DOCKET: 70-7002

CERTIFICATE HOLDER: United States Enrichment Corporation
Portsmouth Gaseous Diffusion Plant
Piketon, Ohio

SUBJECT: COMPLIANCE EVALUATION REPORT: Validation Report POEF-LMUS-13 Revision 1, "Validation of the CSAS25 Sequence in SCALE-4.3 and the 27-Group Cross Section Library for Use at the Portsmouth Gaseous Diffusion Plant."

BACKGROUND

Violation 70-7002/97-203-03 was issued on June 27, 1997, for the failure of USEC to develop an adequate validation report that supported the use of the SCALE computer code at the Portsmouth GDP (PORTS). The inspectors had observed that several PORTS calculations had been performed to establish the safety margin for systems based on an enrichment of 20 wt% ^{235}U. The PORTS validation report at the time of inspection 97-203 did not contain any benchmarks in the range between 5 wt% to 93 wt%. The PORTS validation report concluded that the Average Energy Group of neutrons causing fission was similar between the calculated results and the benchmarks below 5 wt% and above 93 wt% so that the range could be extended by interpolation. The NRC determined that this methodology did not adequately address certificate commitments in that the extension was not statistically supported.

As a result of this finding, USEC committed to identify additional benchmarks and revise the validation report to include benchmarks related to the range of desired parameters. USEC completed the validation report revision in July 1998 and submitted the report to inspectors during inspection 70-7002/98-208 as evidence of completion of open item 70-7002/97-203-03. Subsequent to the inspection, the staff performed an independent review of the revised validation report in order to resolve the open item. This Compliance Evaluation Report closes this issue by determining that the revised PORTS validation report meets certificate requirements and USEC commitments to resolve the violation.

CERTIFICATION COMMITMENTS

Three categories of commitments are applicable to a PORTS validation report, the Portsmouth Safety Analysis Report which is also the certificate application, the Technical Safety Requirements, and American National Standards Institute (ANSI) standard ANSI/ANS-8.1-1983. The commitments are straightforward and nonprescriptive, allowing considerable flexibility in how USEC prepares the validation report.

Enclosure

Portsmouth Safety Analysis Report Section 5.2.3.2, under the heading "Computer Calculations," requires, in part:

> Critical experiments which have specific, well-defined parametric values and are adequately documented are termed benchmark experiments. Computer codes are validated using experimental data from benchmark experiments which, ideally, have geometries and material compositions similar to the systems being modeled.
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> Validation of the computer code determines its calculational bias or uncertainty as well as the effective margin of subcriticality. The PORTS validation involves the modeling of benchmark critical experiments over a range of applicability. Because the k_{eff} value of a critical experiment is essentially 1.0, the bias of the code is taken to be the deviation of the calculated values of k_{eff} from unity. Statistical analysis is employed to estimate the calculational bias, which includes the uncertainty in the bias and uncertainties due to extensions of the area of applicability, as well as the effective margin of subcriticality. Uncertainty in the bias is a measure of both the precision of the calculations and the accuracy of the experimental data. The validation of the computer code specifically defines the maximum acceptable k_{eff} used to determine subcriticality.
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> The margin of subcriticality used at PORTS shall result in a k_{eff} upper safety limit which will ensure that there is a 95 percent confidence that 99.9 of all future k_{eff} values less than this value will be subcritical. The minimum margin of subcriticality of 0.02 in k_{eff} shall be used to establish the acceptance criteria (i.e., upper safety limit) for criticality calculations. The upper safety limit for PORTS calculations is established as $\leq$.9605 in accordance with the validation report POEF-T-3636, Revision 1, "Validation of Nuclear Criticality Safety, Software and 27 Energy Group ENDF/B-IV Cross Sections" dated January 1996.
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> When NCS is based on computer code calculations of k_{eff}, controls and limits are established to ensure that the maximum k_{eff} complies with the computer code validation for that type of system being evaluated.
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> Scoping and analysis calculations can be performed utilizing various unvalidated computer codes; however, computer calculations of k_{eff} used as the basis for NCS approvals are confirmed by, or performed using, configuration-controlled codes and cross-section libraries for which documented validations are performed with at least the same degree of conservatism as that presented in the validation report POEF-T-3636, Revision 1, and are in accordance with the American National Standards Institute (ANSI) standard ANSI/ANS-8.1-1983.

Technical Safety Requirement 3.11.3 states that "A minimum margin of subcriticality of 0.02 in k_{eff}, shall be used to establish the acceptance criteria for criticality calculations."

Technical Safety Requirement 3.11.4 states that "The k_{eff} for criticality calculations shall be $\leq$ 0.9605 which includes the bias, uncertainty, and the margin of subcriticality."

