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STONE & WEBSTER

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LIST OF ACRONYMS

AIVM	Addition of individual volume and masses
ANS	American Nuclear Society
ANSI	American National Standards Institute
AOA	area of applicability
AP	aqueous polishing
CFR	Code of Federal Regulations
DCS	Duke Cogema Stone & Webster
DOE	U.S. Department of Energy
EALF	energy of average lethargy causing fission
FA	fuel assembly
LTB	lower tolerance band
MFFF	Mixed Oxide Fuel Fabrication Facility
MOX	mixed oxide
NRC	U.S. Nuclear Regulatory Commission
ORNL	Oak Ridge National Laboratory
RSICC	Radiation Safety Information Computational Center
USL	upper safety limit

ABSTRACT

This report documents the validation of the nuclear criticality safety codes to be used in the design of the Mixed Oxide (MOX) Fuel Fabrication Facility (MFFF), to be owned by the U.S. Department of Energy (DOE) and operated by the licensee, Duke Cogema Stone & Webster (DCS). This report is applicable to the validation of the SCALE 4.4a code package [1] using the CSAS26 (KENOVI) sequence and the 238 energy group cross section library 238GROUPNDF5.

Title 10 Code of Federal Regulations (CFR) §70.61(d) requires that all nuclear processes remain subcritical under all normal and credible abnormal conditions. In order to establish that a system or process will be subcritical under all normal and credible abnormal conditions, it is necessary to establish acceptable subcritical limits for the operation and then show that the proposed operation will not exceed those values. In order to comply with this requirement, the *American National Standard for Nuclear Criticality in Operations with Fissionable Material Outside Reactors* [2] and the U.S. Nuclear Regulatory Commission (NRC) *Standard Review Plan for the Review of an Application for a Mixed Oxide (MOX) Fuel Fabrication Facility* [3], require that a validation be performed that (1) demonstrates the adequacy of the margin of subcriticality for safety by assuring that the margin is large compared to the uncertainty in the calculated value of k_{eff} and (2) determines the area(s) of applicability (AOA) and use of the code within the AOA, including justification for extending the AOA by using trends in the bias.

A number of design AOAs are established to cover the range of processes and fissile materials in the MFFF. AOAs covering Pu and MOX applications are as follows (1) Pu-nitrate aqueous solutions, (2) MOX pellets, fuel rods, and fuel assemblies, (3) PuO₂ powders, (4) MOX powders, and (5) Aqueous solutions of Pu compounds and Pu precipitates. The first four AOAs are addressed in the validation reports Part I [15] and Part II [16]. This report addresses the fifth AOA: (5) Aqueous solutions of Pu compounds and Pu precipitates.

The report concludes that the upper safety limit (USL) for the fifth design AOA is 0.9411 for Pu-nitrate solutions (H/Pu>50) and 0.9328 for PuO₂ powder-polystyrene mixtures (H/Pu<50). The USL accounts for the computational bias, uncertainties, and a 0.05 administrative margin.

The validation report concludes further that the MFFF application: Aqueous solutions of Pu compounds and Pu precipitates are in the range of the AOA (5). Therefore, the USL of AOA (5) is relevant for these MFFF applications.

The report further demonstrates that the PuO₂F₂ “standard salt” introduced in the criticality safety analysis to cover these aqueous solutions of Pu compounds and Pu precipitates is also in the range of the AOA (5) and represents bounding medium for criticality analysis of these aqueous solutions.

1. Introduction

1.1 Purpose

The purpose of this report is to validate the criticality codes and determine the upper safety limit (USL) to be used for performing nuclear criticality safety calculations and analyses of the Mixed Oxide (MOX) Fuel Fabrication Facility (MFFF), to be owned by the U.S. Department of Energy (DOE) and operated by the licensee, Duke Cogema Stone & Webster (DCS).

1.2 Scope

The scope of this report is limited to the validation of the CSAS26 sequence of the SCALE 4.4a code package [1] with the 238 energy group cross-section library 238GROUPNDF5 for nuclear criticality safety calculations of the MFFF.

1.3 Applicability

The following areas of applicability (AOAs) are identified to cover a range of processes in the MFFF involving Pu and MOX materials:

MFFF Design Application	AOA of Experiments
(1) Pu-nitrate solutions	AOA(1) Pu-nitrate solution
(2) MOX pellets, fuel rods, and FA	AOA(2) MOX pellet lattices in water
(3) PuO ₂ powders-H ₂ O systems	AOA(3) PuO ₂ powder-polystyrene mixture and Pu metal systems
(4) MOX powders-H ₂ O systems	AOA(4) MOX powder-polystyrene mixture
(5) Aqueous solutions of Pu compounds and Pu precipitates and Pu-nitrate solutions	AOA(5) PuO ₂ powder-polystyrene mixture

The first four AOAs are addressed in the code validation reports Part I [15] and Part II [16]. The following sections address AOA(5): PuO₂ powder-polystyrene mixtures and Pu-nitrate solutions (see Section 5.1). Section 4 demonstrates that the AOA(5) covers the design application aqueous solution of Pu compounds and Pu precipitated oxalates.

In order to cover the chemical compounds of Pu-oxalates in the AP process (precipitation of Pu-oxalates), a criticality bounding medium, PuO₂F₂ “standard salt,” is defined and shown to be a bounding computational proxy for design applications within AOA(5).

1.4 Background

1.4.1 Overall MFFF Design

The MFFF is designed to produce MOX fuel assemblies on an industrial scale from a mixture of depleted uranium and plutonium oxides for use in mission light-water reactors. The MFFF will be constructed on a DOE site and will be licensed by the U.S. Nuclear Regulatory Commission (NRC) under Title 10 Code of Federal Regulations (CFR) Part 70. The facility is designed to applicable U.S. codes and standards and operated by DCS, a private consortium under contract to DOE. The goal of the contract is to design, construct, and operate a facility to fabricate MOX fuel based on existing technology from the COGEMA MELOX and La Hague plants in France. To maximize the benefit of the existing technology, process and equipment designs from the MELOX and La Hague plants are duplicated, to the maximum extent possible, in the design of the new plant.

The feed material is depleted uranium dioxide and surplus plutonium dioxide supplied by DOE. The impurities in the plutonium dioxide feed are extracted by the Aqueous Polishing process. The MOX fuel fabrication process blends this “polished” plutonium dioxide with depleted uranium dioxide to form mixed oxide pellets. These pellets are loaded into the fuel rods, which are integrated into fuel assemblies. The nuclear fuel assemblies are transported for use in specific U.S. commercial reactors as nuclear fuel. The MFFF is designed to process 3.5 metric tons annually, for a total disposition of 33 metric tons of plutonium (as dioxide).

1.4.2 Regulatory Requirements, Guidance, and Industrial Standards

Title 10 CFR §70.61(d) requires that “under normal and credible abnormal conditions, all nuclear processes are subcritical, including use of an approved safety margin of subcriticality for safety”. In order to comply with this requirement, NUREG 1718 [3] and ANSI/ANS-8.1-1998 [2] require a validation report that (1) demonstrates the adequacy of the margin of subcriticality for safety by assuring that the margin is large compared to the uncertainty in the calculated value of k_{eff} and (2) determines the AOA and use of the code within the AOA, including justification for extending the AOA by using trends in the bias.

NUREG 1718 [3] further states that the validation report should contain:

A description of the AOA that identifies the range of values for which valid results have been obtained for the parameters used in the methodology. As defined in ANSI/ANS 8.1–1983, the AOA is the range of material compositions and geometric arrangements within which the bias of a calculational method is established. Other variables that may affect the neutronic behavior of the calculational method should also be specified in the definition of the AOA. Particular attention should be given to validating the code for calculations involving mixed oxides of differing isotopics and defining the isotopic ranges covered by the available benchmark experiments. In accordance with the provisions in ANSI/ANS 8.1–1983 (applicable section is Section 4.3.2), any extrapolation of the AOA beyond the physical range of the data should be supported by an established mathematical methodology.

2. Calculational Method

The SCALE 4.4a code package [1] is the computational system used for MFFF criticality analyses. The code package is available from the Radiation Safety Information Computational Center (RSICC). The SCALE 4.4a code package is installed and verified on the SGN PC hardware platform under the operating system “Windows NT 4.0”, as documented in [4].

A recent KENO-VI update published in SCALE Newsletter number 24 (July 2001), available at the SCALE web site, has not been applied to the version of SCALE 4.4a used for calculations. Comparison between patched and unpatched SCALE 4.4a versions do not present significant differences [17].

SCALE 4.4a is a collection of modules designed to perform criticality, shielding, and thermal calculations. The CSAS26 sequence is validated in this report. Functional modules may be run individually or sequentially in a module designated as a criticality safety control sequence (CSAS). A control sequence is also referred to as a control module. The CSAS26 (KENO VI) sequence is used for MFFF criticality analyses using the 238 group cross-section library 238GROUPNDF5 based on the ENDF/B-V data file. The CSAS sequences process the cross sections via the BONAMI and NITAWL-II modules within SCALE. The calculation of k_{eff} is performed with the Monte Carlo code KENO VI.

3. Criticality Code Validation Methodology

In order to establish that a system or process will be subcritical under all normal and credible abnormal conditions, it is necessary to establish acceptable subcritical limits for the operation and then show that the proposed operation will not exceed those values.

Figure 3–1 shows how the validation process fits within the overall MFFF nuclear criticality analysis process. The first step involves the procurement, installation, and verification of the criticality software on a specific computer platform. For the MFFF, the SCALE 4.4a code package has been procured, installed, and verified on the PC [4] hardware platform. This step is followed by the validation of the criticality software, which is the purpose of this report. The final step involves the criticality safety design analysis calculations, which are performed and presented in separate reports.

The criticality code validation methodology can be divided into four steps:

- Identify general MFFF design applications,
- Select applicable benchmark experiments and group them into AOAs,
- Model and calculate k_{eff} values of selected critical benchmark experiments,
- Perform statistical analysis of results to determine computational bias and upper safety limit (USL).

The first step is to identify the MFFF design applications and key parameters associated with the normal and upset design conditions. Table 3–1 lists the key parameters for the MFFF.

The second step involves several substeps. First, based on the key parameters, the AOA and expected range of each key parameter are identified. ANSI/ANS-8.1 [2] defines the AOA as “the limiting range of material composition, geometric arrangements, neutron energy spectra, and other relevant parameters (such as heterogeneity, leakage interaction, absorption, etc.) within which the bias of a computational method is established.” AOAs covering Pu and MOX applications are as follows: (1) Pu-nitrate solutions; (2) MOX pellets, fuel rods, and fuel assemblies; (3) PuO₂ powders; (4) MOX powders; and (5) PuO₂-polystyrene mixture and Pu-nitrate solutions. These AOAs are defined and presented in Section 4. After identifying the AOAs, a set of critical benchmark experiments is selected. Benchmark experiments for the fifth AOA are selected from the references listed in the International Handbook of Evaluated Criticality Safety Benchmark Experiments [5]. A description of all relevant experiments used for each AOA considered here is provided in Section 5.

The third step involves modeling the critical experiments and calculating the k_{eff} values of the selected critical benchmark experiments¹. Attachment 4 presents calculated results.

The final step involves the statistical analysis of the results in order to calculate the computational bias and USL. Section 6 presents the computational bias and USL results.

¹ Note that these models contain simplifications of critical experiments geometry. These simplifications lead to additional uncertainties which are included in the statistical analysis of the results.

3.1 Determination of Bias

ANSI/ANS-8.1-1998 [2] requires a determination of the calculational bias by “*correlating the results of critical and exponential experiments with results obtained for these same systems by the calculational method being validated.*” The correlation must be sufficient to determine if major changes in the bias can occur over the range of variables in the operation being analyzed. The standard permits the use of trends in the bias to justify extension of the area of applicability of the method outside the range of experimental conditions.

Calculational bias is the systematic difference between experimental data and calculated results. The simplest technique is to find the difference between the average value of the calculated results of critical benchmark experiments and 1.0. This technique gives a constant bias over a defined range of applicability.

Another technique is to find the difference between a regression fit of the calculated results of critical benchmark experiments and 1.0, as a function of an independent variable (e.g., enrichment, moderator-to-fuel ratio, etc.). As a rule, the bias is not a constant, but is dependent upon an independent variable, usually the degree of moderation of the neutrons. For example, the bias for an unmoderated system in which fission occurs with fast neutrons would not be expected to be the same as for a moderated system in which fission occurs with thermal neutrons. The AOA for the bias is the limiting range of material composition, geometric arrangement, etc., over which the bias is collectively established.

The recommended approach for establishing subcriticality based on numerical calculations of the neutron multiplication factor is prescribed in Section 5.1 of ANSI/ANS-8.17 [8]. The criteria to establish subcriticality requires that for a design application (system) to be considered as subcritical, the calculated multiplication factor for the system, k_s , must be less than or equal to an established maximum allowed multiplication factor based on benchmark calculations and uncertainty terms that is:

$$k_s \leq k_c - \Delta k_s - \Delta k_c - \Delta k_m \quad (\text{Eq. 3.1})$$

where:

- k_s = the calculated allowable maximum multiplication factor, (k_{eff}) of the design application (system)
- k_c = the mean k_{eff} value resulting from the calculation of benchmark critical experiments using a specific calculation method and data
- Δk_s = the uncertainty in the value of k_s
- Δk_c = the uncertainty in the value of k_c
- Δk_m = the administrative margin to ensure subcriticality.

Sources of uncertainty that determine Δk_s include:

- Statistical and/or convergence uncertainties
- Material and fabrication tolerances
- Limitations in the geometric and/or material representations used.

Sources of uncertainty that determine Δk_c include:

- Uncertainties in critical experiments
- Statistical and/or convergence uncertainties in the computation
- Extrapolation outside of the range of experimental data
- Limitations in the geometric and/or material representations used.

An assurance of subcriticality requires the determination of an acceptable margin based on known biases and uncertainties. The USL is defined as the upper bound for an acceptable calculation.

Critical benchmark experiments used to determine calculational bias (β) should be similar in composition, configuration, and nuclear characteristics to the system under examination. The range of applicability may be extended beyond the range of conditions represented by the benchmark experiments by extrapolating the trends established for the bias. β is related to k_c as follows:

$$\beta = k_c - 1 \quad (\text{Eq. 3.2})$$

$$\Delta\beta = \Delta k_c \quad (\text{Eq. 3.3})$$

Using this definition of bias, the condition for subcriticality in Eq. 3.1 is rewritten as:

$$k_s + \Delta k_s \leq 1 - \Delta k_m + \beta - \Delta\beta \quad (\text{Eq. 3.4})$$

A system is acceptably subcritical if a calculated k_{eff} plus calculational uncertainties lies at or below the USL.

$$k_s + \Delta k_s \leq \text{USL} \quad (\text{Eq. 3.5})$$

The USL can be written as:

$$\text{USL} = 1 - \Delta k_m + \beta - \Delta\beta \quad (\text{Eq. 3.6})$$

Bias is negative if $k_c < 1$ and positive if $k_c > 1$. For conservatism, a positive bias is set equal to zero for the purpose of defining the USL. $\Delta\beta$ is typically determined at the 95% confidence level.

The USL takes into account bias, uncertainties, and administrative and/or statistical margins such that the calculated configuration will be subcritical with a high degree of confidence.

β is related to system parameters and may not be constant over the range of a parameter of interest. If k_{eff} values for benchmark experiments vary as a function of a system parameter, such as enrichment or degree of moderation, then β can be determined from a best fit as a function of the parameter upon which it is dependent. Extrapolation outside the range of validation must take into account trends in the bias.

Both $\Delta\beta$ and β can vary with a given parameter, and the USL is typically expressed as a function of the parameter. Normally, the most important system parameter that affects bias is the degree of moderation of the neutrons. This parameter can be expressed in several different ways, such as

the energy of average lethargy causing fission (EALF), moderator-to-fuel volume ratio (v^m/v^f), or moderator-to-fuel atomic ratio (H/Pu ratio).

In general, the “bias” can be broken down into components caused by system modeling error, code modeling inaccuracies, cross-sectional inaccuracies, etc. Biases associated with individual inaccuracies are usually combined into a total bias to represent the combined effect from all sources that prevent code and cross-sections from calculating the experimental value of k_{eff} (see Section 3.4).

One or two calculations are insufficient to determine calculation bias. In practice, it is necessary to determine the “average bias” for a group of experiments. A statistical analysis of the variation of biases around this average value is used to establish an uncertainty associated with the bias value when it is applied to a future calculation of a similar critical system. The lower limit of this band of uncertainty establishes an upper bound for which a future calculation of k_{eff} for a similar critical system can be considered subcritical with a high degree of confidence.

NUREG/CR-6361 [9] describes two statistical methods for the determination of an USL from the bias and uncertainty terms associated with the calculation of criticality. The first method applies a statistical calculation of the bias and its uncertainty, plus an administrative margin, to a linear fit of critical experimental benchmark data. The second method applies a statistical calculation to determine a combined lower confidence band and subcritical margin. Both methods assume that the distribution of data points is normal. The following discussion of each method is taken from NUREG/CR-6361 [9] and is based on equations and techniques described in Dryer, Jordan, and Cain [10], Easter [11], Bowden and Graybill [12], Johnson [13], and Cain [14].

