Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Disclaimer:

VALIDATION AND BIAS QUANTIFICATION OF CRITICALITY SAFETY CODES FOR SRNS OPERATIONS

Scott Finfrock, David Erickson, Tracy Stover
Savannah River Nuclear Solutions, LLC[I]
Savannah River Site, Aiken, SC
Scott.Finfrock@srs.gov
David.Erickson@srs.gov
Tracy.Stover@srs.gov

ABSTRACT

The validation and bias quantification methods employed by the Criticality Safety Engineering group at Savannah River Nuclear Solutions are discussed. Both SCALE and MCNP are validated against benchmark experiments, where these benchmark models have been divided into subgroups representative of the types of fissile material operations at SRNS. A quantification of the bias is made for each subgroup for each code and the three methods employed for quantification are discussed. The bias information is employed directly in the establishment of the Upper Safety Limit (USL) value of the neutron multiplication factor when using standardized documented SRNS methods. A simple example of validation and bias quantification is given and the procedure for setting the USL using the derived bias information is also presented.

Key Words: **validation, bias, MCNP, SCALE**

1. INTRODUCTION

Savannah River Nuclear Solutions' (SRNS) Criticality Safety Engineering group regularly makes use of the Monte Carlo neutron transport codes MCNP and SCALE (particularly the KENO module in the SCALE package) for estimating the neutron multiplication properties of the various operations occurring on site. Effort has recently been made to upgrade the validated versions to SCALE 6.1 and MCNP 6.1 for use. Validation at SRNS includes not only proving that the two codes satisfactorily reproduce the results of benchmark experiments but also quantitatively establishing the bias, if any, the code has in reproducing those results.

With the voluminous amount of criticality benchmark experiments available in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Ref. 1) hereinafter referred to as the "Handbook", prudence must be used in deciding which to model with the codes given limited resources in time and manpower. A high level qualitative assessment of the fissile material operations that SRNS currently carries out revealed that these operations can be broadly classified as those involving:

[I] This document has been authorized for public release by Savannah River Nuclear Solutions as SRNS-STI-2017-00315.

- Solid plutonium metal having fast neutron spectra
- Solid plutonium oxide having thermal to intermediate neutron spectra
- Solutions of plutonium nitrate having thermal neutron spectra
- Solutions of plutonium nitrate poisoned with gadolinium nitrate having thermal neutron spectra
- Solid highly enriched uranium metal having fast neutron spectra
- Solid highly enriched uranium oxide having thermal to intermediate neutron spectra
- Solutions of highly enriched uranium in uranyl nitrate having thermal neutron spectra
- Solutions of highly enriched uranium in uranyl nitrate poisoned with boron having thermal neutron spectra
- Various solution and solid forms of low enriched uranium having thermal to intermediate neutron spectra
- Material Test Reactor type fuels of solid form highly enriched uranium metal alloy, typically of aluminum, with explicit heterogonous, lattice geometry and having fast neutron spectra.

Bearing in mind these types of operations, benchmarks were selected from the available library which would best support the ability of each code to make predictive simulations of these types of systems. The benchmarks selected for modeling were filtered into these ten subgroups and the methodology discussed herein applied to those subgroups for validation and bias quantification.

The validation program employed at SRNS has been developed to satisfy those requirements in ANSI/ANS-8.24-2007 (Ref. 2). A selection of benchmarks is made and divided into the subgroups mentioned above. Those benchmarks are then modeled in the two code systems used on site. In each of those subgroups, effort is made to establish a bias and bias uncertainty for the resulting data from the modeling effort. Additional margins for area of applicability considerations and minimum subcritical requirements are set as needed. The SRNS treatment for trending, weighting, and rejection of data are discussed in the bias quantification methods section. The specific versions of codes are placed under configuration control on the specific computer system employed before validation proceeds. They remain under configuration control until such time that either the computer system or the code versions are updated.

1.1. Overview and Terminology

The following sections of this document discuss how SRNS implements the validation program. Section 2 discusses documentation requirements, established for both the benchmark modeling and the bias quantification, that meet internal requirements determined to be compliant with ANS-8.24. Requirements and assumptions for generating the models are discussed in Section 3. SRNS employs three accepted methods for quantification of the bias which are the Lower Tolerance Band, Lower Tolerance Limit, and Non-Parametric Value. These methods, along with treatment of positive biases and outlier data are summarized in Section 4. Section 5 presents how the quantified bias is directly used to set a USL for criticality safety analyses and Section 6 demonstrates application with an example data set of benchmark models used to construct a USL.

