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# Validation of SCALE4.4a/CSAS25 for Nuclear Criticality Safety Analyses

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This paper presents calculation results used for establishment of bias, bias trends and uncertainty for validation of the CSAS25 control module from the Standardized Computer Analyses for Licensing Evaluation (SCALE) Version 4.4a, using the 238-group ENDF/B-V cross-section library. Over 1200 benchmark cases were used from Volumes I through VI of the "International Handbook of Evaluated Criticality Safety Benchmark Experiments," published by the Nuclear Energy Agency Organization for Economic Cooperation and Development (NEA/OECD). Associated upper subcritical limits are also discussed.

***KEYWORDS: benchmarks, criticality safety, computer software, validation, SCALE, CSAS25, OECD, Physics Code Validation***

## 1. Introduction

The successful application of computational methods in nuclear criticality safety engineering requires verification, certification and validation of the method. Software validation "calibrates" the calculation results obtained using certified software for agreement with the accepted benchmarks (critical experiments).

This paper presents calculation results used for establishment of bias, bias trends and uncertainty for validation of the CSAS25 control module from the Standardized Computer Analyses for Licensing Evaluation (SCALE) Version 4.4a, using the 238-group ENDF/B-V cross-section library. [1] Over 1200 benchmark cases were used from Volumes I through VI of the "International Handbook of Evaluated Criticality Safety Benchmark Experiments," published by the Nuclear Energy Agency Organization for Economic Cooperation and Development (NEA/OECD). [2] Associated upper subcritical limits are also discussed.

## 2. Description of Work

### 2.1 ANSI/ANS Standards Guidance

In nuclear criticality safety engineering, calculation methods are one of the methods used to establish subcritical limits for operations involving fissionable material. The American National Standards Institute gives fundamental guidance for establishing these limits. [3]

### 2.2 Summary

Calculations were performed for validation of the CSAS25 control module with the 238-group ENDF/B-V cross-section library from the SCALE 4.4a computer code system, for use in evaluating nuclear criticality safety. [1] Based on the results, the CSAS25 module and 238-group library are validated for use with systems that are similar to those included in this validation. [3] Subcritical limits were determined through an analysis of the criticality calculation results. Non-parametric statistical methods were used. [4]

Previously unpublished, internal reports, which are now publicly available, included about 500 validation cases from Volumes II and IV (HEU and LEU) of the OECD Benchmark

Handbook. [5-7] Subsequently, about 400 cases from Volumes I and VI (Pu and mixed U/Pu) were incorporated into revisions of the reports, which have not been publicly available. [8,9] In addition, new results for Volumes III (IEU, 51 cases) and V ($^{233}$U, 140 cases) are now included. Finally, 53 new results for Volume II (HEU), including 26 models developed as part of the Y-12 Nuclear Criticality Safety qualifications program, as well as 32 new results for Volume IV (LEU), including 7 from the qualifications program, have also been added. About 700 new models were added in this revision, for a total of over 1200 models out of approximately 3000 available in the OECD Handbook.

Although many cases are included in this work, analysts are cautioned that they must not assume that all SCALE input options are validated for all applications. They must verify or demonstrate that their options are validated against benchmark experiments that are similar to their applications. Options include material selections, scattering options (i.e. SCT), geometry options (i.e. infinite homogeneous, multi-region, or latticecell), and others. Seemingly minor differences (e.g. for beryllium, "bebound" versus "be") may cause large changes in results, particularly when errors exist in cross section libraries. [10]

Similar work at Y-12 using MCNP with continuous energy cross sections has been previously reported. [11] Future work may include preparing a detailed comparison of the results from SCALE/KENO and MCNP, but this has not yet been performed.

This work provides assurance that the software predicts critical systems reasonably well, however, in general, there is wide variation in performance depending on the type of system, based on bias results. The performance ranges from "very good" or less than about +/- 0.01 to "very poor" or about +0.087/-0.14, depending on the category of experiments, using a rating scale similar to one previously used. [12] This paper includes several benchmark cases that significantly under-predict the expected results.

### 2.3 Criticality Benchmark Database

1217 cases were prepared from experiment descriptions and sample inputs. Table 1 shows the number of cases that were obtained in various categories. This validation comprises a substantial subset of the database of about 3000 cases in the first six volumes of the OECD Benchmark Handbook.