3.2 USL Method 1: Confidence Band with Administrative Margin

This method applies a statistical calculation of the bias (β) and its uncertainty ($\Delta\beta$) plus an administrative safety margin (Δk_m) to a linear fit of calculated results for a selected set of critical experiments. A confidence band (W) is determined statistically based on the existing data and a specified level of confidence; the greater the standard deviation in the data or the larger the confidence desired, the larger the band width will be. This confidence band, W , accounts for uncertainties in the experiments, the calculational approach, and calculational data (e.g., cross sections) and is therefore a statistical basis for $\Delta\beta$, the uncertainty in the value of β . W is defined for a confidence level of $(1-\gamma_1)$ using the relationship:

$$W = \max \{w(x) \mid x_{\min}, x_{\max}\} \quad (\text{Eq. 3.7})$$

where

$$w(x) = t_{1-\gamma_1} s_p \left[1 + \frac{1}{n} + \frac{(x - \bar{x})^2}{\sum_{i=1,n} (x_i - \bar{x})^2} \right]^{\frac{1}{2}} \quad (\text{Eq. 3.8})$$

and

- n = the number of critical calculations used in establishing $k_c(x)$
- $t_{1-\gamma_1}$ = the Student - t distribution for $1 - \gamma_1$ and $n - 2$ degrees of freedom
- \bar{x} = the mean value of parameter x in the set of calculations
- s_p = the pooled standard deviation for the set of criticality calculations.

The function $w(x)$ is a curvilinear function. For simplicity, it is desirable to obtain a constant width margin. Therefore, for conservatism, the confidence band, W , is defined as the maximum of $(w(x_{min}), w(x_{max}))$, where x_{min} and x_{max} are the minimum and maximum values of the independent parameter x , respectively. Typically, W is determined at a 95% confidence level.

The pooled standard deviation is obtained from the pooled variance $S_p = \sqrt{S_p^2}$, where S_p is given as:

$$S_p^2 = S_{k(x)}^2 + S_w^2 \quad (\text{Eq. 3.9})$$

Where $S_{k(x)}^2$ is the variance (or mean square error) of the regression fit, and is given by:

$$S_{k(x)}^2 = \frac{1}{(n-2)} \left[\sum_{i=1,n} (k_i - \bar{k})^2 - \frac{\left\{ \sum_{i=1,n} (x_i - \bar{x})(k_i - \bar{k}) \right\}^2}{\sum_{i=1,n} (x_i - \bar{x})^2} \right] \quad (\text{Eq. 3.10})$$

and S_w^2 is the within-variance of the data:

$$S_w^2 = \frac{1}{n} \sum_{i=1,n} \sigma_i^2 \quad (\text{Eq. 3.11})$$

where σ_i is the standard deviation associated with k_i for a Monte Carlo calculation. It is recommended that the individual standard deviations for Monte Carlo calculations be roughly uniform in value for the best results. For deterministic codes that do not have a standard deviation associated with a computed value of k , the standard deviation is zero. However, this term can also be used as a mechanism to include known uncertainties in experimental data.

In USL Method 1, Δk_m is given an arbitrary administrative value. NUREG-1718 [3] states that a “minimum subcritical margin (Δk_m) of 0.05 is generally considered acceptable without additional justification when both the bias and its uncertainty are determined to be negligible.” The MFFF criticality analyses use a value of 0.05. Section 6 provides further justification of the 0.05 administrative margin.

Having determined the constant W and substituting for $\Delta\beta$ in equation 3.6, the expression for the USL may be written as:

$$USL_1(x) = 1.0 - \Delta k_m - W + \beta(x). \quad (\text{Eq. 3.12})$$

3.3 USL Method 2: Single-Sided Uniform Width Closed Interval Approach

In USL Method 2, sometimes referred to as a lower tolerance band (LTB) approach, statistical techniques are applied to determine a combined lower confidence band plus subcritical margin. In USL Method 1, Δk_m and $\Delta\beta$ are determined independently, and in USL Method 2 (LTB method), a combined statistical lower bound is determined.

The purpose of this method is to determine a uniform tolerance band over a specified closed interval for a linear least-squares model. The level of confidence in the limit being calculated is α and is typically in the range of 0.90 to 0.999.

The USL Method 2 is defined as:

$$USL_2(x) = 1.0 - (C_{\alpha/P} \cdot s_p) + \beta(x) \quad (\text{Eq. 3.13})$$

where s_p is the pooled variance of k_c described earlier. The term $C_{\alpha/P} \cdot s_p$ provides a band for which there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band. For example, a $C_{95/995}$ multiplier produces a USL for which there is a 95% confidence that 995 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the USL.

The analysis is over the closed interval from $x = a$ to $x = b$. $C_{\alpha/P}$ is calculated according to the following equations:

$$g = \sqrt{\frac{1}{n} + \frac{(a - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (\text{Eq. 3.14})$$

$$h = \sqrt{\frac{1}{n} + \frac{(b - \bar{x})^2}{\sum_{i=1}^n (x_i - \bar{x})^2}} \quad (\text{Eq. 3.15})$$

$$\rho = \frac{1}{gh} \cdot \left\{ \frac{1}{n} + \frac{(a - \bar{x})(b - \bar{x})}{\sum_{i=1}^n (x_i - \bar{x})^2} \right\} \quad (\text{Eq. 3.16})$$

$$A = \frac{g}{h} \quad (\text{Eq. 3.17})$$

A , ρ , and $(n-2)$ are used to determine the value of D from Table 3 in Bowden [12], which covers values of $0.5 \leq A \leq 1.5$. The procedure to follow when A is in this range is:

$$C^* = D \cdot g. \quad (\text{Eq. 3.18})$$

When A is outside the above range, A is replaced by $1/A$ for the determination of D , and C^* is given by:

$$C^* = D \cdot h. \quad (\text{Eq. 3.19})$$

Next,

$$C_{\alpha/P} = C^* + z_p \cdot \sqrt{\frac{n-2}{\chi^2}}, \quad (\text{Eq. 3.20})$$

where

$$\begin{aligned} z_p &= \text{the Student t statistic depending on } n \text{ and } P \\ \chi^2 &= \text{the chi square distribution, a function of } n-2 \text{ and } \alpha. \end{aligned}$$

This approach provides a statistically based subcritical margin, Δk_m which can be determined as the difference $(C_{\alpha/P} s_p) - W$. In criticality safety applications, such a statistically determined approach generally, but not necessarily, yields a margin of less than 0.05, which serves to illustrate the adequacy of the administrative margin specified in USL Method 1. The recommended purpose of USL Method 2 is to apply it in tandem with USL Method 1 to verify that the administrative margin is conservative relative to a purely statistical basis.

3.4 Uncertainties

Uncertainties, as used in this report, refer to the uncertainty in k_{eff} associated with experimental unknowns or assumptions and to the uncertainty values associated with Monte Carlo analyses.

Experimental uncertainty (σ_e) – Modeling of validation experiments frequently result in assumptions about experimental conditions. In addition, experimental uncertainties (such as measurement tolerances) influence the development of a computer model. Recent efforts by the OECD – NEA [5] have resulted in the quantification of these uncertainties in validation experiments.

Statistical uncertainty (σ_s) – Monte Carlo calculation techniques result in a statistical uncertainty associated with the actual calculation. This type of uncertainty is dependent of upon many factors, including number of neutron generations performed, variance reduction techniques employed, and problem geometry. For this document, σ_s refers to the statistical Monte Carlo uncertainty associated with the computer modeled validation experiment.

Total uncertainty – This is the total uncertainty associated with a calculated k_{eff} on a benchmark experiment. The total uncertainty for an individual benchmark is the combined error of the experimental and statistical uncertainties:

$$\sigma_i = \sqrt{\sigma_{e,i}^2 + \sigma_{s,i}^2} \quad (\text{Eq. 3.21})$$

where the subscript (i) refers to an individual benchmark calculation.

3.5 Normalizing k_{eff}

In many instances, benchmark experiments used for validation may not be exactly critical. Experimental results may show that the experiment is slightly above or below a $k_{\text{eff}} = 1.0$. For these cases, the calculated k_{eff} values should be normalized to the experimental value. This assumes that any 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 applies:

$$k_{\text{eff}} (\text{normalized}) = k_{\text{eff}} (\text{calculated}) / k_{\text{eff}} (\text{experimental}) \quad (\text{Eq. 3.22})$$

The normalized k_{eff} values are to be used in the determination of the USL. Since only small adjustments to the calculated k_{eff} value are made as a result of normalization, no adjustment to the total uncertainty, σ_i , is made.

3.6 Application of the USL

The equations for USL Methods 1 and 2 (equations 3.12 and 3.13) represent an upper bound to assure subcriticality for a given configuration when the calculated k_{eff} plus uncertainty for the configuration is less than the USL. USLs may be calculated for a number of independent parameters for a given system. Here, the subcritical limit is taken as the minimum of all USLs computed for the specific parameters of the system. This approach is conservative with respect to the guidance provided in NUREG/CR-6361 [9] in which the USL is determined based on the statistical results for the parameter “*with the strongest correlation to the calculated k_{eff} values.*”

Another advantage of the USL is that it may also be used to establish guidelines for quantitatively determining the applicability of the bias (or validation) to specific applications. For a given parameter, the USL is valid over the range of that parameter in the set of calculations used to determine the USL. However, ANSI/ANS-8.1 [2] allows the range of applicability to be extended beyond this range by extrapolating the trends established for the bias. No precise guidelines are specified for the limits of extrapolation. Thus, engineering judgment should be applied when extrapolating beyond the range of the parameter bounds.

Appendix C in NUREG/CR-6361 [9] documents the USLSTATS computer program that was developed to perform the required statistical analysis and calculate USLs based on USL Methods 1 and 2.

In this validation report, USLSTATS is used to trend the following parameters:

- Moderator to fuel atomic ratio (H/Pu)
- Energy of Average Lethargy Causing Fission (EALF)

The H/Pu ratio is a parameter that describes the moderation of the neutrons in the fissile medium. The EALF parameter is a measure of the energy dependent fission efficiency of the fissile medium.

The administrative margin, Δk_m , is fixed in order to have a sufficient confidence that the calculated results are subcritical.

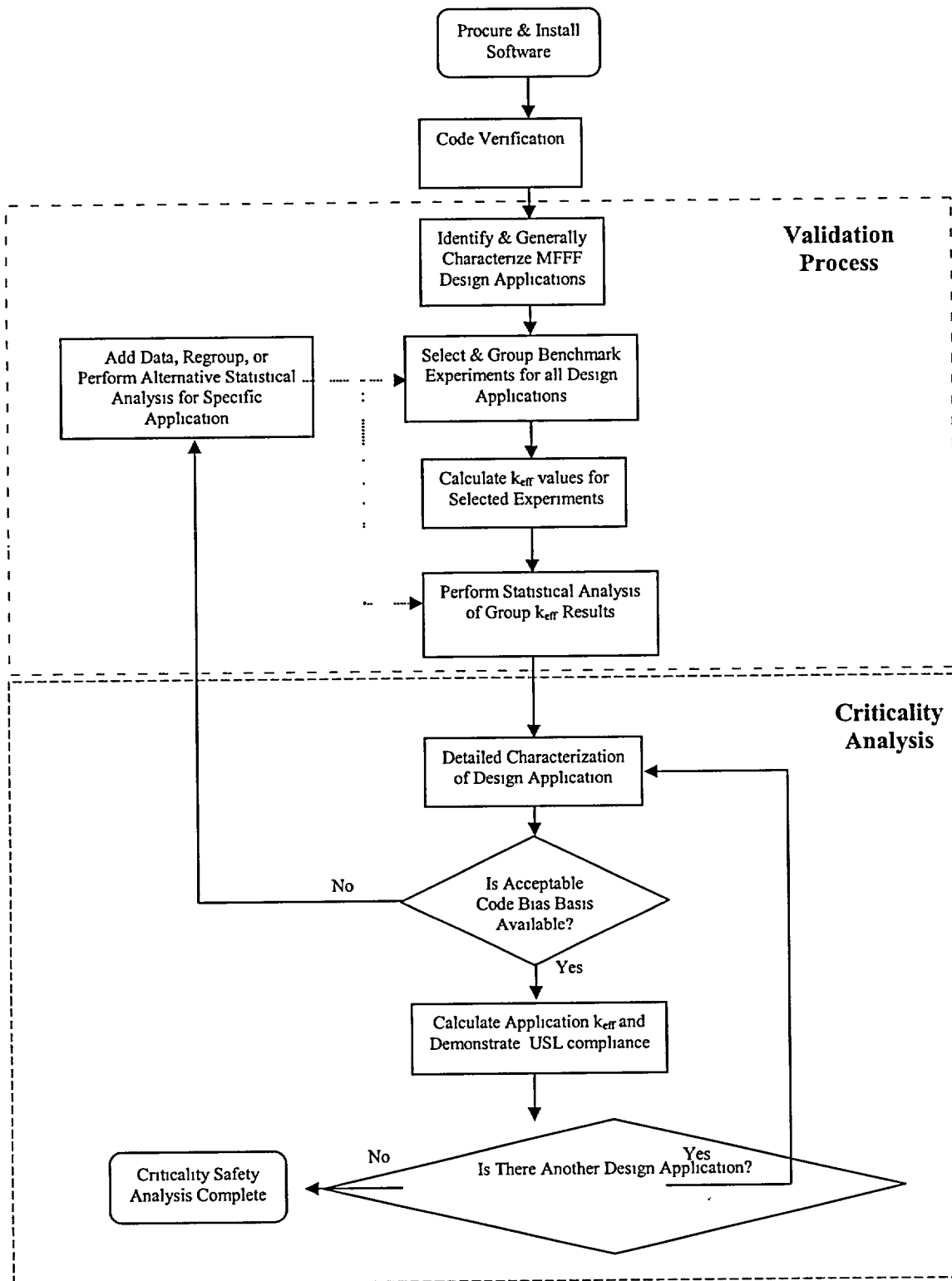


Figure 3–1 Overview of the Criticality Analysis Process of the MFFF

Table 3–1 Characteristics of the MFFF Design Application Areas*

Parameter	Pu-nitrate solution	MOX pellets, fuel rods, FAs	PuO ₂ powder/water mixtures	MOX powder/water mixtures	Aqueous solutions of Pu compounds
Fissile Material Physical/Chemical Form	Pu-nitrate	MOX green and sintered pellets, MOX rods and FAs	PuO ₂ powder	MOX powder	(a) Pu-oxalate (b) PuO ₂ F ₂ “standard salt”
Isotopic composition of fissile material **	96% ²³⁹ Pu 4% ²⁴⁰ Pu	96% ²³⁹ Pu 4% ²⁴⁰ Pu depleted U	96% ²³⁹ Pu 4% ²⁴⁰ Pu	96% ²³⁹ Pu 4% ²⁴⁰ Pu depleted U	96% ²³⁹ Pu 4% ²⁴⁰ Pu
PuO ₂ /(UO ₂ +PuO ₂)	100 %	≤ 6.3 %	100 %	6.3% – 22%	100 %
Maximum oxide density [g/cm ³]	–	7.0, 11.0	3.5, 7.0, 11.46	4.1, 5.5	–
Pu concentration [g/liter]	125 – 237	–	–	–	(a) 242 (b) 767
Type of moderation	Homogeneous	Heterogeneous	Homogeneous	Homogeneous	Homogeneous
Optimum moderation ***	H/Pu=100–200	v ^m /v ^f = 1.9 – 9	H/Pu= 0.3 – 6	H/Pu=1.6 – 291	(a) H/Pu=100 (b) H/Pu=30
Low density moderation [wt.% H ₂ O]	–	≤ 5 ****	≤ 5	≤ 5	–
Anticipated absorber/reflector materials	Water Cd/water Concrete Borated concrete	Water Concrete Borated concrete	Water Borated concrete	Water	Water Cd/water Concrete
Typical geometry	Annular cylinders Cylinders Slabs	Cylinders Arrays Cuboids	Various configurations	Various configurations	Annular cylinders Cylinders Slabs

* Characteristics presented typically refer to optimal or bounding values or ranges associated with respective MFFF design applications

** Bounding design isotopic composition from Aqueous Polishing System basis of design

*** Per calculation

**** Green Pellets (i.e., unsintered pellets) < 5; sintered pellets < 1

4. MFFF Design Application Classification

This section describes the characteristics of the established AOAs based on the various fuel configurations encountered in the MFFF. AOAs covering Pu and MOX applications are as follows (see Table 3–1):

- Pu-nitrate aqueous solution,
- MOX pellets, fuel rods, and fuel assemblies (FA),
- PuO₂ powders,
- MOX powders,
- Aqueous solutions of Pu compounds, precipitated Pu-oxalates.

The following sections address the fifth AOA based on the various fuel configurations encountered in the Aqueous Polishing process (Pu-oxalate solutions and precipitated Pu-oxalates).

It will be demonstrated that for H/Pu ratios greater than 50, AOA(5) is bounded by AOA(1). For the low moderated range, $H/Pu < 50$, the benchmarks used for AOA(3) [15] will also be used for AOA(5) because the PuO₂+polystyrene experiments have Pu concentrations and H/Pu ratios that are typical of wet powders (addressed in AOA(3)), precipitates and powder slurries [6], [7].