The reader should note at the onset that quantification of the bias is a core part of this methodology and the validation effort overall. However, which of the accepted methods listed above to use is not left to the analyst's discretion but a prescribed hierarchy is established. Each bias quantification

analysis begins with the LTB method and examines physical parameters common to the benchmarks to search for a parametric correlation to the bias. If the LTB analysis is unsuccessful, the data is tested for normality to support using the LTL analysis. Provided the data is normally distributed, an LTL value is derived. If the LTB was successful, then this analysis is not performed. If the LTB cannot be used and if the data is not normally distributed, a Non-Parametric Value for the bias is derived. If the data was normal and an LTL value was derived, then this analysis is not performed.

Effort has been made in the validation implementation (and in this document) to maintain consistency with terminology from ANS-8.24. However, there are some unique terms to the methodology which are defined here.

- The best estimate multiplication factor, k_{be}, is defined as (1.0 + bias – bias uncertainty) where both the bias and its uncertainty values are established through implementation of this validation method, using one of the accepted bias quantification methods listed above. The uncertainty used in this definition combines both experimental and statistical uncertainties.

2. DOCUMENTATION REQUIREMENTS

Detailed and consistent documentation is a central and significant portion of the validation effort. Because many different engineers contributed to the documentation, regular communication, review and editing were essential to maintain a high level of homogeneity amongst the individual components of the documents. The final products are modeling documentation, and bias quantification documentation. The basic requirements were to:

- Clearly present the quantified bias and discuss the Area of Applicability so that it can function as a useful tool for the nuclear criticality safety analysts.
- Meet the requirements of the SRNS Criticality Safety Program
- Satisfy all SRNS corporate documentation requirements.
- Clearly and accurately document the process so that an independent reader can review it and, if need be, reproduce the validation.

Specific requirements for the two types of documents produced are discussed in the following subsections.

Once the individual sections of the documents, i.e. those for each subgroup, are complete and meet the documentation requirements, they are collected into a single overall document, one for modeling for each code and one for bias quantification for each code.

2.1. Model Documentation

Documentation of the modeling followed a standardized structure agreed to early on by the developers. The structure required the homogeneous and consistent documentation of information described below. It was found to be a good practice to have regular formal meetings and continual informal communication between developers, analysts, and reviewers.

- Introduction and Scope – the scope of the analysis is broadly stated, in particular the nature of each subgroup is stated, the code version and cross sections identified, and appropriate references indicated to establish traceability.
- Requirements – the internal SRNS requirements for validation, which have been structured specifically to satisfy ANS-8.24 are identified for traceability and briefly discussed.
- Inputs and Assumptions – any guidance on inputs or specific data/code options are discussed. Any assumptions made are enumerated and defined. With limited exception, there were no assumptions made in this effort. The models were generated as described in the benchmark description section of the benchmark reports.
- Analytical Methods – the required results to be documented are identified and the method of calculation is generically discussed including traceable documentation of the computer system upon which the codes are executed.
- Selected Benchmarks – A brief discussion is made of each of the benchmarks selected and the total number and nature of cases is summarized.
- Modeling Methodology – the code system and cross section set being utilized are clearly documented. Many of the benchmark model input files were prepared original in house following the specification in the benchmark description section of the benchmark reports. Select few with simpler geometry were taken from the Handbook sample inputs and were carefully reviewed. Of those, many required some level of modification to align with the approved methodology. Additionally, this section includes specific discussion on the materials including any assumptions in defining compositions, the temperature data, discussions on geometry of the benchmarks, summary of the modeling techniques including any special cross section treatments (e.g. lattice calculations, infinite medium assumptions, etc.), and finally the criteria for convergence of each model is clearly stated.
- Confirmations of Code Output Files – upon completion, verified final model outputs were reviewed and any warnings appearing in the output files were appropriately dispositioned.
- Results – for every model run the benchmark name, multiplication factor, its statistical uncertainty, and the EALF are documented.
- Conclusions - at the end of the process, the model developer and reviewer should be able to conclude that the results meet the objective to provide the multiplication factor, its statistical uncertainty, and the EALF for the selected benchmarks.
- References – references are clearly listed including the individual benchmark reports from the Handbook.
- Input Files – after verification by qualified reviewers, each and every input file for the models was included in its entirety in the document.
- Independent Review – after authorship is complete the document is reviewed by an independent reviewer qualified in the code system and familiar with these requirements

2.2. Bias Quantification Documentation

Equally important to documenting the modeling of benchmarks is documenting the quantification of the bias for each subgroup. Like model documentation, bias quantification documentation followed a standardized structure agreed to early on by the developers. The structure required the homogeneous and consistent documentation of information described below.