The International Criticality Safety Benchmark Evaluation Project (ICSBEP) is now an official activity of the Organization for Economic Cooperation and Development - Nuclear Energy Agency (OECD-NEA). The wide scale evaluation effort has published the "International Handbook of Criticality Safety Benchmark Experiments" (OECD Handbook). The seven-volume set of handbooks, currently available on compact disk, contains criticality safety benchmark specifications derived from experiments that were performed at various nuclear critical facilities around the world. The benchmark specifications are intended for use by criticality safety engineers to validate the application of calculation techniques, such as SCALE 4.4a, for criticality safety analyses. Example calculations presented in the handbook do not constitute a validation of the codes or cross section data sets by themselves, but the information contained in the Handbook can be used to validate SCALE 4.4a.

For this criticality validation of SCALE 4.4a, fissile material forms include uranium systems, plutonium systems, mixed uranium and plutonium systems, and Uranium-233 systems. Table 1 summarizes the evaluated benchmark experiments that are analyzed in this validation. The data from the benchmark experiments represents a sufficiently wide range of fissile and fissionable materials, enrichments, and physical and chemical forms to cover many existing, planned or unforeseen activities for the Y-12 site. These benchmarks include enriched uranium with $^{235}$U only, natural and depleted uranium, intermediate (10-60%) enriched uranium, highly (>60%) enriched uranium, uranium-233, plutonium, and mixed plutonium-uranium systems. Data analyzed from critical experiments in this validation includes systems having fast, intermediate and thermal neutron energy spectra, and they include materials in various physical and chemical forms such as metals, solutions, and oxide compounds. For many benchmark experiments, critical conditions are tabulated in the OECD Handbook for a number of parametric variables (height, concentration, shape, etc.).

Input data for the CSAS25 cases are based on information contained in the OECD distribution CD. Cases were first prepared using the 1998 edition of the CD, and additional cases were taken from the subsequent editions through 2002. Each subsequent revision provides additional experiments and input data. The organization and categorization of the experiments and data on the CD also changes.

Reviews were performed of the input preparation in a graded approach. For models based on sample inputs, reviews generally assume the models are adequate unless reasons are found to think otherwise, at the discretion of the reviewer. Models prepared from scratch, based on experiment descriptions, are given more scrutiny. Mentors review models submitted as part of the Nuclear Criticality Safety qualifications program.

**Table 1** Validation Cases Categorized By Fissile Material Type and Energy

| | Fissile Material Category (OECD Benchmark Volume) | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | II | III | IV | | I | VI | V | |
| Material / Energy | HEU | IEU | LEU | Subtot U-235 | Pu | Mixed Pu-U | U-233 | Total |
| Metal Fast | 106 | 16 | 0 | 122 | 62 | 33 | 10 | 227 |
| Metal Inter | 4 | 0 | 0 | 4 | 0 | 0 | 0 | 4 |
| Metal Therm | 31 | 0 | 13 | 44 | 0 | 0 | 0 | 44 |
| Metal Mixed | 3 | 0 | 0 | 3 | 0 | 0 | 0 | 3 |
| Comp Fast | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Comp Inter | 12 | 4 | 0 | 16 | 1 | 0 | 0 | 17 |
| Comp Therm | 24 | 31 | 99 | 154 | 0 | 92 | 0 | 246 |
| Comp Mixed | 9 | 0 | 0 | 9 | 9 | 0 | 0 | 18 |
| Solution Inter | 0 | 0 | 0 | 0 | 0 | 0 | 33 | 33 |
| Solution Therm | 271 | 0 | 16 | 287 | 198 | 32 | 97 | 614 |
| Solution Mixed | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Misc. Therm | 0 | 0 | 0 | 0 | 0 | 11 | 0 | 11 |
| Total | 460 | 51 | 128 | 639 | 270 | 168 | 140 | 1217 |

## 3. Results

### 3.1 Results Interpretation

This paper presents only a brief summary of the results. More detailed results are available in the full report, which will be released after this paper.

The OECD benchmark reports provide an estimate of the actual $k_{eff}$ for each experiment model. While benchmarks for most experiments were estimated to be exactly critical, or k_exp = 1.0, a number of the estimates were above or below exactly critical. It was considered desirable to account for this difference. The following adjustment was used to calculate adjusted k-effective, k':

$$k' = 1 + bias = 1 + (k\_cal - k\_exp)$$

where k_cal = code calculated $k_{eff}$ result for the modeled experiment, and
k_exp = OECD estimate of actual $k_{eff}$ for the modeled experiment

The assumption inherent in making this adjustment is that the experiments were close to critical, and if a small adjustment could be made so that the experiment would be exactly critical, the bias of the calculation would not change.