4.1 MFFF Design Application (5) – Aqueous Solutions of Pu Compounds

Table 4–1 and Table 4–2 summarize the anticipated criticality calculations to be performed for the design of the MFFF in which aqueous Pu compounds will be processed or stored. The tables provide the relevant parameters (i.e., chemical form, isotopic vector, moderator to fuel atomic ratio [H/Pu], and energy of average lethargy causing fission [EALF]) for each criticality design application under nominal Aqueous Polishing process conditions (Table 4–1) and abnormal process conditions (Table 4–2).

The normal process conditions are characterized by Pu concentrations in the process solution of less than 500 g/liter. On the other hand, the abnormal conditions are characterized by higher Pu concentrations limited by the theoretical density of the Pu compound in the process solution (values as high as 7000 g/liter or higher).

Typically, design parameters for Aqueous Polishing process equipment are based on geometry control mode. This means that the design dimensions are safe for any credible Pu concentration and for any credible degree of moderation (H/Pu ratio). Under normal process conditions (aqueous solution of Pu compounds with low Pu concentrations) the fissile medium is typically overmoderated and a thermal neutron spectrum will be found.

Nevertheless for criticality control the fissile solution is analyzed at the point of optimum moderation to determine a maximum k_{eff} . In this case, the thermal spectrum shifts towards higher energies and epithermal spectra can occur.

The H/Pu range in which the maximum k_{eff} occurs depends on the composition of the Pu compound [19]. For PuO₂+H₂O mixtures the maximum k_{eff} will occur at the maximum Pu

concentration (corresponding to the maximum abnormal PuO_2 density in the aqueous polishing process). For high PuO_2 densities between 7.0 g/cm^3 and the theoretical maximum density of 11.46 g/cm^3 intermediate to fast neutron spectra can occur at the maximum k_{eff} .

In some other abnormal situations, Pu precipitates and slurry powders with high compound densities can occur (see Table 4-11 in Section 4.4). In these cases geometry control is used and the calculations are performed either at the optimum moderation or at the maximum Pu concentration ($H/\text{Pu} = 0$) if there exists a maximum k_{eff} .

The following primary Aqueous Process situations are considered in AOA(5):

- Oxalic mother liquor solution and aqueous solutions of Pu compounds in nominal process concentrations,
- Precipitated Pu^{IV} -oxalates: $\text{Pu}(\text{C}_2\text{O}_4)_2 \cdot 6\text{H}_2\text{O}$, $\text{Pu}(\text{C}_2\text{O}_4)_2 \cdot 2\text{H}_2\text{O}$, $\text{Pu}(\text{C}_2\text{O}_4)_2$.

Homogeneous $\text{PuO}_2 + \text{H}_2\text{O}$ systems and PuO_2 slurry powders that can occur in the Aqueous Polishing process are addressed in AOA(3) [15]. Nevertheless $\text{PuO}_2 + \text{H}_2\text{O}$ systems are also discussed in the following sections for a better understanding of the differences between the $\text{PuO}_2 + \text{H}_2\text{O}$ systems and the Pu compound solutions in the low moderated range.

In the Basis of Design of the MFFF Aqueous Polishing process [18] a bounding fissile media, PuO_2F_2 “standard salt,” is defined to describe all the possible Pu compounds, other than PuO_2 (for instance Pu-oxalate and various other Pu precipitates) in a conservative manner. In these cases it will be shown on a case by case basis whether the maximum k_{eff} occurs at the optimum of moderation or at the maximum possible Pu concentration in the dry compound.

Section 4.2 shows that the selected experiments are sufficient to describe the physical properties of the PuO_2F_2 “standard salt” solution as well as the Pu-oxalate solution. Section 4.3 shows that the EALF values found for the optimum moderation of each solution are in or near the range of the EALF values for the experimental configuration. Section 4.4 shows that the PuO_2F_2 “standard salt” is bounding for the Pu-oxalate solution and Pu-oxalate precipitates over the full range of applicability.

Table 4–1 Anticipated Criticality Calculation Derived Characteristics for Design Applications Involving Aqueous Solutions of Pu Compounds in Nominal Process Conditions

Fuel configuration	Reflector conditions	Chemical form	C(Pu) [g/liter]	H/Pu	EALF [eV]
AP: KCA Oxalic Precipitation Conversion					
Flat Filter FLT 7000	Water/borated concrete	Pu-oxalate solution	1234 ¹⁾	12 ⁴⁾	-
Tanks TK 1000/2000	Water/colemanite concrete	Pu-nitrate solution	40	613	-
Precipitators PREC 5000/6000	Water	Pu-nitrate solution	25.1 - 30.2 ²⁾	871	-
		Pu-oxalate precipitate	1234 ¹⁾	12 ⁴⁾	-
Furnace FUR 8000	Water/concrete	PuO ₂ +H ₂ O ³⁾	2210 - 3087 ³⁾	5.973	66.9
AP: KCD Oxalic Mother Liquor Recovery					
Evaporator EV 3000	Water	Pu-oxalate + H ₂ O	10.1 - 20 ²⁾	2800	-
Evaporator EV 5000	Water	Pu-oxalate + H ₂ O	-	-	-
Tanks TK 1000/1500/2000	Water/colemanite concrete	Pu-oxalate + H ₂ O	0.179 - 0.3 ²⁾	83000	-
Tank TK 6000	Water	PuO ₂ (NO ₃) ₂ +Pu(NO ₃) ₄ solution	1.6E-3	1.7E7	-
Tanks TK 4100/4200/4000	Water/Cadmium	PuO ₂ (NO ₃) ₂ +Pu(NO ₃) ₄ solution	10.1 - 20 ²⁾	2800	-

¹⁾ Maximum Pu concentration in Pu-oxalate Pu(C₂O₄)₂•6H₂O [21], [22]

²⁾ Maximum nominal value

³⁾ Used as bounding medium for Pu-oxalate in the furnace

⁴⁾ Minimum H/Pu value

Table 4–2 Anticipated Criticality Calculation Derived Characteristics for Design Applications Involving Aqueous Solution of Pu Compounds in Abnormal Process Conditions

Fuel configuration	Reflector conditions	Chemical form	C(Pu) [g/liter]	H/Pu	EALF [eV]
AP: KCA Oxalic Precipitation Conversion					
Flat Filter FLT 7000	Water/borated concrete	PuO ₂ F ₂ “standard salt” solution	767 ¹⁾	30	0.70
		Pu-oxalate	446	50	0.33
Tanks TK1000/2000	Water/colemanite concrete	Pu-nitrate solution	180	135	0.25
Precipitators PREC 5000/6000	Water	PuO ₂ F ₂ “standard salt” solution	767 ¹⁾	30	3
		Pu-oxalate	166	150	0.20
Furnace FUR 8000	Water/ concrete	PuO ₂ +H ₂ O	3087 ³⁾	5.973	67
AP: KCD Oxalic Mother Liquor Recovery					
Evaporator EV 3000	Water	PuO ₂ F ₂ “standard salt” solution	767 ²⁾	30	1.39
		Pu-oxalate	178	140	0.16
Evaporator EV 5000	Water	PuO ₂ F ₂ “standard salt” solution	767 ²⁾	30	1.42
		Pu-oxalate	10.1	5700	-
Tanks TK 1000/1500/2000	Water/colemanite concrete	PuO ₂ F ₂ “standard salt” solution	767 ¹⁾	30	3.08
		Pu-oxalate	-	-	-
Tank TK 6000	Water	PuO ₂ F ₂ “standard salt” solution	767 ¹⁾	30	0.78
Tanks TK 4000/4100/4200	Water/Cadmium	PuO ₂ F ₂ “standard salt” solution	767 ¹⁾	30	4.69

¹⁾ PuO₂F₂ “standard salt” is used as a bounding media for Pu-oxalate Pu(C₂O₄)₂·6H₂O.

²⁾ PuO₂F₂ “standard salt” is used as a bounding media for PuO₂(NO₃)₂, Pu(NO₃)₄ and Pu-oxalate Pu(C₂O₄)₂·6H₂O.

³⁾ Pu concentration in PuO₂ with maximum density 3.5 g/cm³ [18].

4.2 Comparison of Neutron Physical Parameters

An atomic comparison between the benchmark fissile medium PuO_2 +polystyrene and the reference fissile media used in the MFFF applications (PuO_2 + H_2O , Pu-oxalate+ H_2O and PuO_2F_2 + H_2O) is presented in Table 4-3 and Table 4-4.

Table 4-3 Atomic Comparison of the PuO_2 -Polystyrene Experiments and of Pu Compounds in the MFFF Applications

Benchmark Experiment	Reference Fissile Media Used in the MFFF Design Application			
PuO_2 in polystyrene $(\text{CH})_n$	PuO_2 in water PuO_2 + H_2O	Pu^{III} -nitrate $\text{Pu}(\text{NO}_3)_3 \cdot 5(\text{H}_2\text{O})$ + H_2O	Pu-oxalate $\text{Pu}(\text{C}_2\text{O}_4)_2 \cdot 6(\text{H}_2\text{O})$ + H_2O	“Standard salt” PuO_2F_2 + H_2O
$\rho_{(\text{comp})}^{1)}$	$\rho_{(\text{comp})} = 11.460^{2)}$ [g/cm ³]	$\rho_{(\text{comp})} = 2.150^{3)}$ [g/cm ³]	$\rho_{(\text{comp})} = 2.700^{4)}$ [g/cm ³]	$\rho_{(\text{comp})} = 4.187^{5)}$ [g/cm ³]
Pu	Pu	Pu	Pu	Pu
O	O	O	O	O
H	H	H	H	H
C	-	-	C	-
-	-	N	-	F

¹⁾ PuO_2 densities in the experiments of both benchmarks PU-COMP-MIXED-01 and PU-COMP-MIXED-02 (cf. Table 5-1) are between 0.425 g/cm³ and 6.581 g/cm³

²⁾ theoretical density [20].

³⁾ compound (crystal) density $\text{Pu}(\text{NO}_3)_3 \cdot 5\text{H}_2\text{O}$ [23].

⁴⁾ compound (crystal) density $\text{Pu}(\text{C}_2\text{O}_4)_2 \cdot 6\text{H}_2\text{O}$ [21], [22] (see Table 4-11). The dilution law used for this assumed homogeneous mixture is a simple AIVM as described in [23].

⁵⁾ The PuO_2F_2 “standard salt” law is used in criticality studies only as a bounding media (cf. Section 4.4) to cover all salt solutions [23]. Therefore, this law is not valid for genuine PuO_2F_2 media. The crystal density of 6.5 g/cm³ [20] is not relevant for the MFFF application because PuO_2F_2 never appears in the process.

Table 4-3 and Table 4-4 show that the most important atoms in the reference fissile media are covered by the experiments. In the well moderated (optimum of moderation) and overmoderated range, the influence of C, F and N on the neutron spectrum (EALF) is small. The increasing influence of C, F, N on the neutron spectrum in the low moderated range is discussed in the following sections.

As discussed in Section 4.1 the physical parameter (H/Pu) of the design application (5) varies from $\text{H/Pu} = 0$ to $\text{H/Pu} = 83000$. To cover the relevant range of H/Pu between 12 and 500 where the maximum of k_{eff} occurs, two groups of benchmark experiments are established:

Group 1: Benchmarks with PuO_2 powder-polystyrene compacts with $\text{H/Pu} < 50$.

Group 2: Benchmarks with Pu-nitrate solution with $\text{H/Pu} > 50$.

Table 4–4 Atomic Comparison of the Pu-nitrate Experiments and of Pu Compounds in the MFFF Applications

Benchmark Experiment	Reference fissile media used in the MFFF Design Application			
Pu-nitrate solution	PuO ₂ in water PuO ₂ +H ₂ O	Pu ^{III} -nitrate Pu(NO ₃) ₃ ·5(H ₂ O) +H ₂ O	Pu-oxalate Pu(C ₂ O ₄) ₂ ·6(H ₂ O) +H ₂ O	“Standard Salt” PuO ₂ F ₂ +H ₂ O
$\rho_{(comp)}^{1)}$	$\rho_{(comp)} = 11.460^{2)}$ [g/cm ³]	$\rho_{(comp)} = 2.150^{3)}$ [g/cm ³]	$\rho_{(comp)} = 2.700^{4)}$ [g/cm ³]	$\rho_{(comp)} = 4.187^{5)}$ [g/cm ³]
Pu	Pu	Pu	Pu	Pu
O	O	O	O	O
H	H	H	H	H
-	-	-	C	-
N	-	N	-	F

- ¹⁾ Pu concentrations in the Pu-nitrate experiments of benchmarks PU-SOL-THERM (cf. Table 5-1) are between 115 g/l and 268.7 g/l.
- ²⁾ theoretical density [20].
- ³⁾ compound (crystal) density Pu(NO₃)₃·5H₂O [23].
- ⁴⁾ compound (crystal) density Pu(C₂O₄)₂·6H₂O [21], [22] (see Table 4-11). The dilution law used for this assumed homogeneous mixture is a simple AIVM as described in [23].
- ⁵⁾ The PuO₂F₂ “standard salt” law is used in criticality studies only as a bounding media (cf. Section 4.4) to cover all salt solutions [23]. Therefore, this law is not valid for genuine PuO₂F₂ media. The crystal density of 6.5 g/cm³ [20] is not relevant for the MFFF application because PuO₂F₂ never appears in the process.

Table 4–5 through Table 4–8 show that the EALF values of the applications are within or near the range of the experimental EALF values. The following experiments are used for this comparison:

- Group 1: PU_COMP_MIXED_001, 002 (Polystyrene moderated PuO₂ powder).
- Group 2: PU_SOL_THERM_001, 008, 014, 015, 016, 017 (Pu-nitrate solutions).

Table 4–5 through Table 4–8 present a comparison of the EALF values of the PuO₂+Polystyrene experiments (Group 1) and the Pu-nitrate experiments (Group 2) in comparison with the EALF values found for water and Plexiglas reflected infinite slabs and infinite cylinders containing different fissile media. The EALF values for the two standard geometry are calculated for a critical full water reflected system as described in [19] and for a full Plexiglas reflected system. The primary result of this comparison is that the EALF values for the different reference fissile media of the MFFF design applications for H/Pu ratios equal or higher than 15 are within or near the experimental EALF range of Group 1. It is also apparent that the Pu nitrate experiments (Group 2) are suitable to describe the Pu compounds in aqueous solution with H/Pu > 50.

For H/Pu ratios lower than 15, larger differences between the different Pu compounds occur. The differences are larger for slab geometry than for cylindrical geometry. On the other hand it is obvious that the EALF value depends not only on the geometrical shape of the fissile media but also on the reflector material composition, because both effects (geometric shape and reflector

material) influence the neutron spectrum in the lateral zones of the fissile medium, particularly if the core dimensions are small compared to the mean free path of the fast neutrons. To study the different factors that affect the neutron energy spectrum in the fissile medium zone and therefore the key parameter EALF, a parametric study of EALF is presented in Section 4.3.

Table 4-5 Comparison of EALF Values Found for the Experiments and in the Design Applications (Infinite Critical Slab with 30 cm Plexiglas Reflector)

Parameter	Experiment ²⁾		PuO ₂ +H ₂ O	Pu-oxalate+H ₂ O	PuO ₂ F ₂ +H ₂ O
H/Pu	EALF [eV]	Geometry	EALF [eV]	EALF [eV]	EALF [eV]
(g1) 0.04	1850 to 4900	Parallelepiped	154	- ⁽¹⁾	140
(g1) 5	56.8 to 92.9	Parallelepiped	17.3	- ⁽¹⁾	16.3
(g1) 15	4.12 to 6.65	Parallelepiped	2.72	2.62	2.67
(g1) 50	0.70 to 0.74	Parallelepiped	0.41	0.41	0.41
(g2) 85.03	0.55	Sphere	0.22	0.22	0.22
(g2) 88.43	0.52	Sphere	0.21	0.21	0.21
(g2) 155.27	0.24	Cylinder	0.13	0.13	0.13
(g2) 210.18	0.17	Cylinder	0.10	0.10	0.10

(g1) Group 1: Critical experiments with PuO₂ powder in polystyrene (CH)_n [5], [6], [7].

(g2) Group 2: Critical experiments with Pu-nitrate solutions [5].

(1) H/Pu > 12 in Pu(C₂O₄)₂·6H₂O [21], [22].

(2) cf. Table 5-1.

Table 4-6 Comparison of EALF Values Found for the Experiments and in the Design Applications (Infinite Critical Slab with 30 cm Water Reflector)

Parameter	Experiment ²⁾		PuO ₂ +H ₂ O	Pu-oxalate+H ₂ O	PuO ₂ F ₂ +H ₂ O
H/Pu	EALF [eV]	Geometry	EALF [eV]	EALF [eV]	EALF [eV]
(g1) 0.04	1850 to 4900	Parallelepiped	323	- ⁽¹⁾	286
(g1) 5	56.8 to 92.9	Parallelepiped	26.9	- ⁽¹⁾	25.2
(g1) 15	4.12 to 6.65	Parallelepiped	3.56	3.41	3.48
(g1) 50	0.70 to 0.74	Parallelepiped	0.47	0.46	0.47
(g2) 85.03	0.55	Sphere	0.24	0.24	0.24
(g2) 88.43	0.52	Sphere	0.23	0.23	0.23
(g2) 155.27	0.24	Cylinder	0.13	0.13	0.13
(g2) 210.18	0.17	Cylinder	0.11	0.11	0.11

(g1) Group 1: Critical experiments with PuO₂ powder in polystyrene (CH)_n [5], [6], [7].