ANSI/ANS-8.1-1983 Section 4.3 under the heading "Validation of a Calculational Method" requires:

> There are many calculational methods suitable for determining the effective multiplication factor (k_{eff}) of a system or for deriving subcritical limits. The methods vary widely in basis and form, and each has its place in the broad spectrum of problems encountered in the nuclear criticality safety field. However, the general procedure to be followed in establishing validity is common to all.
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> 4.3.1 Bias shall be established by correlating the results of all criticality experiments with results obtained for these same systems by the method being validated, Commonly the correlation is expressed in terms of the values of k_{eff} calculated for the experimental systems, in which case the bias is the deviation of the calculated values of k_{eff} from unity. However, other parameters may be used. The bias serves to normalize a method over its area(s) of applicability so that it will predict critical conditions within the limits of the uncertainty in the bias. Generally neither the bias nor its uncertainty is constant; both should be expected to be functions of composition and other variables.
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> 4.3.2 The area(s) of applicability of a calculational method may be extended beyond the range of experimental conditions over which the bias is established by making use of the trends in the bias. Where the extension is large, the method should be supplemented by other calculational methods to provide a better estimate of the bias in the extended areas(s).
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> 4.3.4 A margin in the correlating parameter, which margin may be a function of composition and other variable, shall be prescribed that is sufficient to ensure subcriticality. This margin of subcriticality shall include allowances for the uncertainty in the bias and for uncertainties due to any extensions of the area(s) of applicability.
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> 4.3.5 Nuclear properties such as cross sections should be consistent with experimental measurements of these properties.
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> 4.3.6 A written report of the validation shall be prepared. This report shall:
> (1) Describe the method with sufficient detail, clarity, and lack of ambiguity to allow independent duplication of results.
> (2) State computer programs used, the options, recipes for choosing mesh points where applicable, the cross section sets, and any numerical parameters necessary to describe the input.
> (3) Identify experimental data and list parameters derived therefrom for use in the validation of the method.

(4) State the area(s) of applicability.

(5) State the bias and the prescribed of subcriticality over the area(s) of applicability. State the basis for the margin."

The staff believes that for a particular safety limit to be considered adequately validated, the above requirements must be complied with and documented in a validation report combined with analyses of the specific situations to which the safety limits apply. All of the above requirements do not need to be addressed explicitly in the validation report but must be addressed in the combination of validation report and analysis to establish confidence in the safety limit.

BENCHMARK SELECTION

Fissile material is found in a variety of forms at PORTS, thereby requiring a relatively broad area of applicability to be established. USEC enriches uranium using the gaseous diffusion process. UF_6 is brought into the facility in cylinders and withdrawn into the process cascade in gaseous or liquid form. UF_6 is withdrawn from the cascade in liquid form and returned to cylinders. While in the process cascade, UF_6 encounters atmospheric moisture which causes UO_2F_2 deposits in the cascade equipment.

UF_6 deposits are removed from cylinders by flushing with steam. USEC has facilities for removing UO_2F_2 deposits from equipment by spraying with nitric or citric acid. Uranium is recovered from waste by a solvent extraction process involving uranyl nitrate and tri-butyl phosphate. Calciners in the uranium recovery area produce U_3O_8 powder. Other significant uranium systems encountered are uranium-freon, uranium-alumina, and uranium contaminated lube oil.

The USEC validation report uses 301 benchmark cases divided into areas of LEU, IEU, and HEU which are further subdivided into 10 areas:

- LEU - Uranium/U-metal
- LEU - U_3O_8
- LEU - UF_4
- LEU - UO_2F_2
- LEU - UO_2 Arrays
- LEU - $UO_2(NO_3)$
- HEU - UO_2F_2
- HEU - $UO_2(NO_3)$
- HEU/IEU - U-metal
- IEU - UF_4

The staff believes that the benchmarks selected explicitly model the major uranium systems in the facility with the exception of UF_6 and various waste configurations. USEC argues that UF_6 and waste configurations are accurately represented by UF_4 and Uranium/U-metal benchmarks. This argument is reasonable but not supported by anything in the validation report. Therefore, the adequacy of UF_4 and Uranium/U-metal benchmarks for UF_6 and waste systems must be determined by review of specific analysis. This does not detract from the overall usefulness of the revised validation report.

STATISTICAL ANALYSIS

Benchmarks were broken down by USEC into the ten representative groups for statistical analysis. USEC performed standard tests for normality on the data within the groups using the Shapiro-Wilk and Lilliefors tests which are widely accepted tests. Benchmark data was analyzed by USEC using one of three methods based on the results of the normality tests:

- weighted, single sided, lower tolerance limit
- weighted confidence interval
- distribution free confidence interval based on the sign test

The staff believes that the lower tolerance limit method incorporates relevant uncertainties in the bias as required by certificate commitments. The staff further believes that confidence interval methods may not adequately represent uncertainty in the bias, depending on the specific formulation, and therefore require additional discussion concerning how uncertainties are addressed. The staff believes that both the standard and the non-parametric confidence interval methods used in the validation report were otherwise a suitable methods based upon the wide acceptance of these methods in the literature and their previous wide and successful use in validation.

The PORTS validation report analyzed benchmarks for trends based on two parameters; enrichment and average energy group causing fission. The staff believes that, due to the relative simplicity of and long experience with the systems concerned, these two parameters adequately to represent the physics of thermalized fissile systems involving uranium with enrichments between 1.4 and 92.3 wt% and will allow a suitable comparison of analytical models with benchmarks.

