NUREG/CR-6698
Guide for Validation of Nuclear Criticality Safety Calculational Methodology

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Introduction

The U.S. Nuclear Regulatory Commission (NRC) licenses nine facilities for uranium enrichment and fuel fabrication under Title 10 of the Code of Federal Regulations, Part 70 and Part 76. These NRC licensed fuel cycle facilities use nuclear criticality safety (NCS) evaluations to ensure that fissile material will remain subcritical under both normal and credible off-normal conditions. Licensee NCS evaluations typically rely upon computer based computational techniques to establish criticality safety limits and these methods must, therefore, be validated in accordance with ANSI/ANS-8.1[1]. The NRC has observed wide variation in the methods employed at these facilities to validate computational techniques and has noted that some validation methods in use do not provide a clearly defined technical basis for establishing the safety margin. NUREG/CR-6698[2], "Guide for Validation of Nuclear Criticality Safety Calculational Methodology," was developed under contract by Science Applications International Corporation to review widely used procedures and assemble specific guidance for validation of criticality safety calculational methodology.

This paper reviews the validation methods discussed in NUREG/CR-6698 which were taken substantially from the Westinghouse Savannah River Company Criticality Safety Methods Manual[3]. These methods establish an upper safety limit (USL) based on statistical evaluation of the calculational bias which is the difference between critical experimental conditions similar to the area of applicability of interest and the calculated results of those experiments. Calculated neutron multiplication or k_{eff} values must fall under the USL to be considered subcritical. NUREG/CR-6698 describes procedures by which NRC fuel cycle facility licensees may perform validation including selection of critical experiments, establishing an area of applicability, determination of calculational bias and bias uncertainty, and establishing an USL. Also included are suggested topics for inclusion in formal documentation of the validation activity, along with complete examples and key data useful for statistical analysis.

Validation Methodology

During the licensing and subsequent inspection of fuel cycle facilities, the NRC must be assured of the adequacy of the safety margin when criticality safety limits have been established through computer based calculational methods. Therefore, the license reviewer or inspector must understand the bias of the calculational methodology used at the facility. The bias is the difference between calculated and experimental results and reflects the accuracy of the calculational methodology. Understanding a calculational methodology's bias is key to understanding the margin and is obtained through the validation process. The bias and the uncertainty associated with the bias are used in combination with additional subcritical margin to establish an upper safety limit (USL). Adequate subcritical margin is considered assured if calculated results are below the USL and are within the area of applicability of the validation.

The USL is represented by the following equation:

$$USL = 1.0 + Bias - \sigma_{Bias} - \Delta_{SM} - \Delta_{AOA} \quad (1)$$

Assuming the critical experiments have a k_{eff} of unity, the bias is calculated as the difference between the calculated k_{eff} and the modeled critical experiment. Because a positive bias may be nonconservative, a bias is set to zero if the calculated average k_{eff} is greater than one. The statistical uncertainty in the bias is represented by σ_{Bias} and the minimum subcritical margin is represented by Δ_{SM}. The term Δ_{AOA} is an additional subcritical margin to account for extensions in the area of applicability and a value of zero is assigned to Δ_{AOA} if not extending the area of applicability.

The following condition must be demonstrated for all normal and credible off-normal operating conditions:

$$k_{calc} + 2\,\sigma_{calc} < USL \quad (2)$$

where:

k_{calc} is the calculated k_{eff} returned by the method and σ_{calc} is the uncertainty.

2σ is related to 95/95 confidence values suggested by the examples. Although 95/95 confidence is typical, license commitments will normally determine final confidence requirements.

Elements of Validation

The ANSI/ANS-8.1-1998 standard provides basic requirements for validation of a calculational method. The common validation practice is comparison of the calculated k_{eff} to a critical or near critical system. NUREG/CR-6698 defines common elements of validation as:

- Define operation/process to identify range of parameters to be validated. Prior to the initiation of the validation activity, the operating conditions and parameters for which the validation is to apply must be identified. The fissile isotope, enrichment of fissile isotope, fuel density, fuel chemical form, types of neutron absorbers, moderators and reflectors, range of moderator to fissile isotope, and physical configurations are among the parameters to specify. These parameters define the area of applicability for the validation effort.

- Select critical experiment data. After the desired range of operating conditions and parameters are identified, appropriate critical experiments can be selected for use in the validation. Many critical experiments have been performed and documented with varying degrees of quality. Although peer reviewed critical benchmarks are preferred for use in validating calculational methodologies, there may be some instances where only critical experiment data are available. Care should be taken to make appropriate allowances for larger, and perhaps unspecified, uncertainties inherent with such data. Use of subcritical benchmark experiments should be appropriately justified.