(g2) Group 2: Critical experiments with Pu-nitrate solutions [5].

(1) H/Pu > 12 Pu(C₂O₄)₂·6H₂O [21], [22].

(2) cf. Table 5-1.

Table 4–7 Comparison of EALF Values Found for the Experiments and in the Design Applications (Infinite Critical Cylinder with 30 cm Plexiglas Reflector)

Parameter	Experiment ²⁾		PuO ₂ +H ₂ O	Pu-oxalate+H ₂ O	PuO ₂ F ₂ +H ₂ O
H/Pu	EALF [eV]	Geometry	EALF [eV]	EALF [eV]	EALF [eV]
(g1) 0.04	1850 to 4900	Parallelepiped	6945	- ⁽¹⁾	1386
(g1) 5	56.8 to 92.9	Parallelepiped	95.1	- ⁽¹⁾	58.7
(g1) 15	4.12 to 6.65	Parallelepiped	6.69	-5.68	5.96
(g1) 50	0.70 to 0.74	Parallelepiped	0.62	0.61	0.62
(g2) 85.03	0.55	Sphere	0.30	0.29	0.30
(g2) 88.43	0.52	Sphere	0.28	0.28	0.28
(g2) 155.27	0.24	Cylinder	0.15	0.15	0.15
(g2) 210.18	0.17	Cylinder	0.12	0.12	0.12

(g1) Group 1: Critical experiments with PuO₂ powder in polystyrene (CH)_n [5], [6], [7].

(g2) Group 2: Critical experiments with Pu-nitrate solutions [5].

(1) H/Pu > 12 in Pu(C₂O₄)₂.6H₂O [21], [22].

(2) cf. Table 5-1.

Table 4–8 Comparison of EALF Values Found for the Experiments and in the Design Applications (Infinite Critical Cylinder with 30 cm Water Reflector)

Parameter	Experiment ²⁾		PuO ₂ +H ₂ O	Pu-oxalate+H ₂ O	PuO ₂ F ₂ +H ₂ O
H/Pu	EALF [eV]	Geometry	EALF [eV]	EALF [eV]	EALF [eV]
(g1) 0.04	1850 to 4900	Parallelepiped	9049	- ⁽¹⁾	1988
(g1) 5	56.8 to 92.9	Parallelepiped	113.0	- ⁽¹⁾	72.3
(g1) 15	4.12 to 6.65	Parallelepiped	7.46	6.40	6.71
(g1) 50	0.70 to 0.74	Parallelepiped	0.66	0.64	0.65
(g2) 85.03	0.55	Sphere	0.24	0.30	0.31
(g2) 88.43	0.52	Sphere	0.23	0.29	0.29
(g2) 155.27	0.24	Cylinder	0.13	0.16	0.16
(g2) 210.18	0.17	Cylinder	0.11	0.12	0.12

(g1) Group 1: Critical experiments with PuO₂ powder in polystyrene (CH)_n [5], [6], [7].

(g2) Group 2: Critical experiments with Pu-nitrate solutions [5].

(1) H/Pu > 12 in Pu-oxalate Pu(C₂O₄)₂.6H₂O [21], [22].

(2) cf. Table 5-1.

4.3 Sensitivity Studies on EALF for Different Pu Compounds

In MFFF design applications, the H/Pu ratio of the reference fissile media is defined on the basis of the Pu isotopes ^{239}Pu and ^{240}Pu since other Pu isotopes are assumed to be absent. In addition to the Pu isotopes, the presence of other atoms in the compound with significant macroscopic scattering and absorption cross sections can have an influence on the system reactivity.

As shown in the MFFF document “Minimum critical and maximum permissible parameters of Pu containing media” [19] a potential criticality risk ($k_{\text{inf}} > 1$) exists over a wide range of Pu concentrations from 10 g/liter up to the highest possible concentration defined by the crystal density of the dry Pu-compound. Figure 4–1 shows the basic physical parameter k_{inf} versus H/Pu in the range $0 < \text{H/Pu} < 1000$ for different Pu compounds in aqueous solution.

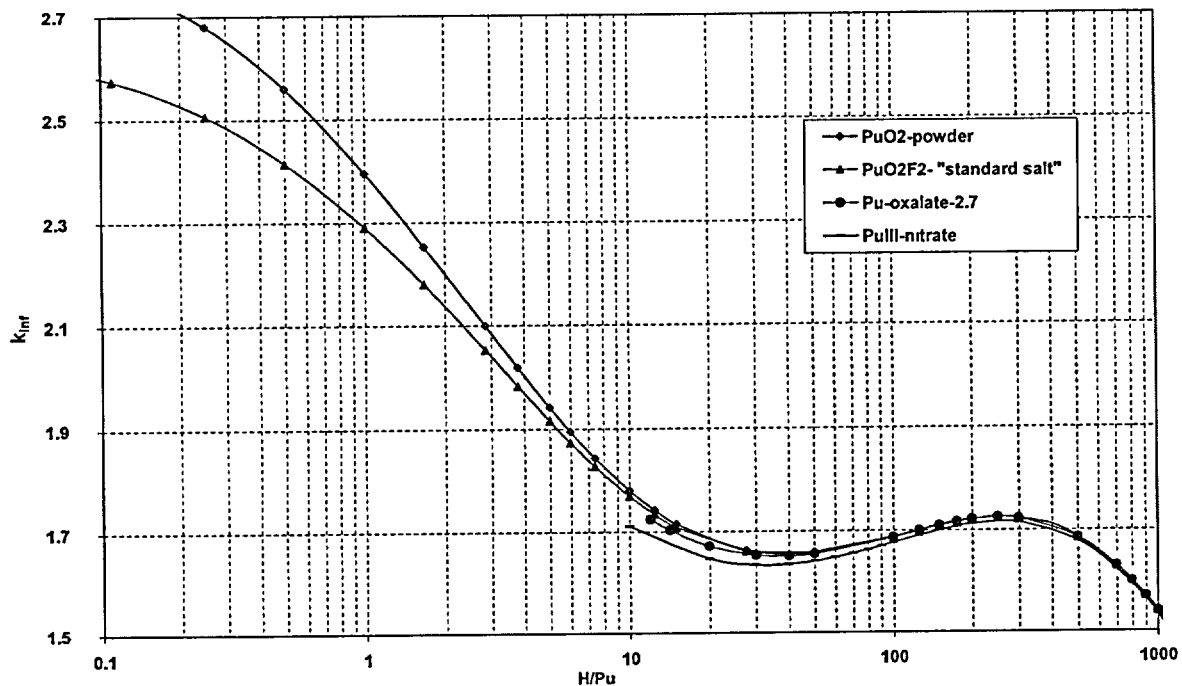


Figure 4–1 k_{inf} versus H/Pu for different Pu compounds in aqueous solution

It can be seen from the Figure 4–1 that for higher H/Pu ratios (lower Pu concentrations) the k_{inf} is determined only by the H/Pu ratio. The influence of other atoms in the compound on k_{inf} can be neglected. This means the k_{inf} in the range of higher H/Pu values is only influenced by hydrogen, oxygen (coming from H_2O) and the Pu isotopes.

If the Pu concentration in the aqueous solution increases (H/Pu decreases) the different numbers of oxygen, nitrogen and carbon atoms per Pu isotope in the Pu compound (molecule) changes the neutron flux spectrum and therefore affects the k_{inf} and the EALF value.

In the following, the influence of three factors on the EALF value will be determined as a function of the H/Pu ratio:

- Composition of the Pu compounds,
- Geometric shape of the fissile medium zone,
- Reflector material composition.

4.3.1 Plutonium Compound Composition

Figure 4–2 shows the EALF value versus the H/Pu ratio for different Pu compounds. The EALF values shown are calculated for full water reflected cylinders in admissible dimensions ($k_{\text{eff}} = 0.93$). It is apparent that the difference in the EALF values for the different compounds increases with lower H/Pu values.

The $\text{PuO}_2 + \text{H}_2\text{O}$ system leads for a given H/Pu to the highest EALF value. The more complex compounds lead to smaller values because of their lower Pu density. If the H/Pu is fixed the density of the fissile media (Pu concentration in case of solutions) as well as the geometrical shape and dimensions have an influence of EALF.

For higher H/Pu ratios the differences between the EALF values found for the different Pu-compounds decreases so that there is practically no significant difference between the different Pu compounds in water above $\text{H/Pu} = 50$. Figure 4–3 shows the relative difference DELTA-EALF between the EALF values versus the H/Pu ratio for different Pu compounds over the full range of moderation. The PuO_2 -polystyrene media (exp) is used as the basis media. Thus the difference in EALF expressed as:

$$\text{DELTA-EALF} = (\text{EALF}(\text{media } i) - \text{EALF}(\text{exp}))/\text{EALF}(\text{exp})$$

is a measure of how far the EALF value of a reference medium of the MFFF application is from the EALF value found for the experiment at the same H/Pu ratio.

Figure 4–4 shows the DELTA-EALF values versus the H/Pu in the low moderated range: $0 < \text{H/Pu} < 30$ in a linear scale.

Therefore, it can be concluded that all design applications with H/Pu values higher than 50 have similar EALF values as was also shown in Figure 4–2. Significant differences between EALF values appear only in the low moderated and unmoderated range with H/Pu values lower than 50. This is also significant by comparison of the neutron flux spectrum obtained for infinite full water reflected slabs filled with PuO_2 and Pu-oxalate, cf. Attachment 1, Figure A1-1 and Figure A1-2. It is obvious that differences in the dry neutron spectrum occur over the full energy range at $\text{H/Pu} = 0.04$. In the dry moderated range ($\text{H/Pu} = 0.04$), the PuO_2 -polystyrene experiments are in a good agreement with the PuO_2 -powder application, whereas significant differences occur when H/Pu ratio increases.

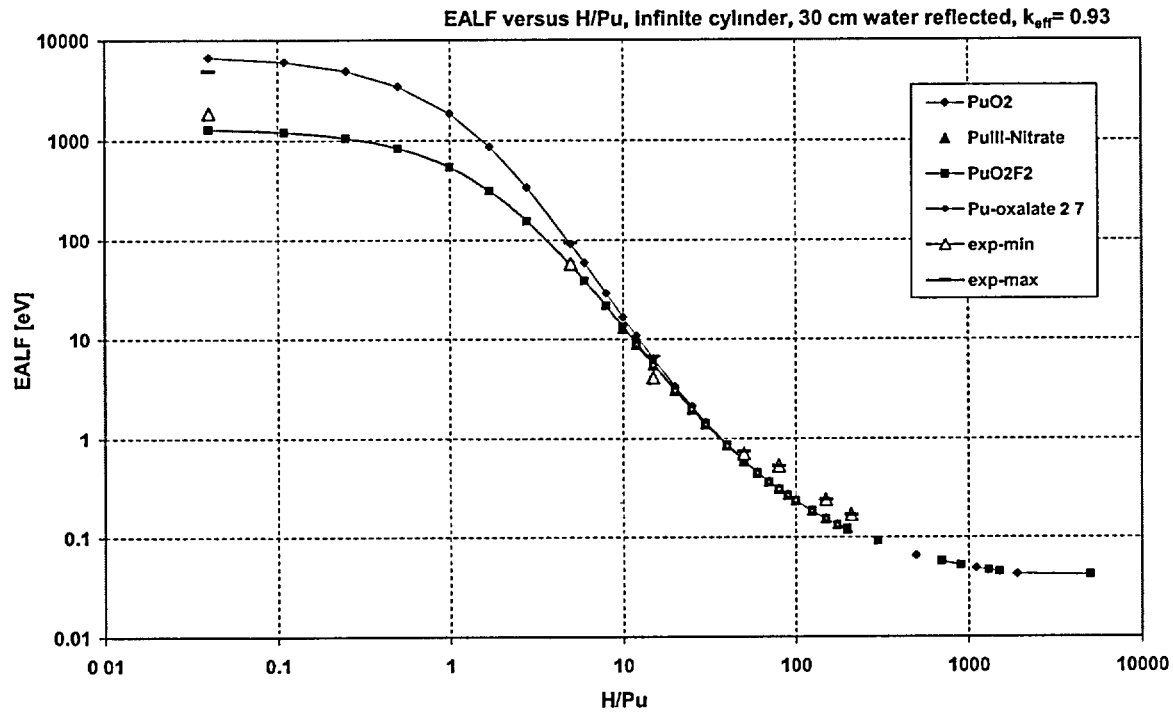


Figure 4–2 EALF versus H/Pu for different Pu compounds in aqueous solution over the full range of H/Pu

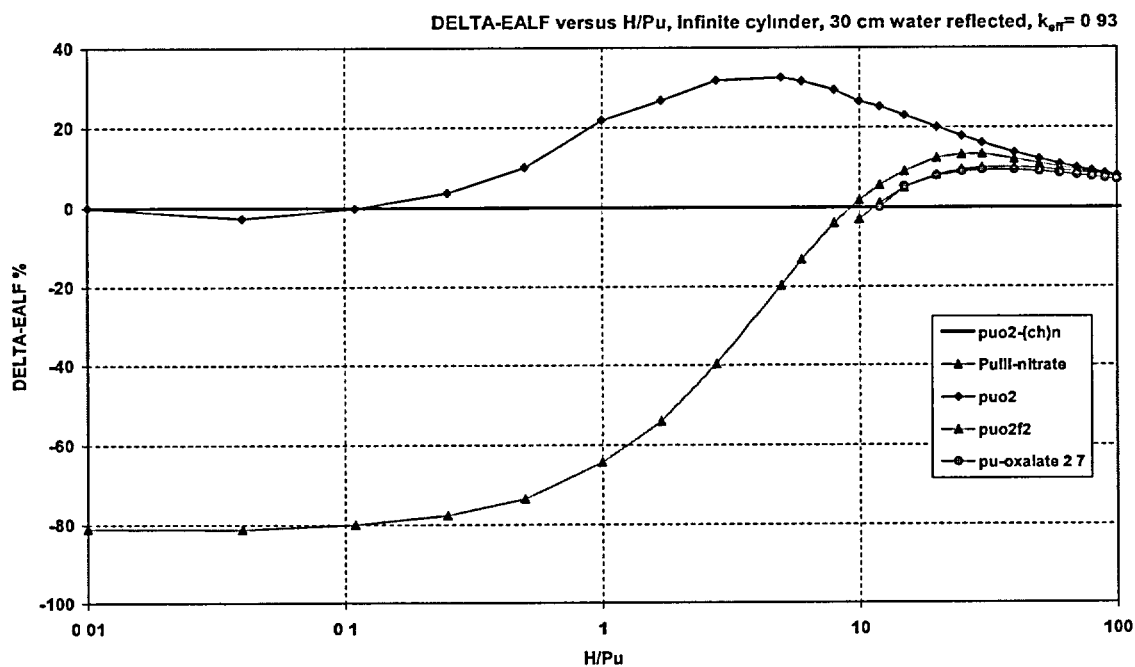


Figure 4-3 DELTA-EALF versus H/Pu for different Pu compounds in water over the full range of H/Pu

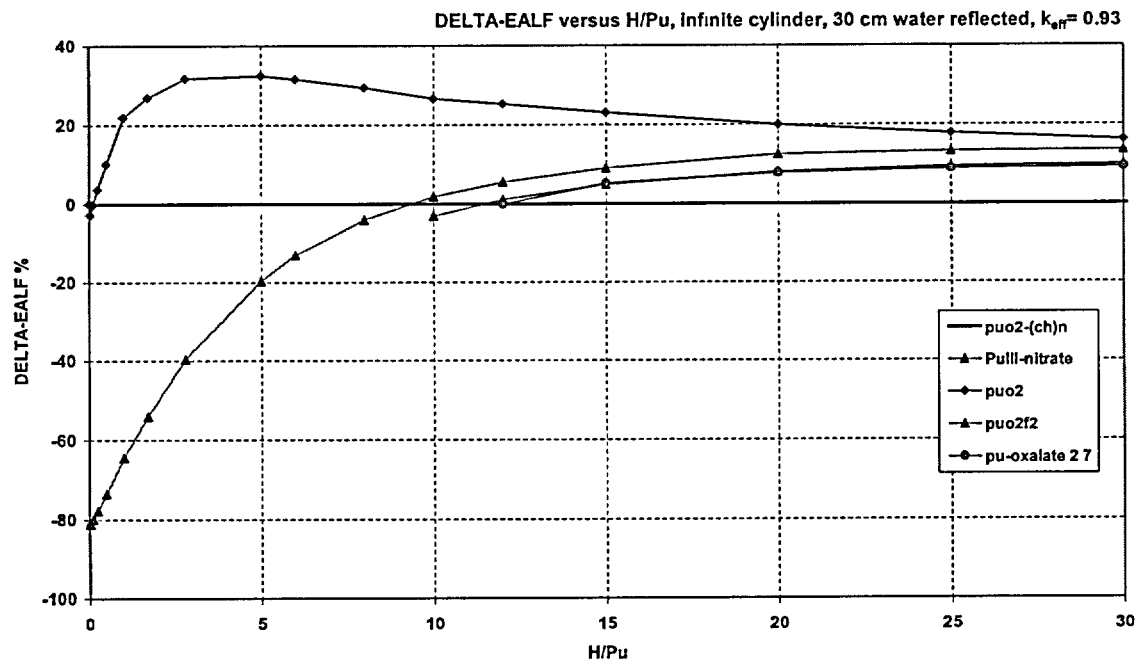


Figure 4-4 DELTA-EALF versus H/Pu for different Pu compounds in water in the range of $0 < H/Pu < 30$

4.3.2 Geometrical Shape

Calculations also show that the geometrical shape has a significant influence on the EALF values. In order to eliminate this geometrical shape effect, the experimental configuration geometry of the PuO₂-polystyrene experiments (parallelepiped compacts) is used to model different Pu compounds. This means the PuO₂-polystyrene compacts filled with the reference fissile media instead of the PuO₂-polystyrene medium (exp) preserving the same H/Pu ratio as in the experimental fissile medium. Table 4-9 shows the differences in the EALF values in the function DELTA-EALF.