- Introduction and Scope – documentation of the scope includes the subject of the subgroup of benchmarks, code version and cross section set, computers and operating systems used, and the referenced benchmark Handbook edition. The general purpose of the document is also discussed and the modeling documentation appropriately referenced.
- Requirements – bias quantification must meet the requirements referenced in this section, which are largely internal specific requirements to satisfy ANS-8.24.
- Inputs and Assumptions – as with modeling documentation, any inputs or assumptions that go into the bias quantification are clearly enumerated and summarized.
- Analytical Methods and Computations - general documentation is made of the calculation of the biased multiplication factor, the accepted methods for bias quantification, and clear statement of the intent to satisfy ANS-8.24. Appropriate references are cited.
- Selected Benchmarks – the benchmarks used in the analysis are discussed in terms of the general design of the system and physical parameters each benchmark represents/spans. The appropriateness of the benchmark was assessed for the scope of the intended application. At the time of this authorship this assessment process extended to assigning the selected benchmarks to one of ten generic groups which encompassed the fissile material operations at SRNS.
- Benchmark Models – the multiplication factor and uncertainty data from the modeling effort is reproduced in this report and paired with the corresponding benchmark values and experimental uncertainties. All four of these quantities are typically used in determining the bias.
- Bias Term Analysis – the approach used to quantify the bias is documented in detail.
    - The analysis proceeds through the bias quantification method hierarchy of LTB, LTL, and Non-Parametric Value, as appropriate, until an acceptable bias value is established.
    - The treatment of the positive bias, if one exists, is documented.
- Area of Applicability Discussion – for the models evaluated in each particular subgroup, a discussion is made of the important parameters, which typically include:
    - Code version and cross-section set
    - Calculational methods and analysis techniques
    - Fissionable isotope enrichment
    - Moderator material
    - Moderator H/X (typically for homogenous systems)
    - Reflector material and associated reflector thickness
    - Poison isotope concentration
    - Incidental materials (isotopes present in small concentrations or in locations that have only a small impact on the reactivity)
    - Neutron spectrum (typically represented by EALF)
    - Geometry (simple solid, complex/concave solid, array, etc.)
    - Fissionable material form (metal, oxide, etc. – this is relevant only if the modeling method makes a distinction between the forms)
    - Temperature
- Results – the quantified bias is clearly presented. Additionally, the code system, cross section library, specific code options, and the range of the physical parameters associated with the benchmarks modeled are all explicitly stated and summarized.

- Conclusions – at the end of the process, the analyst and reviewer should be able to conclude that the results meet the objective in that the code system has been validated to acceptably reproduce experimental results and that a quantification has been made of the code's bias in multiplication factor prediction for systems similar to those in each subgroup.
- References – references are clearly listed including the individual benchmark reports from the Handbook.
- Independent Review – after authorship is complete the document is reviewed by an independent reviewer qualified in the code system and familiar with these requirements

3. BENCHMARK EXPERIMENT MODELING

Modeling of the selected benchmark experiments was completed in both code packages so that personnel at the various SRS facilities, and supporting the various operations, could use either code for criticality safety evaluations. Modeling of the benchmarks was based on the benchmark description (i.e. Section 3 of benchmark reports). Emphasis was placed on establishing a consistent set of models, documenting assumptions, and establishing the required precision of inputs and outputs. Specific nuances of the modeling effort can be broadly divided into geometry specifications and compositions specifications.

3.1. Geometry Specifications

MCNP and SCALE have moderately dissimilar language when it comes to specifying input geometry. Likewise, different model developers have different approaches to how each chooses to construct their input decks. This being recognized, the overarching requirement of this method and effort was to model the geometry specified in the benchmark description verbatim to the extent allowed by the code. Each code had limitations of the capability to define various geometric configurations. So long as this modeling requirement was satisfied, model development was left to the individual engineers.

Each and every model developed for this effort was subjected to an iterative, multi-pass peer review by subject matter experts in the two code packages to ensure that geometry specified in the benchmark description section of the benchmark report was indeed what was modeled. To the extent possible, dimensions entered are directly traceable to values in the benchmark report.

