 4, the recommended non-parametric margin

(NPM) correction is 0.0 for confidence values greater than 90%, as also indicated in Table 2.2 of Reference 4.

3.5 DESCRIPTION OF THE CRITICAL EXPERIMENTS

Reference 2 is the primary source for most of the experiments used in this suite; Reference 3 is used to supplement the selected experiments to ensure coverage over all of the important parameters. The Haut Taux de Combustion (HTC) experiments designed to represent irradiated UO_2 fuel with mixed oxide rods are also included in the validation suite (References 6, 7, and 8). Each set of experiments is described in detail below. All experiments used in this validation are judged acceptable as benchmark data.

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Table 3-1 [ ]a,c

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3.5.13 HTC Experiments

The HTC experiments are a series of experiments performed with mixed oxide rods designed to have a U and Pu isotopic composition equal to that of U(4.5%)O_2 PWR fuel with 37,500 MWd/MTU burnup. No fission products are included in the composition. Up to this point, all the experiments modeled in this suite represent fresh fuel; the HTC experiments are included to ensure the validation suite covers spent fuel as well. The HTC critical experiment set is organized into four phases. [

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4.0 RESULTS

4.1 DETERMINATION OF BIAS AND BIAS UNCERTAINTY AND NORMALITY CHECK

This validation suite is intended to be used for [

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Table 4-1 [ ]a,c

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Table 4-2 [ ]^{a,c} a,c

Table 4-3 [ ]^{a,c} a,c

4.2 TRENDING ANALYSIS

The regression fits and goodness of fit tests described in Section 3.3 are applied to [

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4.2.1 [ ]^{a,c}

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Figure 4-1 [ ]^{a,c}

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Figure 4-2 [ ]a,c

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Figure 4-3 [ ]a,c

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Figure 4-4 [ ]a,c

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Table 4-4[ ]a,c

Table 4-5 [

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Table 4-6 [ ]a,c

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4.2.2 [ ]a,c

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Figure 4-5 [ ]a,c

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Figure 4-6 [ ]a,c

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Figure 4-7 [ ][a.c]

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Figure 4-8 [ ][a.c]

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Figure 4-9 [ ]a,c

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Figure 4-10 [ ]a,c

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Table 4-7 [ ]a.c

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Table 4-8 [

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Table 4-9 [ ]a,c

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Figure 4-11 [ ]a,c

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Figure 4-12 [ ]a,c

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Figure 4-13 [ ]a,c

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Figure 4-14 [ ]a,c

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Figure 4-15 [

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Figure 4-16 [**]a,c**

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Table 4-10[ ]a,c

Table 4-11 [

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Table 4-12 [

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4.2.4 Summary of Trend Results

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Table 4-13 [ ]a,c

5.0 VALIDATION SUMMARY

The area of applicability (AOA) of this benchmark is defined by the range of parameters in the validation suite and is summarized in Table 5-1.

Table 5-2 summarizes the results of the validation. [

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Table 5-1 Area of Applicability

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Table 5-2 Summary of Bias and Bias Uncertainty

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Table 5-2 Summary of Bias and Bias Uncertainty

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