From Table 4-9, the PuO₂-polystyrene experiments describe the EALF situation in the Pu-oxalate solution at H/Pu = 15 nearly exactly (differences lower than 2%). The differences with the PuO₂F₂ “standard salt” solution are smaller than 11%, whereas the differences with the PuO₂ systems is between 45% and 55%.

Detailed EALF values are presented in Attachment 1.

Table 4-10 shows the range of EALF values obtained for the reference fissile media assumed in the experimental configuration. The EALF values for a given H/Pu ratio of 15 calculated for the Pu-oxalate systems are in excellent agreement with the EALF values of the PuO₂-polystyrene experiments.

Besides the application with Pu-oxalate solution and Pu-oxalate precipitates the PuO₂ powder H₂O systems with high powder densities between 3.5 g/cm³ (H/Pu = 5.973) and 7.0 g/cm³ (H/Pu = 1.674) are an important application in the MFFF.

The following figures illustrate how far the PuO₂ powder application (full saturated powder with full H₂O reflector) is from the critical experiment with PuO₂-polystyrene and full Plexiglas reflector. Figure 4-5 shows the EALF as a function of H/Pu for critical full reflected infinite cylinders and critical full reflected infinite slabs representing the experimental configuration and the PuO₂+H₂O application. Figure 4-6 and Figure 4-7 show the differences between the EALF values in the relevant application range of $1 < \text{H/Pu} < 10$.

The differences between the experimental EALF value and the EALF value found for the same H/Pu = 1.674 for the PuO₂-powder application are 87% in case of slab geometry and 78% in case of cylindrical geometry.

Table 4–9 Comparison of DELTA-EALF Values of the Experimental Configuration Filled with PuO₂-Polystyrene and Other Reference Fissile Media

Case	C (Pu) [g/cm ³]	wt. % Pu-240	H/Pu	DELTA EALF PuO ₂ [%]	DELTA EALF PuO ₂ F ₂ [%]	DELTA EALF Pu-Oxalate [%]
10	1.12	2.2	15	55.1	11.4	0.4
11	1.12	2.2	15	53.5	10.3	0.2
12	1.12	2.2	15	53.4	9.8	0.2
13	1.12	2.2	15	52.5	9.8	0.2
14	1.12	2.2	15	52.2	10.4	0.9
15	1.12	2.2	15	51.5	9.4	1.7
16	1.12	2.2	15	51.9	10.6	0.5
17	1.05	8.06	15	51.5	11.8	1.2
18	1.05	8.06	15	48.2	9.4	1.5
19	1.05	8.06	15	46.9	9.5	1.8
20	1.05	8.06	15	46.5	9.3	1.4
21	1.05	8.06	15	46.2	9.1	1.5
22	1.05	8.06	15	48.2	9.9	1.2

$$\text{DELTA-EALF} = (\text{EALF}(\text{media i}) - \text{EALF}(\text{exp})) / \text{EALF}(\text{exp})$$

Table 4–10 Comparison of the Range of EALF Values of the Experimental Configuration Filled with PuO₂-Polystyrene and Other Reference Fissile Media

Cases	PuO ₂ +H ₂ O	PuO ₂ F ₂ +H ₂ O	Pu-oxalate+H ₂ O	Experiments [5], [6] PuO ₂ +(CH) _n
Cases 10 – 16	6.39 – 8.48	4.59 – 6.15	4.14 – 5.66	4.12 – 5.57
Cases 17 – 22	7.47 – 9.77	5.51 – 7.29	4.99 – 6.78	4.93 – 6.68

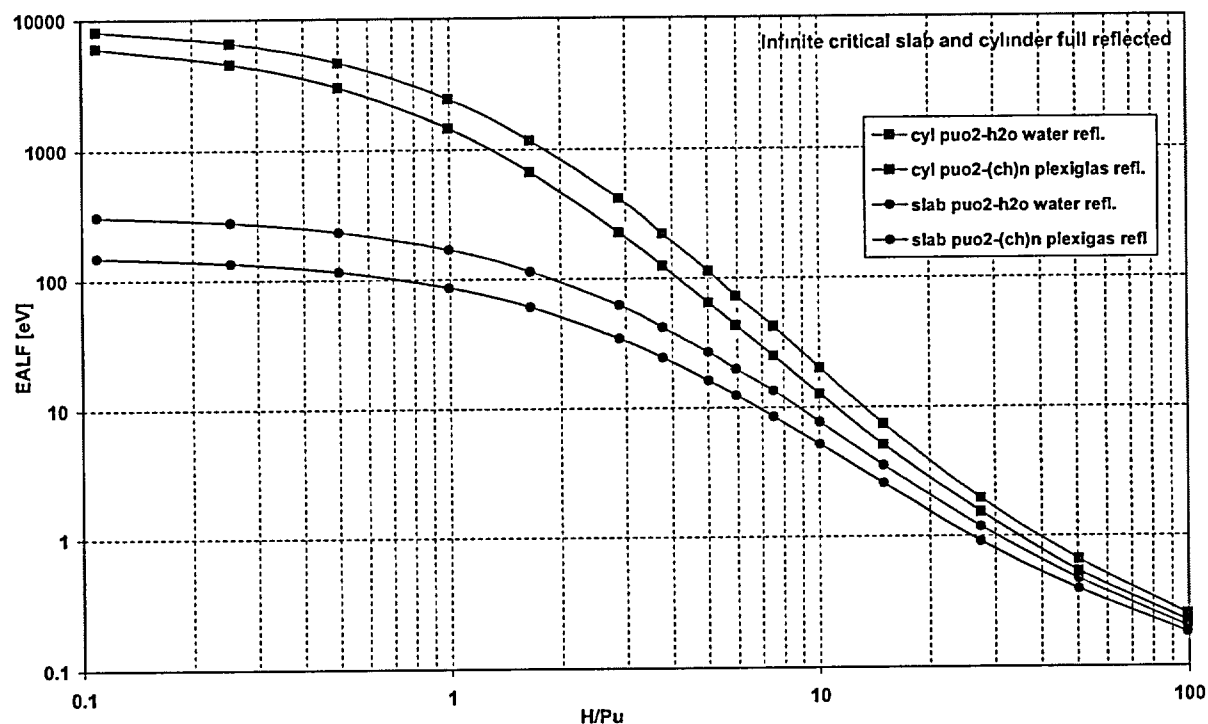


Figure 4-5 EALF versus H/Pu for a critical full reflected infinite cylinder and slab for PuO_2 -polystyrene with Plexiglas reflector and $\text{PuO}_2 + \text{H}_2\text{O}$ with water reflector over the full range of H/Pu

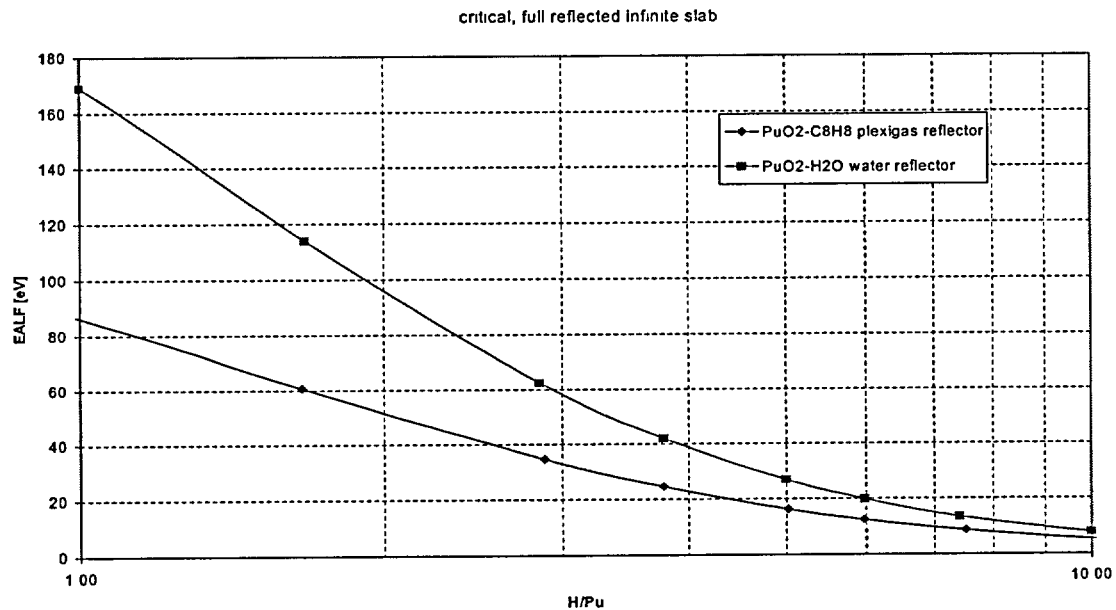


Figure 4-6 EALF versus H/Pu for different reflector materials in the range of $1 \leq H/Pu \leq 10$, infinite critical slab

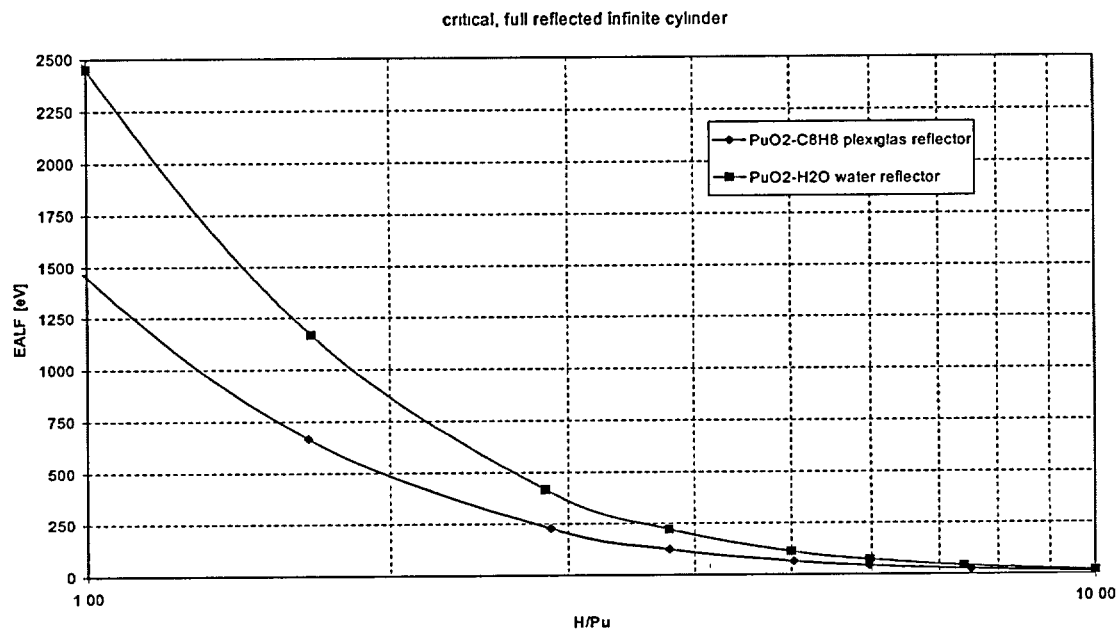


Figure 4-7 EALF versus H/Pu for different reflector materials in the range of $1 \leq H/Pu \leq 10$, infinite critical cylinder

4.3.3 Reflector Material Composition

The comparison of the EALF values presented in Table 4–6 and Table 4–7 shows the increasing influence of the reflector material composition on EALF with decreasing H/Pu.

Figure 4–8 compares the EALF values for four different reflector materials used in the MFFF for the case of slab geometry. It was shown in Table 4–6 and Table 4–7 that the slab geometry shows the strongest influence of the reflector materials on EALF.

Therefore, in the following figures the influence of Plexiglas reflector, water reflector, concrete reflector and borated concrete reflector materials on the EALF is studied for an infinite slab filled with PuO₂-polystyrene mixture corresponding to the experiments of Group 1 and Pu-nitrate experiments of Group 2.

Figure 4–8 shows the strong influence of borated concrete and Cd-steel+water reflectors on the EALF value in the $H/Pu < 50$ range. Again in the range over $H/Pu = 50$ there is no significant difference between concrete, Plexiglas and water reflectors whereas the differences to the borated concrete still remain but with decreasing influence. In the range between $10 < H/Pu < 1000$, It is evident that these differences between concrete reflector, Plexiglas reflector and water reflector are small.

Therefore Figure 4–9 shows the DELTA-EALF values as a function of the H/Pu for three different reflector materials used in MFFF design applications over the full range of H/Pu (DELTA-EALF is defined as: $(EALF(\text{refl } i) - EALF(\text{plex})) / EALF(\text{plex})$). The reference reflector material is Plexiglas (plex) used in the experiments of Group 1.

In the H/Pu range between 10 and 1000, the differences between concrete reflector and Plexiglas reflector in this range are smaller than 20%. Hence, the MFFF applications of AOA(5) with concrete reflector (e.g., the tanks filled with Pu-oxalate in the AP cells) are well described by the PuO₂-polystyrene experiments of Group 1.

Next the influence of different reflector materials is studied for a infinite slab filled with Pu-nitrate solution. Figure 4-10 shows the EALF values as a function of the H/Pu for an infinite slab filled with Pu-nitrate solution with different reflector materials in the H/Pu range between 10 and 1000. There is no other trend in this H/Pu range as in the case of Pu-oxalate solution.

Figure 4–11 shows DELTA-EALF as a function of H/Pu in the range of $10 < H/Pu < 1000$. The reference EALF value in this case is the EALF value of the full water reflected slab (water) to be in agreement with the experiments of Group 2.

The difference between the EALF values of regular concrete (reg-concrete) reflected slabs with Pu-nitrate solution at $H/Pu = 100$ and water reflected slabs with the same solution is lower than 10 %. The difference between colemanite concrete reflected slabs and water reflected slabs filled with Pu-nitrate solution at $H/Pu = 100$ is larger. Therefore in applications with colemanite concrete the EALF values found for the application have to be compared with the experimental EALF values in a case by case manner.