3.2. Composition Specifications

Compositions specifications were taken verbatim from the benchmark description section of the benchmark report. In most cases this section of each report has the compositions specified in atom density (atoms per barn-centimeter) and this value was taken directly so as to be traceable to the benchmark reports, with the few nuances discussed below. All atom densities were entered in scientific notation. Temperatures for each composition were assigned based on the temperature specified in the benchmark description and entered in Kelvin. In cases where the temperature was not specified or specified as "ambient" or "room temperature" a value of 293 K was assumed.

The overall nuance of composition specification was that each composition was specified isotopically, even when the benchmark description provided only the elemental atom density. This

requirement, which was consistent for all benchmarks modeled, led to the following set of guidelines for composition specification.

- Atom densities specified in the benchmark description for individual isotopes were entered directly into the inputs
- Atom densities specified for elements only were decomposed into isotopic number densities using the following method
    - Assume natural abundances and reference the Handbook guide for natural isotopic abundances by atom percent.
    - Decompose the element atom density into atom densities for each isotope by the naturally occurring fraction. This action precipitated additional guidance:
        - In cases where the cross section library used did not contain an isotope that was specified in the naturally occurring abundance list, the most prominently occurring isotope was substituted as a place holder. This occurred for only a few isotopes having very low natural abundances. Specifically, Oxygen-16 was substituted in place of Oxygen -18 and Tungsten-184 was substituted in place of Tungsten-180.
        - In cases where the cross section library used contained only the elemental cross section, the atom density for that element was used directly. This occurred for SCALE and MCNP which did not have individual cross sections for Carbon-12 and Carbon-13 in the libraries used.
        - In cases where the element had only one naturally occurring isotope, the elemental atom density from the benchmark description was used directly. This occurred for Manganese which was stated in the Handbook as consisting only of Manganese-55.

For clarification it should be noted that the above guidance did result in hydrogen being isotopically specified as the appropriate ratio of protium and deuterium. Also, in benchmarks where the composition of air was specifically stated, that composition was modeled per the same guidance and the environment filled with the specified air. Otherwise air was modeled as void space.

Each and every model developed for this effort was subjected to an iterative, multi-pass peer review by subject matter experts in the two code packages to ensure that compositions specified in the benchmark description section of the benchmark report were translated into the inputs per the guidance specified above. Where isotopic atom densities were available these were verified to be directly traceable to the benchmark description. All atom densities decomposed from element to isotopic were verified to sum to the element atom density provided in the benchmark description and that the ratios matched the naturally occurring abundances assumed.

4. BIAS QUANTIFICATION METHODS

Quantification of the bias each code exhibits in reproducing certain types of experimental systems is a central component of this work as it directly influences how the USL is established per standard SRNS procedures. Three methods were made available to the analyst in an effort to quantify the bias of each subgroup of benchmarks. The first two are parametric in nature and based on the lower tolerance of the data – lower tolerance band and lower tolerance limit. If both of those methods

failed to yield a bias quantification due to the nature of the data, the third option available was the non-parametric value method. These three methods are discussed in the subsections below.

4.1. Lower Tolerance Band

The results of benchmark modeling are calculated multiplication factors from the code output, k_{calc}. The k_{calc} values vary about 1.0 but the systems they represent have an experimentally determined multiplication factor, typically at or very near critical. The lower tolerance band (LTB) approach begins by examining the data as a function of physical parameters which affect neutronic behavior of the system (e.g. neutron energy, fissile material concentration, etc.). These data are examined to determine if a linear correlation exists between the bias value and the physical parameter. If such a correlation is determined to exist, a lower tolerance band is established. This LTB is a bounding quadratic polynomial derived from the parametric fit of the data. The best estimate multiplication factor, k_{be}, (1.0 + bias – bias uncertainty) may then be determined directly from the LTB equation by evaluating it at the value of the physical parameter for the system being analyzed.

The reader should note that the nature of the parametric studies for the LTB method inherently involve trending of the data which is accomplished in accordance with the requirements of ANS-8.24 Section 6.2.

4.2. Lower Tolerance Limit

If the data fails to exhibit a clear relationship between the bias and a physical parameter (i.e., LTB is not applicable), then the next option is to establish a lower tolerance limit (LTL) which is a single bounding value best estimate multiplication factor. The data is tested for normality and if it is statistically determined to be a normal distribution then an LTL is determined. The LTL value is derived from the average multiplication factor result adjusted by the variance and scaled by a (95/95) tolerance factor. A confidence factor of 95% and a proportion factor of 95% are normally used. The LTL value is typically more restrictive than a value computed from an LTB relationship within given range of a physical parameter. This is often due to larger variance in the data set which both drives the LTL lower and makes determination of clear relationship for the LTB difficult. This is not true of every LTL analysis however; some data sets have a narrower variance band and the LTL could be less restrictive than the LTB in those cases.