When calculation methods are employed, the subcritical limit is a quantitative value used for implementation of NCS policy, which is established in accordance with DOE Orders, Standards, or by NRC regulations for those activities under NRC jurisdiction. Evaluation criteria are usually the calculated reactivity, $k_{eff}$, for the model of the case being evaluated, uncertainty in the calculated value of reactivity, bias introduced by the code used to calculate reactivity, and bias introduced by the model. Code bias is determined by a validation performed in accordance with ANSI/ANS 8.1. The statistical results determine code bias based on comparison of code calculations with experimental results. Model bias is due to uncertainties in the modeled parameters describing the physical reality; approximations made for the model to conform to the input requirements of the code, and any significant simplifications by the analyst. The acceptance criterion requires that the evaluation criteria be bounded by the subcritical limit. In the case of code calculations, the subcritical limit is often a criterion based on calculated $k_{eff}$ and estimated bias and uncertainties.

It is recognized that it may also be possible to determine subcritical limits based on adjustment of correlating parameters other than $k_{eff}$, as allowed by ANSI/ANS-8.1. These parameters could include physical parameters such as mass or radius, for example, or other calculated parameters besides $k_{eff}$, if they can be shown to provide subcritical margin. This work does not address other potential correlating parameters, but an analyst could determine them as part of an evaluation and use them to determine subcritical limits in conjunction with the code bias results in this work.

### 3.2 Discussion of Results

Figure 1 shows a plot of all adjusted k-effective results versus EALCF, or the Energy corresponding to the Average Lethargy of neutrons Causing Fission. EALCF or average energy group has traditionally been used as a trending variable for SCALE/KENO $k_{eff}$ results. The amount of data in the middle energy range is somewhat sparse relative to the low and high ends; however, with a few exceptions there are at least some results in almost every energy range. As expected, most $k_{eff}$ results are centered about 1.0, and are generally within a range of about 1.0 +0.04/-0.03, with the exception of a few results that are outside the range. These high and low data will be discussed in more detail below.

There appears to be a small systematic more negative bias for U-233 results, relative to other fissile categories, in the thermal to intermediate energy range, and some indication of a slight trend in the bias with energy. Otherwise, none of the fissile species appears to consistently have a different bias than other categories, and no other major trends in results are seen.