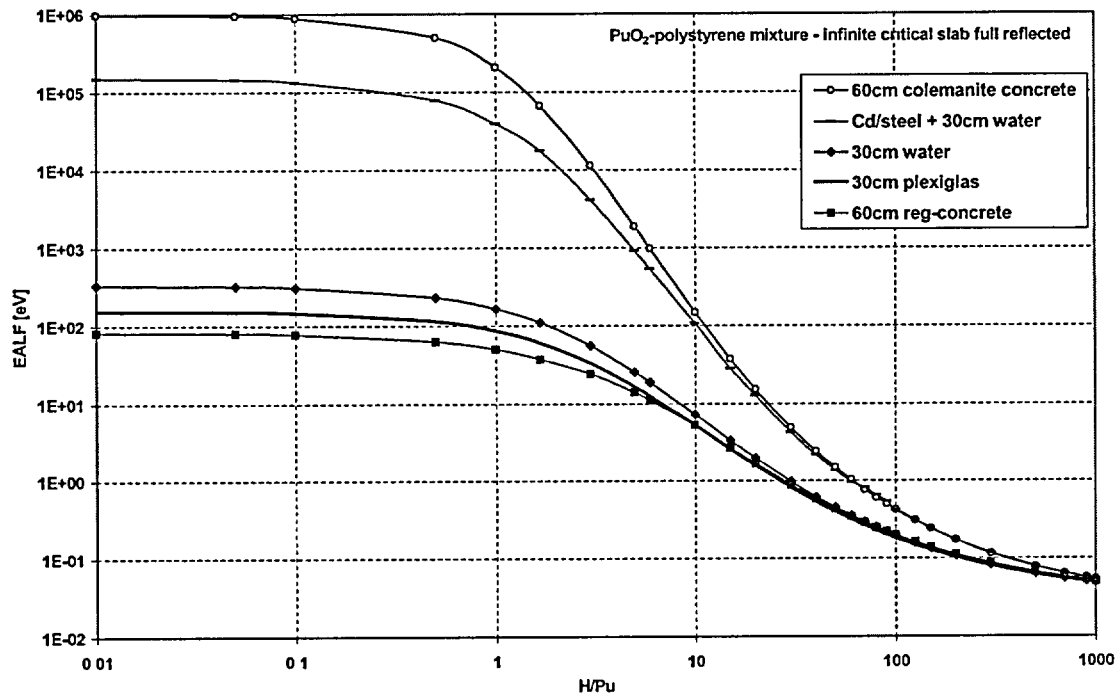


Figure 4-8 EALF versus H/Pu for different reflector materials over the full range of H/Pu, critical infinite slab with PuO₂-polystyrene mixtures

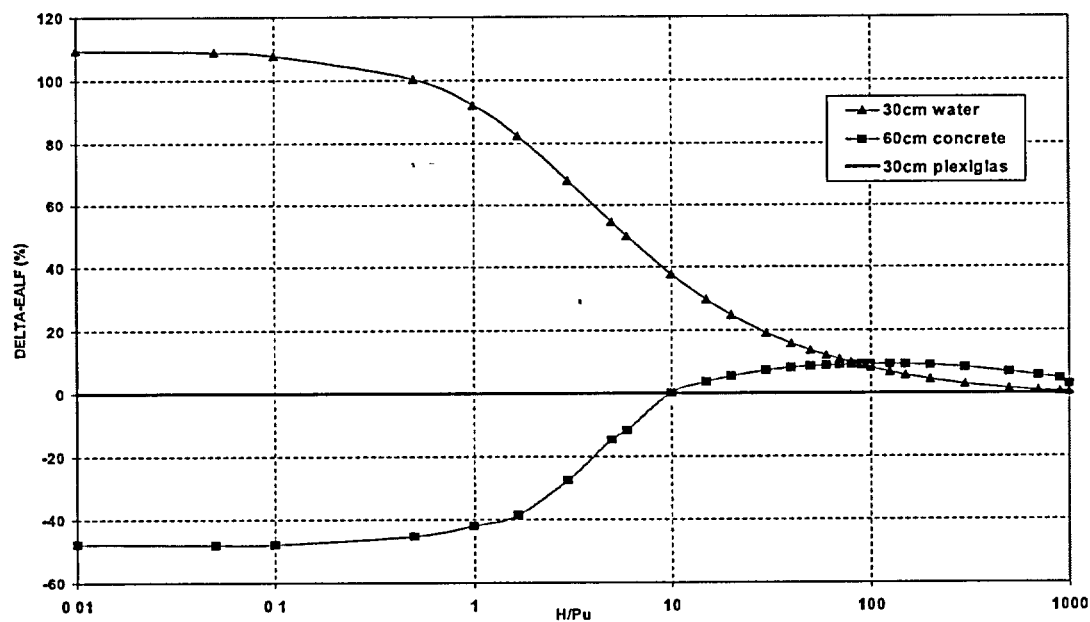


Figure 4-9 DELTA-EALF versus H/Pu for different reflector materials over the full range of H/Pu, critical full reflected slab filled with PuO₂-polystyrene mixtures

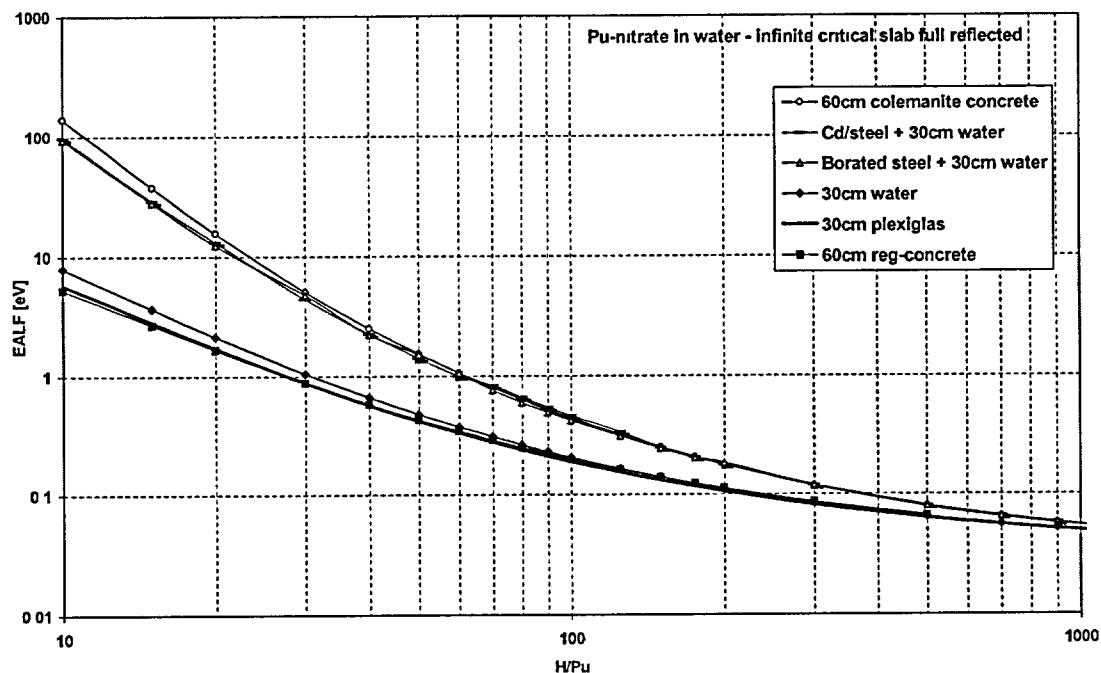


Figure 4-10 EALF versus H/Pu for different reflector materials over the range of $10 < H/Pu < 1000$, critical full reflected slab filled with Pu-nitrate solution

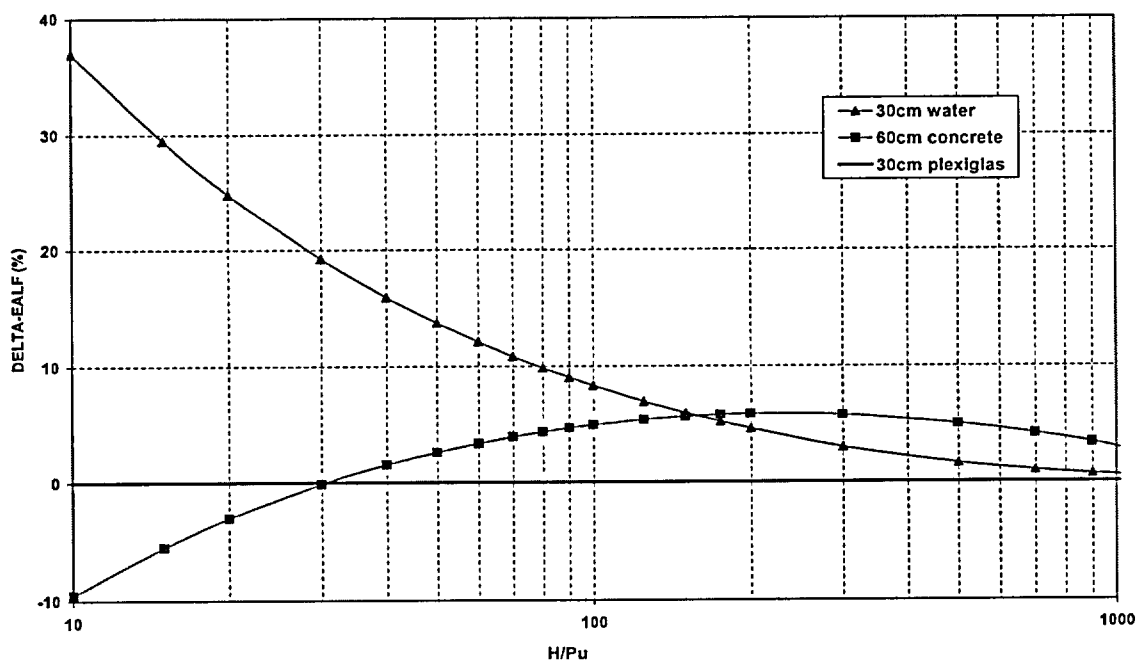


Figure 4-11 DELTA-EALF versus H/Pu for different reflector materials in the range of $10 \leq H/Pu \leq 1000$, critical full reflected slab filled with Pu-nitrate solution

4.4 Determination of a Reactivity Bounding Fissile Medium

Due to the Aqueous Polishing process the range of the fissile media concentrations in the different process stages vary from nominal Pu concentrations of 10 g/liter ($H/Pu < 1000$) up to the highest possible concentrations of the Pu-oxalate and PuO_2 powders of 3.5 g/cm^3 [18] (see Table 4-11).

For the criticality safety analysis it is important to know at which Pu concentration or H/Pu ratio the absolute maximum of k_{eff} occurs and whether a second relative maximum exists. The code validation for this AOA(5) has to cover the EALF range or H/Pu range where the maximum k_{eff} values of the application occur. The height of the maximum depends on the Pu compound density. In order to cover the variety of Pu compounds and compound densities that can occur in the AP process, a bounding media, PuO_2F_2 “standard salt,” is introduced in the MFFF application [18]. This approach was first employed in the criticality studies of Paxton et al. [27] and justified for application in the French reprocessing plants by Fruchard et al. in [28].

The advantage of the PuO_2F_2 “standard salt” defined in [23] is that it also describes the low moderated range between $H/Pu = 0$ and $H/Pu = 12$. Furthermore, it is demonstrated in Table 4-11 that PuO_2F_2 bounds all possible Pu^{IV} oxalate compounds in the MFFF.

Table 4-11 Comparison of experimental and estimated Pu compounds densities

Pu compound	Density [g/cm^3]	Reference
$Pu(C_2O_4)_2 \cdot 6H_2O$	2.70	Experimental Pu^{IV} -oxalate density deduced from the unit cell parameters in [21], [22]
$Pu(C_2O_4)_2 \cdot 2H_2O$	3.05	Experimental Pu^{IV} -oxalate density deduced from the unit cell parameters in [21], [22]
$Pu(C_2O_4)_2$	$3.225^{1)}$	Estimated Pu^{IV} -oxalate density by linear extrapolation from the values of $Pu^{IV} \cdot 6H_2O$ -2.70 and $Pu^{IV} \cdot 2H_2O$ -3.05
“Standard salt” PuO_2F_2	4.187	Estimated PuO_2F_2 “standard salt” density used in criticality studies only to covers the MFFF Pu compounds [23]. This law is not valid for genuine PuO_2F_2 media (crystal density of 6.5 g/cm^3 [20])
PuO_2	3.50	Basis of Design [18]

1) An estimated conservative value of 3.50 g/cm^3 is used in the calculations as shown in Figure 4-13

In the following figures, typical k_{eff} curves are presented as a function of H/Pu for slab geometry. Figure 4-12 shows the k_{eff} for a slab filled with different Aqueous Process reference fissile media versus H/Pu over a wide range of H/Pu .

All k_{eff} -values corresponding to the Figure 4-12 through Figure 4-14 are presented in Attachment 2, Table A2-1. The fissile media number densities are addressed in [19].



For the Aqueous Polishing process the range of H/Pu between 0 ($C(\text{Pu}) \approx 3.0 \text{ g/cm}^3$) and 500 ($C(\text{Pu}) \approx 0.05 \text{ g/cm}^3$) is of interest. Therefore Figure 4-13 and Figure 4-14 compares k_{eff} -values respectively versus H/Pu and C(Pu) in this range to demonstrate that the PuO_2F_2 “standard salt” bounds various Pu^{IV} -oxalate solutions which can occur in the AP process. It appears that the number of crystal water molecules in the Pu precipitate is as important as the density. Thus, the most reactive Pu-oxalate is the following one: $\text{Pu}(\text{C}_2\text{O}_4)_2 \cdot 6\text{H}_2\text{O}$ with a crystal density of 2.7 g/cm^3 . Based on measurements of Pu-oxalate density, [29] provides a maximum density of 2.7 g/cm^3 with six H_2O crystalline water molecules. This value is considered in the MFFF AP process.

It is also obvious from Figure 4-12 and that the maximum of k_{eff} occurs for Pu-nitrate and Pu-oxalate in the same range around $\text{H/Pu} = 100$, whereas the maximum of PuO_2F_2 occurs at $\text{H/Pu} = 30$. Therefore the calculational bias for Pu oxalate solutions is better described by the Pu-nitrate experiments with H/Pu values between 78 and 211 whereas the calculational bias for PuO_2F_2 “standard salt” solutions is better described by the PuO_2 -polystyrene experiments.

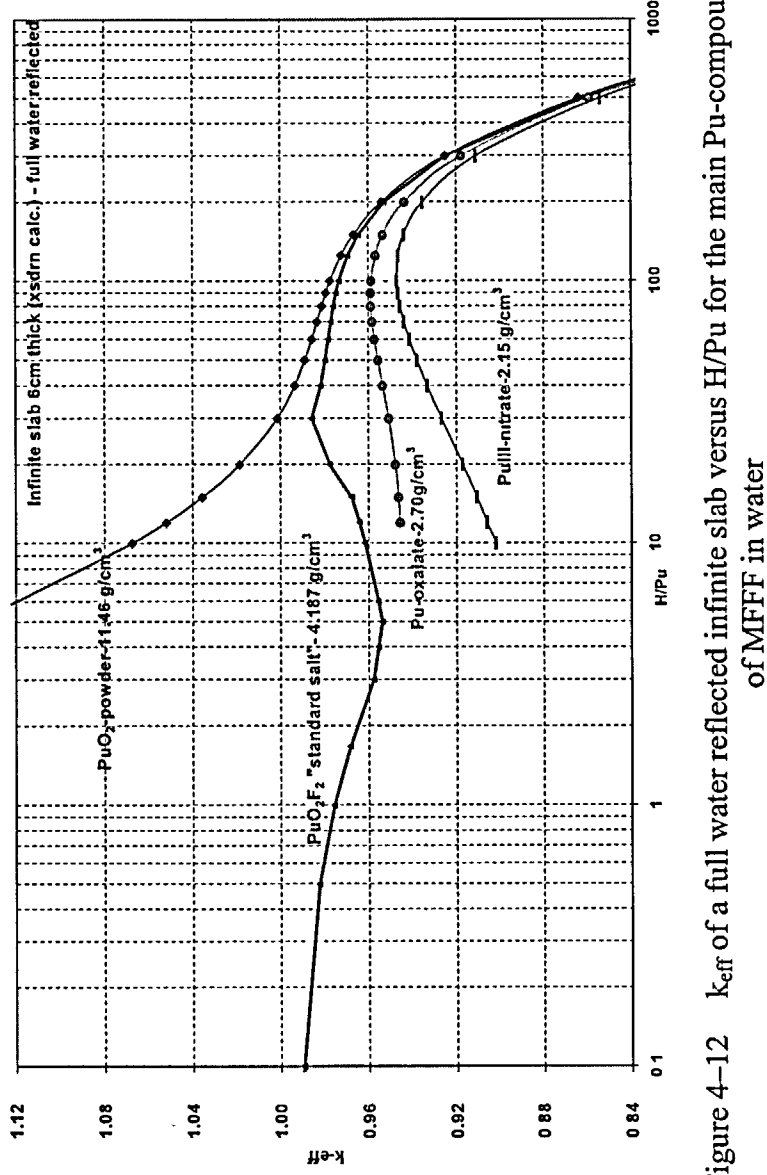


Figure 4-12 k_{eff} of a full water reflected infinite slab versus H/Pu for the main Pu-compounds of MFFF in water

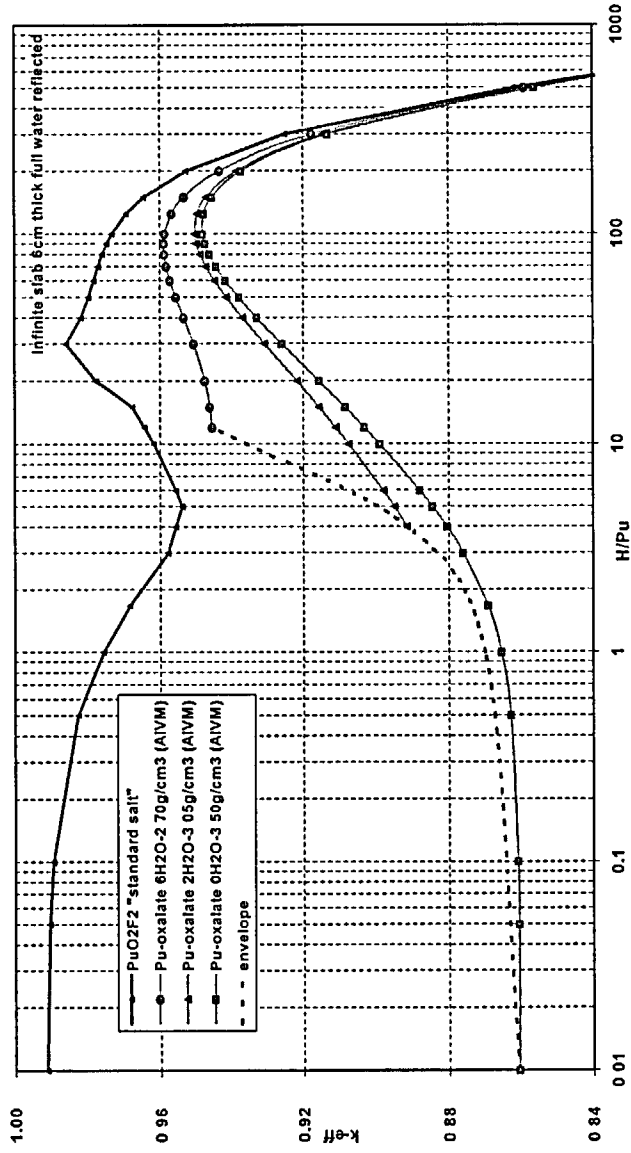


Figure 4-13 k_{eff} of a full water reflected infinite slab versus H/Pu for PuO_2F_2 "standard salt" and different Pu-oxalate in water (*), (**)