4.3. Non-Parametric Value

If the LTL method cannot be used because the data is not statistically determined to be normal, the last method to quantify the bias is to set a k_{be} that is a non-parametric value. The minimum bias (i.e. the most negative bias) from the modeling effort is identified. From this value is subtracted a non-parametric margin set based on a pre-defined table of values related to the degree of confidence in the data population and also the root sum of the statistical and experimental uncertainties squared. Of the three methods, the non-parametric value usually yields the most restrictive bias.

4.4. Positive Bias Treatment

A positive bias is defined as the situation wherein the average weighted bias for the subgroup of benchmarks, as determined by one of the methods above, have value greater than unity. This means that the code will tend to over predict multiplication factor. In most cases the bias is negative which, as will be discussed in the following section, reduces the USL. Positive biases may be used but only if they are appropriately justified. This justification is required because use of a positive bias will raise the USL value rather than lower it. Theoretically, this could result in a USL, barring any other margins being introduced, that would be greater than 1.

4.5. Outlier Treatment

Outlier data points for specific benchmark cases which fall outside of the expected trend of the data are not ignored simply to prevent data skewing, normalize the data set, or for any other statistical argument. Outliers were only excluded in rare cases as supported by the benchmark report. If the benchmark report made explicit discussion of outlier data as being suspect due to actual, physical complications or errors in the experimental setup, data acquisition, etc. only then was the outlier excluded. Outlier rejection is accomplished in accordance with the requirements of ANS-8.24 Section 6.3.

5. APPLICATION OF BIAS TO SETTING K_{SAFE}

For SRNS criticality safety analyses, the USL is defined as largest value of the multiplication factor for which the system in question can be safely said to be subcritical and is bestowed the label k_{safe}. The multiplication factor output by SCALE or MCNP plus two times the statistical uncertainty of the calculation is the accepted conservative k_{eff}. If the acceptably conservative multiplication factor is less than k_{safe}, then the system is subcritical under those specified conditions. Standard methodology used across SRNS Criticality Safety Engineering is to develop k_{safe} using the following formula:

$$k_{safe} = (1.0 + \text{Bias} - \text{Bias Uncertainty}) - \Delta k_{MSM} - \Delta k_{AoA} \quad (1)$$

In this formulation the quantity of $(1.0 + \text{Bias} - \text{Bias Uncertainty})$ is the k_{be}, Δk_{MSM} is an additional margin applied to meet the ANS-8.24 margin of subcriticality, and Δk_{AoA} is an additional margin applied for the Area of Applicability. These terms are discussed in greater detail in the subsections below.

5.1. Bias Value

The k_{be}, $(1.0 + \text{Bias} - \text{Bias Uncertianty})$, is the value determined by the bias quantification method for the subgroup of benchmarks relevant to the system in question for which the user seeks to set a k_{safe}. This is, in general, the lower bound multiplication factor value the code will predict for systems of a given type known to be critical.

5.2. Area of Applicability

The benchmark systems evaluated are representative of the types of operations at SRNS but are not exact cases of each and every operation or contingency situation in any given analysis. In general, the benchmarks that went into establishing a k_{be} have a range of parameters affecting multiplication such as mass, moderation, geometry, reflection, temperature, position, enrichment, and neutron energy spectrum. The system being analyzed may not always fall exactly within these same ranges of parameters, i.e. the Area of Applicability (AoA) for the bias quantification. Therefore it is left to the prudent engineering judgement of the analyst to apply an appropriate additional margin to the k_{safe} value to account for known differences between the system being analyzed and the benchmarks. A typical value for this margin, when it is necessary, is $\Delta k_{AoA} = 0.01$.

5.3. Margin of Subcriticality

SRNS standard criticality safety methodology requires an additional margin be applied in accordance with ANS-8.24 Section 6.4. This is to ensure the system is actually subcritical via a margin to account for the sensitivity of the system or process to variations in fissile form, geometry, physical characteristics (e.g. differences in as-built and as-analyzed geometry), etc. This additional value is meant to protect against these unknown but reasonable variations and is called the minimum subcritical margin (MSM). Since a single value might not always be appropriate, even within different applications of the same validation subgroup, guidance was developed to help the engineer select an appropriate MSM. A typical value is $\Delta k_{MSM} = 0.02$.