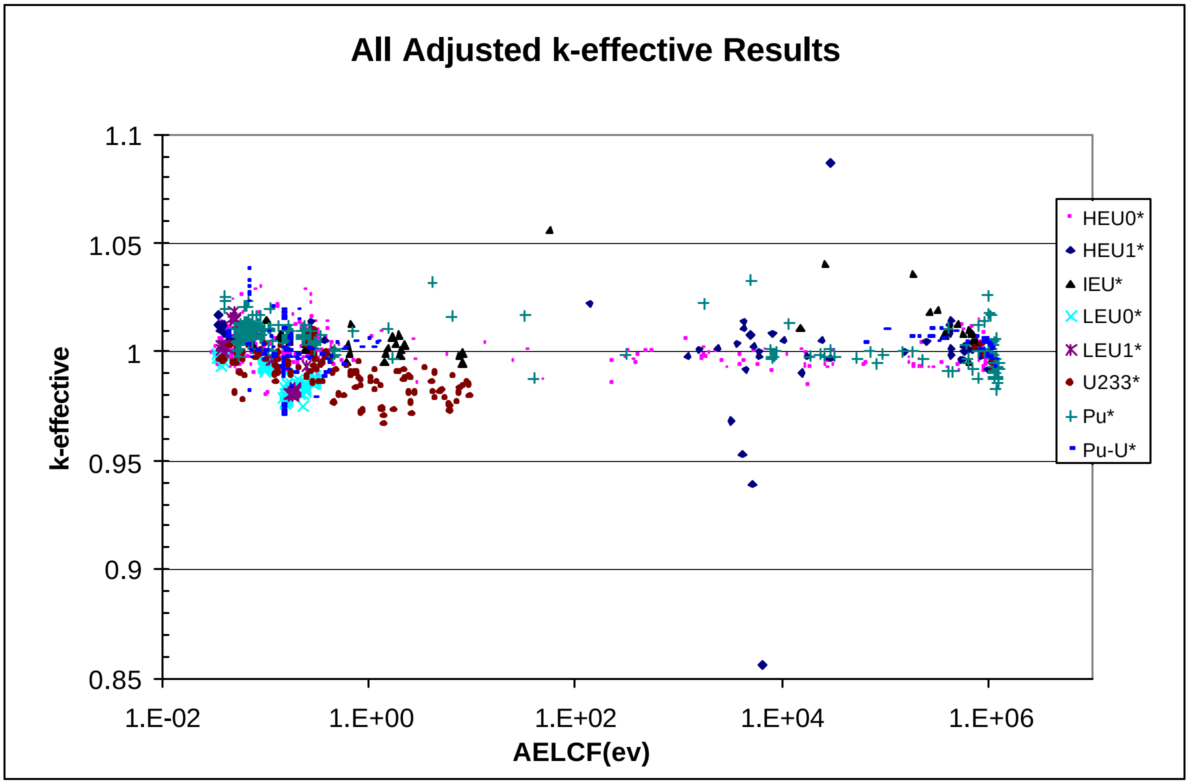


**Fig.1** Adjusted neutron multiplication factors versus neutron energy

### 3.3 High Positive and Negative Bias Results

Table 2 lists eight results having adjusted k-effective results less than 0.97 or greater than 1.04, or correspondingly, bias results more negative than -0.03 or more positive than +0.04. These high bias results are consistent with the sample calculation results in the OECD Handbook.

Six of the high bias results are for benchmark experiments that were modeled as infinite in extent, and thereby amplified the effects of imperfections in cross section data. These experiments were all performed at the COBRA facility in the Russian Federation. Unlike most other benchmarks, these models required additional interpretation and adjustment from the actual finite experimental configuration to create an infinite benchmark model. It is noted, however, that other, somewhat similar, infinite models had better results. As an example, see HEU-COMP-INTER-004, which included graphite and boron.

In addition to involving infinite models, particular materials were also involved. The four results from HEU-COMP-INTER-005 with high negative bias included relatively large amounts of chromium, nickel, zirconium, or stainless steel, in infinite models. The two results from IEU-COMP-INTER-001 with high positive bias included relatively large amounts of thorium, in infinite models. HEU-MET-INTER-001, with very high bias, involved relatively large amounts of iron in the core, and stainless steel as a reflector. No particular problem was found with U233-SOL-THERM-015 case 9. The U-233 results appear to have a slightly more negative bias, in general, as a category, for low energies.

Because of the unusual aspects of the benchmark models, as discussed above, when establishing subcritical limits for general applications, consideration should be given to eliminating, or giving separate treatment to, the high positive and negative bias models HCI005-07,09,15,16; ICI001-002, 003, and HMI001. UST015_09 should be included, but it may be advisable to establish separate, slightly lower subcritical limits for U-233 applications.

**Table 2** High Positive and Negative Bias Results

| Case | nubar | AFG | EALCF(ev) | k_calc | k_exp | Bias | Adjusted $k_{eff}$ | Comment |
|---|---|---|---|---|---|---|---|---|
| hci005-15 | 2.45 | 60.7 | 6.50E+03 | 0.92044 | 1.064 | -0.14356 | 0.85644 | k-inf, Cr |
| hci005-07 | 2.45 | 63.8 | 5.09E+03 | 0.9712 | 1.032 | -0.0608 | 0.9392 | k-inf, Ni |
| hci005-16 | 2.45 | 64.1 | 4.18E+03 | 0.95005 | 0.997 | -0.04695 | 0.95305 | k-inf, Zr |
| ust015_09 | 2.50 | 170 | 1.43E+00 | 0.96649 | 1.0 | -0.03351 | 0.96649 | |
| hci005-09 | 2.45 | 66.5 | 3.21E+03 | 1.01827 | 1.05 | -0.03173 | 0.96827 | k-inf, St. Steel |
| ici001-002 | 2.47 | 52.1 | 2.66E+04 | 1.02029 | 0.980 | 0.0403 | 1.04029 | k-inf |
| ici001-003 | 2.45 | 124 | 5.59E+01 | 1.06991 | 1.014 | 0.0559 | 1.05591 | k-inf |
| hmi001 | 2.46 | 51.6 | 2.93E+04 | 1.08365 | 0.9966 | 0.08705 | 1.08705 | Iron cross section problem |