- Model experiments. Once the computer code is selected for validation and installed and verified on the computer platform, the selected critical experiments are coded into the format required by the computer program. An inexperienced user can affect the bias through the modeling of critical experiments; therefore, it is essential that the validation modeling be performed by appropriately trained and qualified staff. It is also essential that the user carefully review any input files (benchmark models) used in previous validations or benchmark databases to insure consistency in modeling technique and code options.

- Analyze the Data. Input files are executed using the code system being validated to calculate k_{eff} for the selected critical experiments. The k_{calc} and associated σ_{calc} values are tabulated with other descriptive information and subjected to statistical analysis.

    - Determine bias and bias uncertainty. The validation uses a statistical analysis to determine bias and bias uncertainty in the calculation of k_{eff}.

    - Identify Trends in Data, Including Discussion of Methods for Establishing Bias Trends. Trends are determined through the use of regression fits to the calculated results.

    - Test for Normal Distribution. The statistical evaluation performed must be appropriate for the distribution of the data. One technique described requires normally distributed data. A non-parametric analysis method is used when data does not have a relationship with a parameter of interest that can be usefully represented.

    - Select Statistical Method. The approach to establishing the USL relies on selection of an appropriate statistical treatment. It is the responsibility of the facility or site performing the validation to justify the method selected.

    - Identify and Support Subcritical Margin. The subcritical margin is not intended to account for process upset conditions or for uncertainties associated with a process. The subcritical margin is used solely to establish the maximum value of k_{eff} that can be considered to remain subcritical based on the validation results.

    - Calculate Upper Safety Limit. The USL has been defined as follows:

$$USL = K_L - \Delta_{SM} - \Delta_{AOA} \,. \quad (3)$$

Where:

$$K_L = 1.0 + Bias - \sigma_{Bias} \quad (4)$$

- Define the area of applicability of the validation and limitations. The area of applicability refers to a range of the key physical parameters that define a particular fissile configuration.

Statistical Methods

Many statistical methods are available and capable of producing reasonable results. Regardless of the method chosen to perform the statistical evaluation, the methodology must be clearly defined and technically defensible. NUREG/CR-6698 provides specific statistical treatments that produce adequate results, are readily applied, and are acceptable to the NRC:

- Single-Sided Tolerance Limit. A weighted single-sided lower tolerance limit is a single lower limit above which a defined fraction of the true population of k_{eff} is expected to lie, with a prescribed confidence and within the area of applicability. A lower tolerance limit should be used when there are no trends apparent in the critical experiment results. Use of this limit requires the critical experiment results to have a normal statistical distribution. If the data does not have a normal statistical distribution, a non-parametric statistical treatment must be used.

- Tolerance Band. 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 is a conservative method that provides a fitted curve above which the true population of k_{eff} is expected to lie. The tolerance band equation is actually a calibration curve relation and a given tolerance band may be used multiple times to predict bias.

- Nonparametric Statistical Treatment. Data that do not follow a normal distribution can be analyzed by non-parametric techniques. 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. The more data available in the sample, the higher the degree of confidence.

Area of Applicability

Determination of the area of applicability is key to validation of a calculational method. Once critical experiments have been selected, areas of applicability are identified for each experiment and experimental data is used to establish the area of applicability for each parameter. The analyst must consider the overall parametric span and ensure that experiments encompass the desired operational range. If the operational range cannot be covered by critical experiments, interpolation or extrapolation must be considered.

Validation Report

The validation activity must be documented in a formal report which must have sufficient detail to allow for independent review by qualified individuals. This report should describe the methodology for determining the USL and areas of applicability for the code system. The validation report should provide a summary description of the facility or site for which the validation is to apply, including details relevant to NCS (i.e., fissile isotope(s), enrichment, chemical compounds, density ranges of fissile material, moderators, reflectors, etc.). There should also be a description of the computer code system used, applicable code execution sequences, cross section libraries, and the computer system for which the validation is performed. For each area of applicability, each critical experiment used to determine the bias and associated bias uncertainty for that area of applicability should be listed in the validation report. The input files used in the validation should be included. The statistical methods used in the determination of the USL should be described or a citation provided where such descriptions exist. Finally, a comprehensive list of references used in the validation should be provided such as sources of critical experiment data, statistical methods employed, and other relevant information.

Summary

NUREG/CR-6698, "Guide for Validation of Nuclear Criticality Safety Calculational Methodology," presents a validation methodology which may be useful to fuel cycle licensees to establish a reproducible and understandable basis for safety margin at facilities where criticality safety limits have been based upon computer calculations.

References

1. ANSI/ANS-8.1 1983, *"Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors*," American Nuclear Society, La Grange Park, IL.

2. NUREG/CR-6698, "Guide for Validation of Nuclear Criticality Safety Calculational Methodology," U.S. Nuclear Regulatory Commission, Washington DC.

3. WSRC-IM-96-133, "*Nuclear Criticality Safety Methods Manual,*" Westinghouse Savannah River Company, Aiken, SC.