6. EXAMPLE ANALYSIS: MTR TYPE FUELS USING SCALE 6.1

6.1. Benchmarks

The used material test reactor (MTR)-type fuels stored and processed by SRNS are mostly aluminum clad, aluminum alloyed highly enriched uranium fuels. These fuel types are similar in many physics aspect to those in the Handbook benchmark set HEU-MET-THERM-006 containing 23 cases. HEU-MET-THERM-006 benchmarks are based on a series of experiments involving SPERT-D fuel assemblies performed at Oak Ridge National Laboratory in 1964-65. The experiments considered in this set involved arrangements of fuel assemblies with a reflector and moderator of either demineralized water or uranyl nitrate solution in a large stainless steel tank. Assemblies were composed of up to 22 fuel plates (full assembly) which could be varied to achieve a critical configuration using less than 22 plates (partial assembly). Fuel plates were comprised of uranium (enrichment of 93.17 wt. % U-235) which was alloyed with aluminum at 23.8 wt. % uranium and clad in 0.020 inch thick aluminum. A full assembly contained an average of 306.46 grams U-235.

6.2. Modeling Results

The benchmark cases were modeled in SCALE 6.1 as described in the methods above (Ref. 3). Table I shows the calculated multiplication factor, k_{calc}, the statistical uncertainty, σ_{calc}, the benchmark value for the multiplication factor, k_{bench}, the biased multiplication factor, $k_{bias} = k_{calc} / k_{bench}$, the critical mass of the assembly in kg, and the energy at the average lethargy of fission

(EALF) in eV. Of the cases available, Case 13 will be omitted as unacceptable data based upon supporting argument from the benchmark report. Case 13 was derived as a coarse interpolation between a subcritical state (involving a partial assembly of 6 plates) and a delayed supercritical state (involving a partial assembly of 8 plates). It is therefore not surprising that modeling the configuration may give an erroneous result.

Table 1. Results of Modeling HEU-MET-THERM-006.

Benchmark Case	k_{calc}	σ_{calc}	K_{bench}	k_{bias}	Critical Mass (kg)	EALF (eV)
HEU-MET-THERM-006-01	0.99964	0.00043	1.00000	0.99964	4.63	8.10198E-02
HEU-MET-THERM-006-02	0.99858	0.00047	1.00000	0.99858	3.87	6.76207E-02
HEU-MET-THERM-006-03	1.00357	0.00037	1.00000	1.00357	3.79	6.08894E-02
HEU-MET-THERM-006-04	0.99770	0.00035	1.00000	0.99770	3.48	5.95276E-02
HEU-MET-THERM-006-05	0.99757	0.00045	1.00000	0.99757	3.87	5.64380E-02
HEU-MET-THERM-006-06	0.99556	0.00048	1.00000	0.99556	4.54	5.40184E-02
HEU-MET-THERM-006-07	0.99570	0.00039	1.00000	0.99570	6.16	5.23666E-02
HEU-MET-THERM-006-08	0.99240	0.00037	1.00000	0.99240	9.82	5.06118E-02
HEU-MET-THERM-006-09	0.99702	0.00037	1.00000	0.99702	14.33	5.02947E-02
HEU-MET-THERM-006-10	1.00690	0.00041	1.00000	1.00690	11.78	7.87653E-02
HEU-MET-THERM-006-11	0.99880	0.00039	1.00000	0.99880	9.28	6.00230E-02
HEU-MET-THERM-006-12	1.00178	0.00039	1.00000	1.00178	14.71	5.22491E-02
HEU-MET-THERM-006-13	1.02026	0.00043	1.00000	1.02026	--	7.91011E-02
HEU-MET-THERM-006-14	0.99466	0.00046	1.00000	0.99466	14.71	5.49328E-02
HEU-MET-THERM-006-15	0.99269	0.00042	1.00000	0.99269	19.62	5.44561E-02
HEU-MET-THERM-006-16	0.99981	0.00040	1.00000	0.99981	19.62	6.09099E-02
HEU-MET-THERM-006-17	0.99744	0.00040	1.00000	0.99744	6.19	7.14023E-02
HEU-MET-THERM-006-18	0.99898	0.00047	1.00000	0.99898	8.64	7.67550E-02
HEU-MET-THERM-006-19	0.99849	0.00054	1.00000	0.99849	2.86	5.05823E-02
HEU-MET-THERM-006-20	0.99754	0.00047	1.00000	0.99754	5.15	6.21880E-02
HEU-MET-THERM-006-21	1.00103	0.00046	1.00000	1.00103	6.76	6.64997E-02
HEU-MET-THERM-006-22	1.00045	0.00041	1.00000	1.00045	8.90	7.08939E-02
HEU-MET-THERM-006-23	1.00279	0.00035	1.00000	1.00279	10.15	7.27112E-02