### 3.4 Upper Subcritical Limits

Based on the calculation results, the following subcritical limits are recommended:

**Table 3** Upper Subcritical Limits (Before subtraction of any additional margin)

| Fissile Category | Number of Cases | Upper Subcritical Limit |
|---|---|---|
| Combined category for HEU, IEU, LEU | 639 | 0.975 (Note 1) |
| Plutonium or Mixed Pu-U | 438 | 0.971 |
| Uranium-233 | 140 | 0.966 |
| All Categories Combined | 1217 | 0.966 |

Note 1: Experiment Series HEU-COMP-INTER-005, cases 7,9, 15 and 16 showed that particular caution should be used with large arrays with large amounts of nickel, chromium, zirconium or stainless steel. These results indicated a potential for limits in the 0.856 to 0.968 range.

This recommendation is subject to the following restrictions:

- Models must be similar to those included in the benchmarks.
- Models must not be similar to the cases with high negative bias described in Table 2.
- Models must use options, materials and arrangements similar to benchmarks.
- Only code bias is included. No additional margin is included for model bias

(simplifications or uncertainties in analyzed conditions) or additional margin of safety. A different margin may be applicable, depending on the process analysis.

With 1214 experiments (of 1217 total) included in the determination of the subcritical limit, there is a good basis for having very high confidence that systems and conditions (similar to those included in this work) calculated by this method to be subcritical, will actually be subcritical. Allowance for additional margin for model bias, safety margin or area of applicability margin, if needed, would be subtracted from this upper subcritical limit. Additional margins of 0.02 to 0.05 have typically been used; however, the appropriate value depends on the details of the analysis, and administrative policy, if any. In determining these upper subcritical limits, the systems were not sub-divided into detailed categories based on materials and forms. Rather, conservative combined limits were determined.

The 238-group library is the only one included in this work. There may be applications where the 44-group library performs better (e.g. Low Enriched LWR and MOX lattices, and $^{233}U$). [12]

Although four or more decimal places are shown in results, the actual accuracy of the software, for a particular calculation, may be on the order of +/- 0.02 to 0.03 (or more) based on the spread in the bias results. Also, the standard deviation of the mean for a particular calculation was approximately 0.001 for benchmark cases, and may be somewhat higher for applications. Therefore, more than two or three decimal places are, in essence, not very meaningful or significant for developing limits. Too much importance should not be placed on small differences in the third or fourth decimal place.

### 3.5 Area of Applicability and Additional Margin

The Area of Applicability (AoA) must be considered in using these results. Correlating parameters (i.e., mass, enrichment, geometry, absorption, moderation, reflection, etc.) and values additional margin to subcritical limits are application dependent. The determination of correlating parameters and additional margin is an integral part of the process analysis. For the critical experiment results, no correlation between calculation results and neutron energy causing fission was found. In using these results, the criticality analyst must exercise sound engineering judgment and use strong technical arguments to develop a margin in $k_{eff}$, or other correlating parameter. The margin must be sufficiently large to ensure that conditions (calculated by this method to be subcritical by this margin) will actually be subcritical. Documentation and justification of the margin in the analyst's evaluation, in conjunction with the validation report, will constitute the complete Validation Report in accordance with ANSI/ANS-8.1-1998. [3]

## 4. Conclusion

This paper addresses the validation of SCALE4.4a and the associated 238-group library for performance of criticality calculations (CSAS25). This evaluation is directed at systems consisting of fissile and fissionable material in metallic, solution and other physical forms, as described in the OECD Handbook. The focus is on comparison of calculated neutron multiplication factors ($k_{eff}$) with the associated experimental results, and on establishment of bias, bias trends, and uncertainty as a final step. Compiled data for 1217 critical experiments is used as the basis for the calculation models.

This work provides assurance that the code predicts critical systems reasonably well, however, in general, there is wide variation in performance depending on the type of system, based on bias results. The performance ranges from "very good" or less than about +/- 0.01 to "very poor" or about +0.087/-0.14. Several benchmark cases significantly under-predicted the expected results. No correlation between calculation results and neutron energy causing fission (or any other parameter) was observed.

Subcritical limits were determined from the results. The determination of correlating parameters and appropriate margin is an integral part of the process analysis. There is no guarantee against the possibility of an unusual scenario that could produce non-conservative results, and analysts must be always vigilant for this possibility.


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