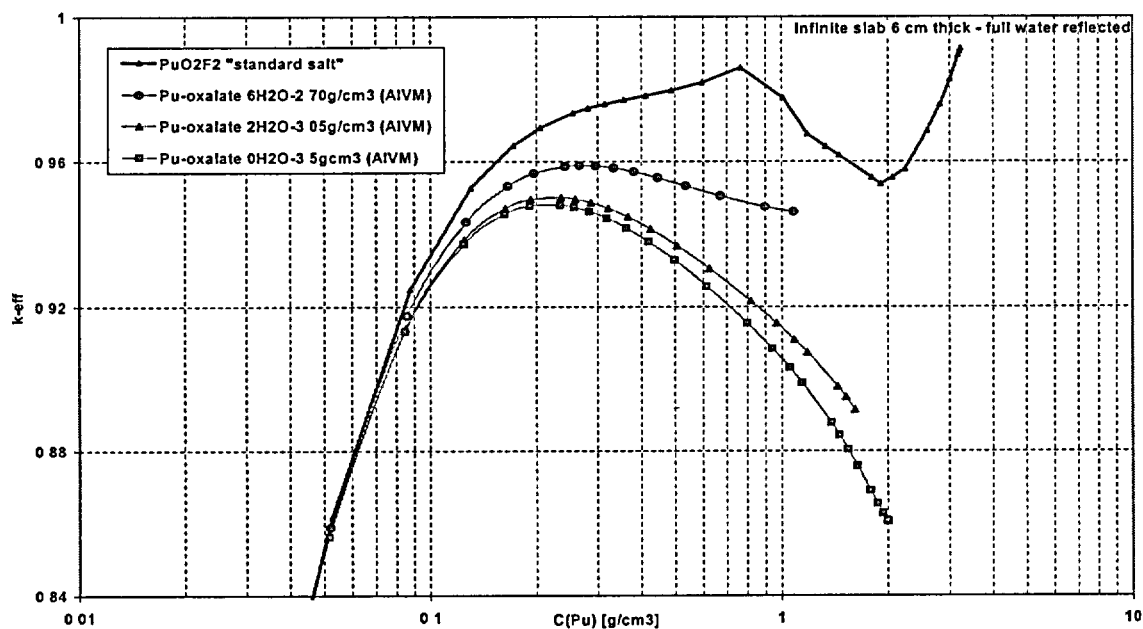


Figure 4-14 k_{eff} of a full water reflected infinite slab versus $C(Pu)$ for PuO_2F_2 "standard salt" and different Pu-oxalate in water^(*)

- (*) AIVM means that the dilution law used for these assumed homogeneous Pu oxalate-water mixtures is a simple Addition of Individual Volumes and Masses as described in [23],
- (**) The envelope curve points out the k_{eff} -values corresponding to the minimum H/Pu of Pu^{IV} -oxalate compounds depending from the number of crystalline water molecules in the complex.

5. Benchmark Experiments

5.1 AOA (5) – PuO₂-Polystyrene Mixtures and Pu-Nitrate Solutions

The MFFF design applications include Pu compound solutions and Pu-oxalate precipitates. For these compounds, no benchmark experiments are available. To cover this range of design applications (see Table 5-2), two benchmark sets of thirty two experiments with PuO₂-polystyrene compacts and six benchmark sets of Pu-nitrate solution experiments are selected from the ICSBEP Handbook [5]. These experiments cover a suitable range of H/Pu ratios, EALF values, geometry and reflectors which correspond to AOA (5). Table 5-1 lists the experiments along with a description and key parameters.

Table 5-2 provides a comparison of the key AOA parameters of the critical experiments and design applications parameters. The experiments involving Pu-nitrate solutions are chosen to cover the range of the EALF values for MFFF design applications from low moderated Pu precipitates to well moderated solutions of Pu compounds.

Table 5-1 Critical Experiments Selected for AOA(5)

Experiment of AOA 5 *	H/Pu	EALF [eV]	Reflector and Geometrical form	²⁴⁰ Pu [wt. %]	Description
PU-COMP-MIXED-001	5 to 49.6	1.548 to 175000	Bare rectangular parallelepipeds	2.2 to 18.35	PuO ₂ -polystyrene compacts
PU-COMP-MIXED-002	0.04 to 49.6	0.685 to 4900	Plexiglas-reflected rectangular parallelepipeds	2.2 to 18.35	PuO ₂ -polystyrene compacts
PU-SOL-THERM-001	87-354	0.35-0.09	Water reflected sphere	4.67	11.5" Diameter sphere
PU-SOL-THERM-008	85-858	0.55-0.05	Concrete reflected and concrete /Cd reflected sphere	4.67	14" Diameter sphere
PU-SOL-THERM-014	210	0.17-0.14	Unreflected array of cylinders	4.23	Interacting cylinders in air with 115.1 g Pu/l
PU-SOL-THERM-015	155	0.24	Unreflected array of cylinders	4.23	Interacting cylinders in air with 152.5 g Pu/l
PU-SOL-THERM-016	155-210	0.24-0.17	Unreflected array of cylinders	4.23	Interacting cylinders in air with 152.5 and 115.1 g Pu/l
PU-SOL-THERM-017	210	0.17	Unreflected array of cylinders	4.23	Interacting cylinders in air with 115.1 g Pu/l

* From (Nuclear Energy Agency 1999) [5]

Table 5–2 AOA (5) – Comparison of Key Parameters

Parameter	Design application (cf. Table 4–1)	Benchmarks (cf. Table 5–1)
Geometric shape	Parallelepipeds Arrays of cylinders Spheres	(a) Parallelepipeds (b) Arrays of cylinders
Absorber/reflector	Water, Cd, Borated concrete	(a) Plexiglas, air (b) Air/ water
Chemical form	Pu compounds in water and precipitated oxalates	(a) PuO ₂ -polystyrene mixture (b) Pu-nitrate solution
Isotopic composition	4 wt. % ²⁴⁰ Pu	(a) 2.2 to 18.35 wt. % ²⁴⁰ Pu (b) 4.23 to 4.67 wt.% ²⁴⁰ Pu
H/Pu	10 to 50 50 to 250	(a) 0.04 to 49.6 (b) 78 to 858
EALF [eV]	0.1 to 30	(a) 0.685 to 4900 (b) 0.135 to 0.551

a) Group 1

b) Group 2

6. Analysis of Validation Results

6.1 AOA (5) – PuO₂-Polystyrene Mixtures and Pu-Nitrate Solutions

Eight benchmarks (cf. Table 5–1) are modeled with CSAS26/KENO VI using the 238 group library 238GROUPNDF5. These experiments are grouped as follows:

- Group 1 (for use with $H/Pu < 50$): Thirty-two experiments with PuO₂-powder in polystyrene.
- Group 2 (for use with $H/Pu > 50$): Eighty-seven experiments with Pu-nitrate solution.

Two benchmark sets, PU-COMP-MIXED-001 and PU-COMP-MIXED-002 are used for Group 1 ($0.4 < H/Pu < 49.9$). From the PU-SOL-THERM benchmarks, four sets with $H/Pu < 250$ are chosen to cover the EALF values of the design application in the range of $H/Pu > 50$. The selection of the Pu-nitrate solution experiments for Group 2 in addition to the PuO₂-polystyrene experiments of Group 1 is necessary to cover the full range of H/Pu and EALF values met in the applications, cf. Table 4–1 and Table 4–2.

The calculated k_{eff} values for the two groups of AOA(5) are presented in Attachment 4. As can be seen from the USLSTATS results shown in Attachment 5, all cases are normally distributed. Figure 6–1 shows the distribution of the calculated k_{eff} values for Group 1 experiments calculated with SCALE 4.4a on the PC platform. Similarly, Figure 6–2 shows the distribution of the calculated k_{eff} values for Group 2 experiments.

The k_{eff} values of the two groups are analyzed statistically using the USLSTATS computer code². (see Attachment 5). For Group 1 EALF ranges from 0.7 eV to 4900 eV. (cf. Table A3-1). For Group 2 EALF ranges from 0.135 eV to 0.551 eV (cf. Tables A3-2). Table 6–1 and Table 6–2 in Section 6.1.2 summarize the statistical results of the USLSTATS program for both groups (PuO₂-polystyrene and Pu-nitrate solutions). Note that the range of EALF obtained with these experiments covers the EALF values of AOA(5), cf. Table 4–1. Figure 6–3 through Figure 6–6 show the results graphically.

² Many of the benchmark experiments in the International Handbook of Evaluated Criticality Safety Benchmark Experiments (Nuclear Energy Agency 1999) are considered to be critical (i.e., $k_{eff} = 1.000$), while other experiments are not considered critical (i.e., $k_{eff} \neq 1.000$). Therefore, all calculated k_{eff} values are normalized to the handbook values (cf. Section 3.5)

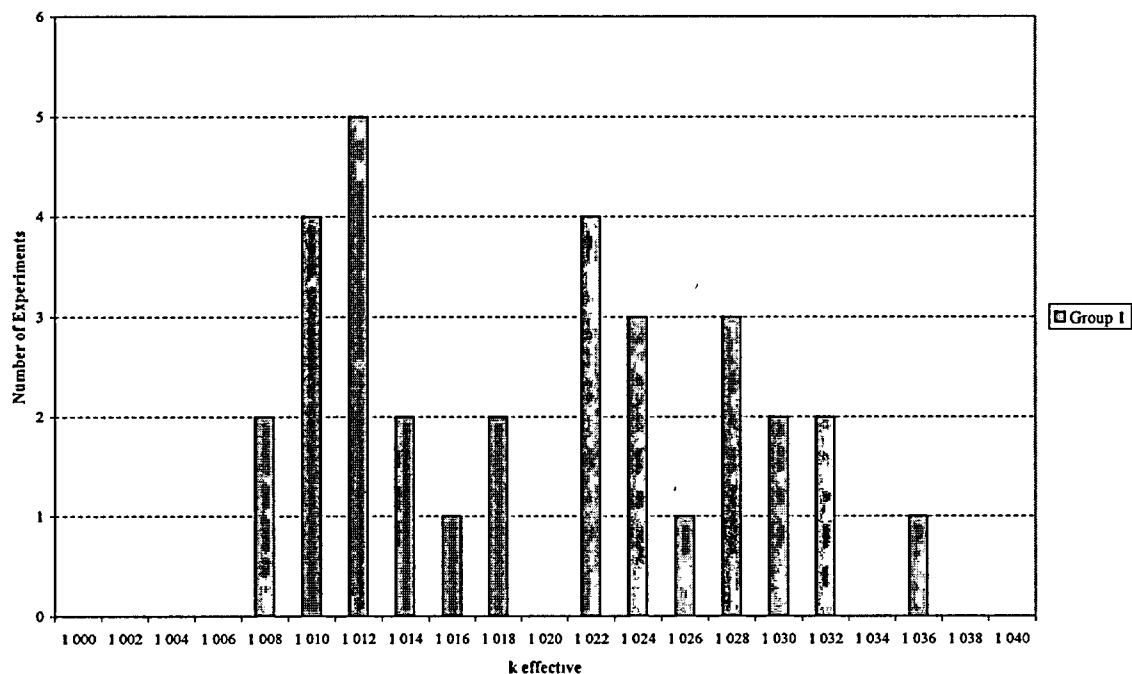


Figure 6–1 Histogram of k_{eff} Occurrences for AOA(5) Group 1

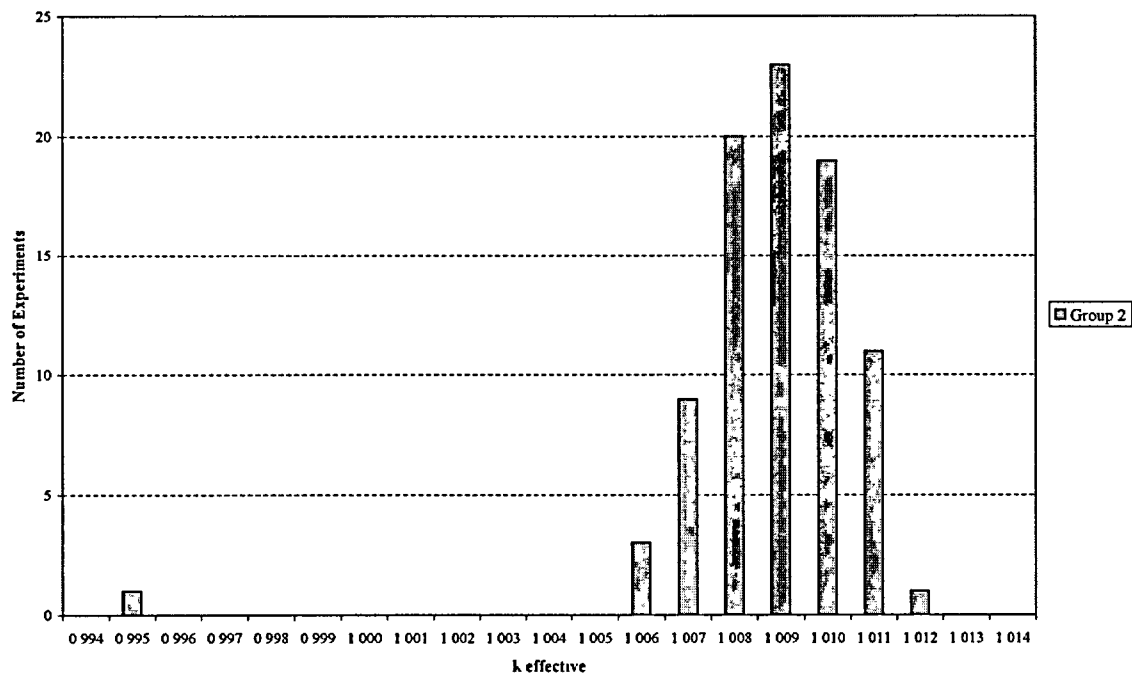


Figure 6–2 Histogram of k_{eff} Occurrences for AOA(5) Group 2

6.1.1 USL with EALF and H/Pu Ratio

Figure 6–3 and Figure 6–4 show the k_{eff} values and the corresponding values of USL-1 and USL-2 values versus the trending parameters EALF and H/Pu for the Group 1 experiments (PuO₂-polystyrene).

The k_{eff} values calculated for Group 2 (experiments with Pu-nitrate solution) are shown in Figure 6–5 and Figure 6–6 as a function of EALF and H/Pu, respectively.

The corresponding USLSTATS output listings are provided in Attachment 5.

Table 6–1 shows that for AOA(5) Group 1 the minimum USL-1 with a 0.05 administrative margin is 0.9328. The minimum USL-2 found for the PuO₂ systems is 0.9534.

Table 6–2 shows that for the AOA(5) Group 2 the minimum USL-1 with a 0.05 administrative margin is 0.9411. The minimum USL-2 found for the Pu-metal systems is 0.9779.