6.3. Bias Quantification

Bias quantification for this data set was documented in Ref. 4. Lower Tolerance Band evaluations were conducted to attempt to correlate the k_{be} to EALF (Figure 1) and to the critical mass of the system (Figure 2). Equations for the linear parametric fit and the quadratic LTB may be seen on each graph. The EALF data has only a weak trend and no trend could be determined from the critical mass data. Therefore the Lower Tolerance Limit method was examined.

The Shapiro-Wilk normality test, applied to the 22 data points, indicated the data may be said to be normally distributed. The mean multiplication factor was found to be 0.99859. The lower tolerance factor was then found to be 2.35. The average uncertainty squared, variance about the mean, and resulting square root of the pooled variance were 1.6306E-05, 1.1843E-05, and 5.3056E-03, respectively. The resulting Lower Tolerance Limit k_{be} is 0.99859 – 2.35*0.0053056 = 0.9861.

Since the LTL method was applicable, there was no need to establish a more restrictive non-parametric value limit.

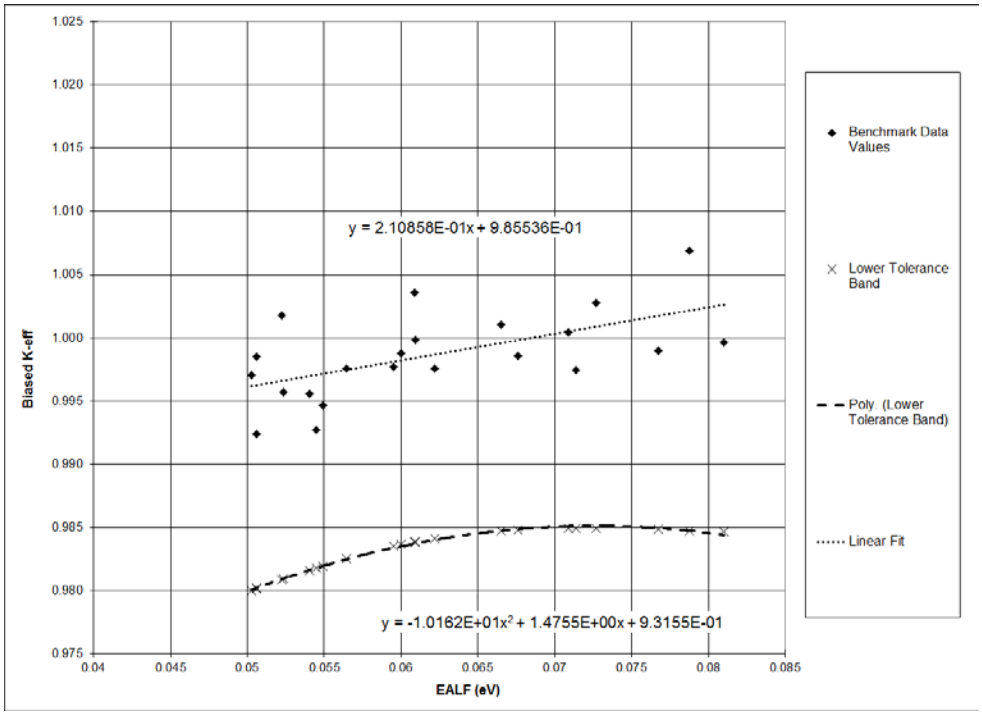

Figure 1. EALF Correlation Check for LTB Analysis.