The PORTS validation report displays the results of the statistical analysis in Table 3 of the report as either an Upper Safety Limit or a k_{min}. The validation report does not explicitly state that the lower of either the TSR limit, USL, or k_{min} must be used to support calculations which rely solely on the validation report to comply with validation requirements. In accordance with certificate commitments, a PORTS analysis is allowed to produce a result which exceeds the USL or k_{min} so long as it does not exceed the TSR limit. In this situation, the staff believes that additional justification is required to support the reduction in the established margin. The staff believes that this position is supported by the USEC commitment to comply with ANS-8.1.

AREA OF APPLICABILITY

The area of applicability that is encompassed by the USEC validation report is explicitly stated in Table 4 of the report. UF_6 is absent from the "Fissile Material" section of the table along with oil from the "Moderating Materials" section. Although these materials can be dealt with by discussion in separate analyses, they are such broad issues that the staff believes they should reasonably be covered in the validation report. The staff believes that a validation report does not necessarily need to cover all situations in a facility in order to be valid for that facility. Other situations may be addressed by an analysis that uses the validation report as a base to extend the area of applicability or by selecting applicable benchmarks for the specific situation and performing separate statistical analysis.

The staff believes that a validation report is not a procedure and does not establish requirements. Therefore, a calculation which does not fall within the area of applicability established by the validation report must independently establish that all applicable certificate commitments have been met even though additional restrictions imposed by the validation report have been complied with by the analysis. An example is using UF_4 and Uranium/U-metal benchmarks for UF_6 and waste systems as discussed above.

The USEC validation report includes limitations on code options in section 6.0 "Conclusions." The staff believes that allowed code options should be tabulated in the area of applicability statement where there are issues regarding their use. Justification for the use of additional code options where an impact on the bias may result should be justified in individual analyses through sensitivity analysis.

The validation report does not include benchmarks between 10.07 and 29.8 wt%. USEC argues that enrichment is equivalent to the concentration of ^{235}U, an isotope for which the physics is well understood and that the benchmarks selected give a good feel for the behavior of the subject systems across the stated range of enrichments. The staff believes that enrichment can be adequately viewed as ^{235}U concentration and that adequate benchmarks are now available in the validation report to predict the behavior of related systems so long as additional margin is used in accordance with ANS-8.1 paragraph 4.3.4.

CONCLUSION

The staff believes that the validation report POEF-LMUS-13 Revision 1, is adequate to resolve the issue underlying Open Item 70-7002/97-203-03 which was inadequate validation due to lack of benchmark experiments for uranium systems with between 5 wt% and 20 wt% enriched ^{235}U.

Several weaknesses were noted in the validation report:

- Allowed code options should be tabulated in the area of applicability statement where there are issues regarding their use.
- UF_6 should be included in the "Fissile Material" section of Table 4.
- Oil should be included in the "Moderating Materials" section of Table 4.
- The report does not explicitly state that the lower of either the TSR limit, USL, or k_{min} must be used to support calculations which rely solely on the validation report to comply with validation requirements.
- Confidence interval methods may not adequately represent uncertainty in the bias.
- The Safety Analysis Report refers to a different validation report than the one in use.

- Item 4 on page 32 states that care should be taken with enrichments between 40 - 80 wt% ^{235}U. Actually, additional margin should be used between 10.07 and 29.8 wt% and 36 and 92.6 wt% or a justification for not using additional margin included in the analysis.

The staff believes that these issues may be easily corrected in a subsequent revision of the validation report and do not detract from the overall acceptability of the submitted report to resolve the original open item. The validation and determination of adequate margin for specific cases may be documented in the relevant analysis, as stated previously. Although there is no benchmark data available at 20 wt% (where the original calculations were performed), and additional margin may be warranted in this region, the staff believes there is no safety issue for the particular cases leading to the violation. The licensee is authorized to operate up to 10 wt% enrichment; modeling at 20 wt% instead of 10 wt% provides more than sufficient margin to compensate for increased uncertainty in the bias in this range. The staff concludes that the revised PORTS validation report now contains adequate benchmarks to validate calculations between 5 wt% and 20 wt% ^{235}U, in principle. The staff concludes that the subcritical margin and statistical analysis for highly thermalized systems with compositions similar to the benchmark experiments is adequate between 5 and 10.07 wt%. The staff also concludes that the revised PORTS validation report identifies benchmarks with geometries and material compositions similar to the systems being analyzed; employs a suitable approach to grouping the benchmarks for analysis; identifies a k_{eff} upper safety limit which will ensure that there is a 95 percent confidence that 99.9% of all future k_{eff} values less than this value will be subcritical; and does not view bias as constant. The documentation is therefore adequate for the purposes of resolving this violation. Open item 70-7002/97-203-03 is considered closed.

PRINCIPAL CONTRIBUTORS

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REFERENCES

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2. D. Lurie and R. H. Moore, "*Applying Statistics*," NUREG/-1475, U. S. Nuclear Regulatory Commission, Washington, DC (1994).

3. M. Hollander, and D. A. Wolfe, "*Nonparametric Statistical Methods*," John Wiley & Sons, 1973.