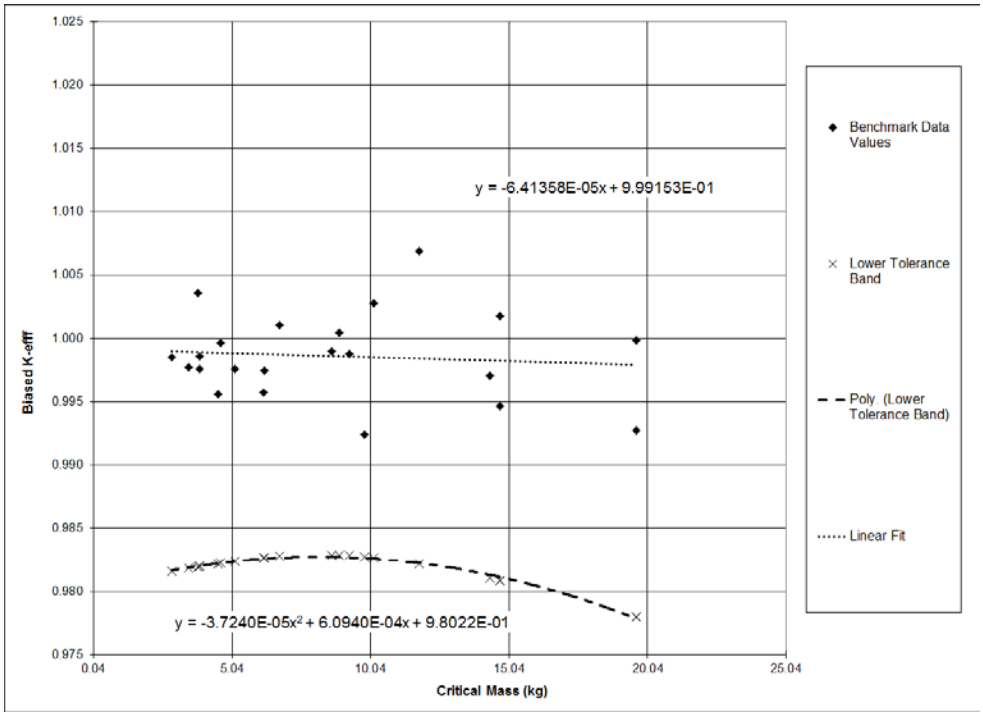

Figure 2. Critical Mass Correlation Check for LTB Analysis.

6.4. A Typical k_{safe} for MTR-type Systems

Using the typical values discussed above for AoA and MSM margins, a typical USL for an MTR-type system under analysis would then be:

$$k_{safe} = (1.0 + \text{Bias} - \text{Bias Uncertainty}) - \Delta k_{MSM} - \Delta k_{AoA} = 0.9861 - 0.02 - 0.01 = 0.9561 \quad (1)$$

Any acceptably conservative multiplication factor calculated for this type of system being modeled found to be less than 0.9561 could be said to be safely subcritical. In this manner, the quantified bias directly influences the criticality safety analysis.

7. CONCLUSIONS AND FUTURE WORK

Developing a validation suite for SCALE 6.1 and MCNP 6.1 for use at SRNS has been divided into a two phase process. At the time of this authorship Phase I has been completed and Phase II is underway. The Phase I effort represented several man years of effort spread out over more than a dozen engineers.

In Phase I, a validation suite for the two code packages has been established, somewhat independently of each other but both adhering to the requirements set forth in the methods described in this paper. Each code system was used to model benchmark experiments fitting into the 10 subgroups discussed herein. The SCALE 6.1 validation included 591 models with the largest subgroups being the unpoisoned plutonium solutions and HEU metal groups. The MCNP 6.1

validation included 599 models with the largest subgroups being unpoisoned plutonium solutions, HEU metal, and LEU groups. Among the subgroups, all three bias quantification methods were employed depending on the nature of the data for each subgroup.

Phase II involves an effort to align the SCALE and MCNP validations so that they both model the same benchmarks in each subgroup. Effort will then be placed on expanding the selection of benchmark models based on customer (U.S. DOE) and internal requests. The revised suite will incorporate the new data points into the bias quantification evaluations and update the biases accordingly. Phase II work is underway at the time of this authorship.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the efforts of everyone who worked on the Phase I validation including (alphabetically) James Baker, Nathan Devine, Andrew Goslen, Stephen Kessler, J. Michael Low, Martin Macher, Austin Meredith, Dorin Musat, Michael Ratliff, and Nicholas Schira.

REFERENCES

[1] *International Handbook of Evaluated Criticality Safety Benchmark Experiments*, NEA/NSC/DOC(95)03, NEA No. 7281, Organization for Economic Co-operation and Development – Nuclear Energy Agency, September 2015.
[2] *Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations*, ANSI/ANS-8.24-2007, American Nuclear Society, March 2007
[3] S.H. Finfrock, et. al., "SCALE 6.1 Benchmark Model Calculations," *N-CLC-G-00162, Rev. 0*, Savannah River Nuclear Solutions, June 2016
[4] S.H. Finfrock, et. al., "SCALE 6.1 Validation for SRNS Personal Computers," *N-CLC-G-00166, Rev. 0*, Savannah River Nuclear Solutions, June 2016