For the PuO₂-polystyrene experiments, the conservative minimum margin to subcriticality $\Delta k_m = 0.0239$ calculated with the USL-2 method suggests that the administrative margin ($\Delta k_m = 0.05$) applied to the USL-1 value is adequate for the AOA(5) provided the EALF and H/Pu ratio fall within this range of applicability³. The same is found for the Pu nitrate experiments with a conservative minimum margin to subcriticality $\Delta k_m = 0.0121$

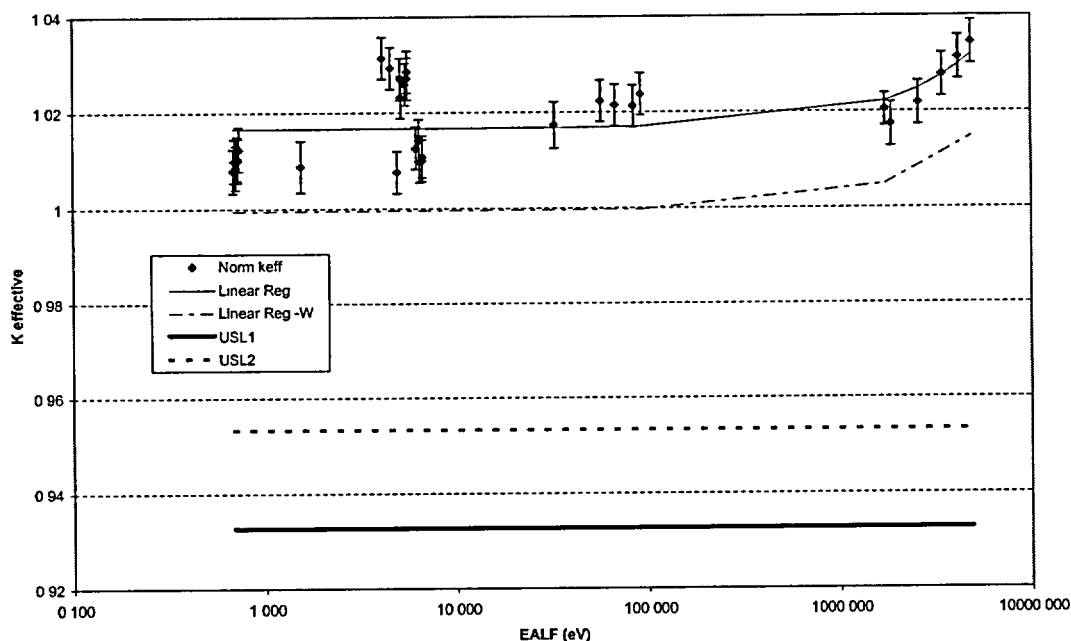


Figure 6–3 k_{eff} as Function of EALF (Pu-Comp-Mixed) AOA(5) Group 1

³ ANSI/ANS-8.1 allows the range of applicability to be extended beyond this range by extrapolating the trends established for the bias; however, no precise guidelines are specified for the limits of extrapolation. Therefore, engineering judgment must be applied when extrapolating beyond the range of the parameter bounds. If extrapolation is necessary, it will be discussed on a case-by-case basis in the individual criticality calculations.

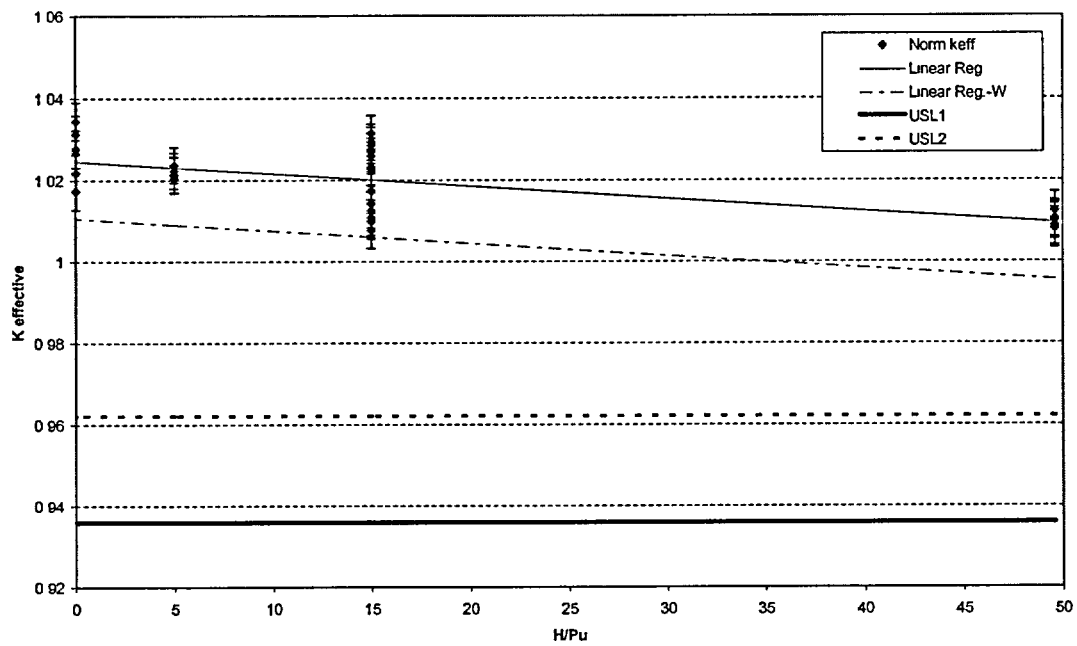


Figure 6-4 k_{eff} as Function of H/Pu (Pu-Comp-Mixed) AOA(5) Group 1

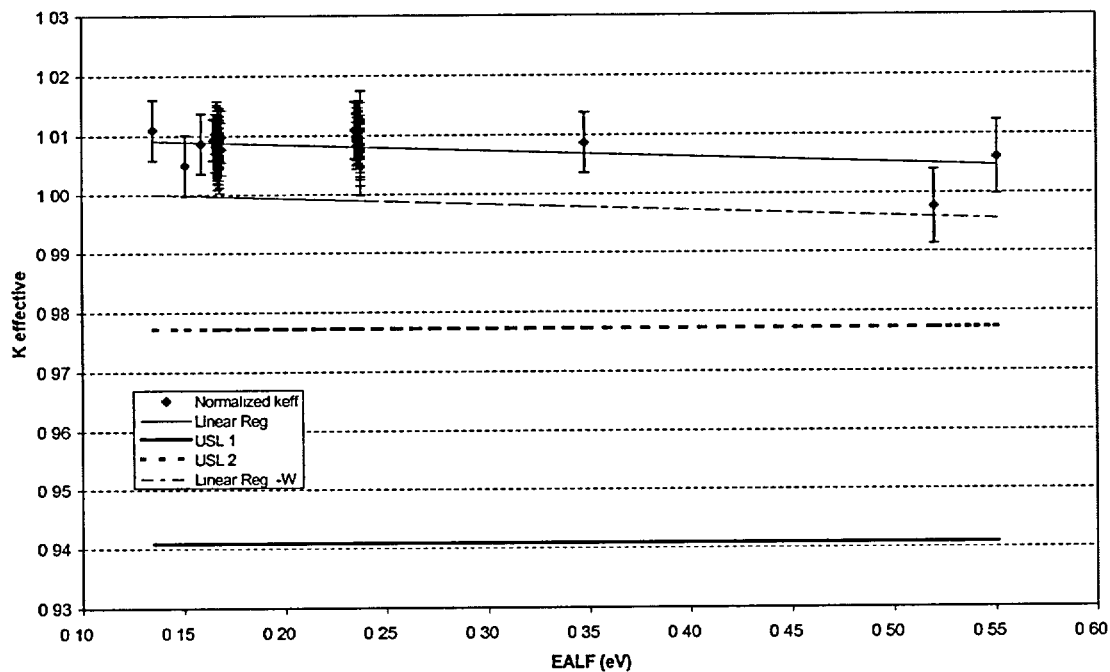


Figure 6-5 k_{eff} as Function of EALF (Pu-Nitrate Solution) AOA(5) Group 2

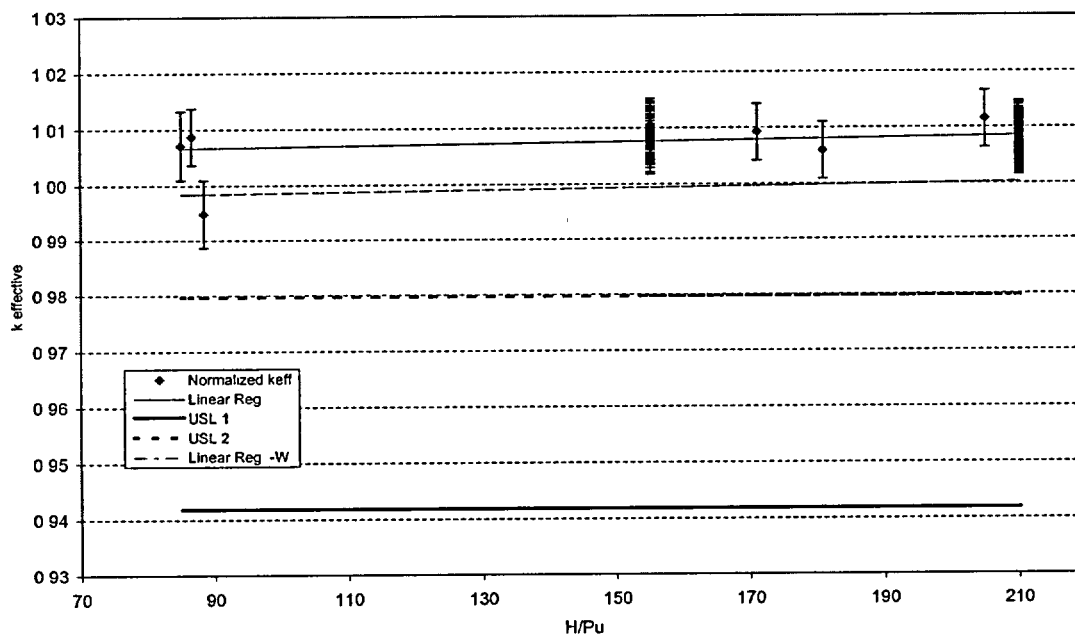


Figure 6-6 k_{eff} as Function of H/Pu (Pu-Nitrate Solution) AOA(5) Group 2



6.1.2 Summary of USL for AOA(5)

The USL-1 for the Group 2 experiments involving plutonium nitrate solution with a thermal fission spectrum (USL-1 of Group 2 is 0.9411) is found to be significantly higher than the USL-1 for the Group 1 experiments involving PuO_2 -polystyrene mixture systems with intermediate to fast fission spectrums. Therefore, the minimum USL for AOA(5) is based on the Group 1 result of 0.9328. This value includes a 0.05 administrative margin and consideration for calculational bias and uncertainties. The adequacy of the administrative margin is further discussed in Section 7.1. The calculated USL values for AOA(5) are summarized in the following tables.

Table 6–1 Summary of USL Calculations from SCALE 4.4a on PC Platform AOA(5)
Group 1: PU-COMP-MIXED-001 and PU-COMP-MIXED-002

Correlated Parameter (X)	No. of Exp.	Range of X	$k_c(X)$ Linear regression	Average k_c	Min USL ₁ ($\Delta k_m=0.05$)	Min USL ₂	Min Δk_m (USL ₂)
EALF [eV]	32	0.686 to 4900	$1.0167+(3.1025E-06)*X$	1.0186	0.9328	0.9534	0.0294
H/Pu	32	0.04 to 49.60	$1.0246+(-3.0367E-04)*X$	1.0186	0.9360	0.9621	0.0239
²⁴⁰ Pu [wt. %]	32	2.20 to 18.35	$1.0237+(-4.5199E-04)*X$	1.0186	0.9338	0.9561	0.0277

Table 6–2 Summary of USL Calculations with SCALE 4.4a on PC Platform AOA(5),
Group 2: Pu-Nitrate Solution

Correlated parameter (X)	No. of Exp.	Range of X	$k_c(X)$ Linear regression	Average k_c	Min USL ₁ ($\Delta k_m=0.05$)	Min USL ₂	Min Δk_m (USL ₂)
H/Pu	87	85.03 to 210.18	$1.0054 + (1.4797E-05)*X$	1.00824	0.9418	0.9797	0.0121
EALF [eV]	87	0.135 to 0.549	$1.0108 +(-1.3126E-02)*X$	1.00824	0.9411	0.9779	0.0132

7. Conclusions

The SCALE 4.4a code package using the CSAS26 (KENO-VI) sequence and the 238 energy group cross section library 238GROUPDF5 has been validated to perform criticality calculations for the MFFF. It has been validated for the fifth area of applicability AOA (5). Two groups of experiments are established to cover the range of design applications: PuO₂-polystyrene mixtures and Pu-nitrate solutions.

The USLs for the two groups of AOA (5) are as follows:

- AOA(5) Group 1 representative of design applications with $H/Pu < 50$ USL = 0.9328.
- AOA(5) Group 2 representative of design applications with $H/Pu > 50$ USL = 0.9411.

The USL accounts for the computational bias, uncertainties, and an administrative margin. The administrative margin is established at 0.05 such that $k_{eff} + 2\sigma - bias \leq 0.95$ for all normal and credible abnormal conditions. Section 7.1 contains a detailed justification of the administrative margin.

No extrapolation outside the range of applicability is expected for AOA(5) USL values; however, ANSI/ANS-8.1 [2] does allow for extrapolation outside the area of applicability by extrapolating the trends established for the bias and USL. If extrapolation is necessary, for instance with the design application involving colemanite concrete reflectors or Cd/water reflectors, it will be discussed on a case-by-case basis in the respective calculation.

7.1 Justification for Administrative Margin

The administrative margin applied in the determination of the USL is intended as an added level of conservatism. The code validation effort accounts for all code bias and the effects of both code and experimental benchmark uncertainties. The administrative margin is applied *in addition* to the code bias and bias uncertainty in determining the USL.

The USL values determined here are based on an administrative margin of 0.05. Based on actual process conditions, including 1) the degree to which application parameters fall within the validated Area of Applicability (AOA) of the calculational method and 2) the results of sensitivity analyses demonstrating the sensitivity of k_{eff} values to variations in controlled parameters, the USL may be adjusted. Each NCSE and criticality calculation will include a discussion of the appropriateness of the USL applied for each specific design application.

Typically, the NCSEs and criticality calculations will present k_{eff} results for various scenarios, including normal operation and credible abnormal situations. The results of these analyses permit a quantitative assessment of the degree of subcriticality of the system measured in terms of variation of one or more controlled parameters. Hence, the NCSEs/criticality calculations for specific design applications will verify the conformance with the AOA used in the validation reports.

In general, based on the discussion below, the administrative margin used in criticality analyses is 0.05. This assessment is based on a comparison against administrative margin practices at both NRC and DOE facilities, and past NRC guidance and practice, and is further substantiated by a statistical analysis of the benchmark validation results.

7.1.1 Fuel Cycle and Industry Practice

A review of NRC materials licensees and analogous DOE facilities (including plutonium facilities) indicates that administrative margins range from 0.02 to 0.05 as shown in Table 7-1. These values apply to applications within the validated AOAs; adjustments to the administrative margin are typically made for application outside the validated region.

These values are consistent with precedent information provided by the NRC Staff [26], which indicates administrative margins with a similar range to those indicated in Table 7-1. An administrative margin of 0.05 is greater than or equal to the most conservative margins identified in Table 7-1 and other NRC precedent [26] for analysis of credible abnormal conditions.

This margin is consistent with guidance provided in NUREG-1718 [3], which supports an administrative margin of 0.05 for the MFFF. It is also consistent with past NRC-accepted practice in reactor operations (10 CFR 50) [25], and transportation (10 CFR 71) and on-site storage (10 CFR 72) of spent nuclear fuel. Examination of various precedents indicates 0.05 is a conservative administrative margin for activities falling within the validated AOA. For criticality analyses applied outside the validated AOA, specific guidance is provided in ANSI/ANS-8.1-1998 which indicates that the administrative margin may be adjusted based on established trends in the bias, if necessary.

7.1.2 USLSTATS Method 2 Quantitative Assessment

Once an administrative margin has been determined (in this case, based on NRC guidance in NUREG-1718 [3] and based on conservative comparison with applicable precedent), NUREG/CR-6361 [9] provides a quantitative method of assessing the suitability of the administrative margin based on a statistical analysis which generates a recommended minimum margin of subcriticality. NUREG/CR-6361 suggests that this minimum margin of subcriticality be compared against the administrative margin in order to verify that the administrative margin is conservative relative to a purely statistical basis⁴.

This mechanism provides an independent, quantitative means of substantiating the administrative margin selected based on the statistics of the benchmarks themselves. The use of this methodology requires the specification of two important statistical parameters: α , the level of confidence in the limit being calculated and P , the probability future calculations will lie within the statistical band. The result of this methodology is the assurance that by using at least the calculated minimum margin of subcriticality, there is a probability P with a confidence α that an additional calculation of k_{eff} for a critical system will lie within the band. For example, a calculation with $\alpha=0.95$ and $P=0.95$ would yield a USL for which there is a 95% confidence that 95 out of 100 future calculations of critical systems will yield a value of k_{eff} above the USL (which is conservative). This level of statistical treatment is consistent with the statistics usually employed in the inclusion of 2σ in the treatment of Monte Carlo criticality calculations. It is also consistent with the statistical recommendations in NUREG/CR-6698 [24]. As can be seen in the figures in Section 6, use of this traditional statistical treatment would lead to the conclusion that,

⁴ See NUREG/CR-6361 §4.1.3. For example, Westinghouse is approved to use a 0.02 Δk administrative margin unless a higher margin of subcriticality is calculated using USL-2 methodology.



based on the usual statistical approach, a margin as low as 0.01 to 0.02 would be necessary to ensure that the USL was conservative based upon a statistical evaluation of the data.

However, this report uses USLSTATS to examine the statistics at a higher level of certainty. That is, values of $\alpha = 0.95$ and $P = 0.999$ were used. This means that the derived USL-2 is such that there is a 95% confidence that 999 out of 1000 future calculations of critical systems will yield a value of k_{eff} above the USL. The resulting conclusion using 95/99.9 statistics is that the added conservatism over the 1-2% amount, which would be required using traditional statistical levels, is available to ensure that the results are conservative for other potential mechanisms for which conservatisms would be prudent.

An analysis of the benchmarks using a value of $\alpha = 0.95$ and $P = 0.999$ yield the subcritical margins listed in Table 7-2. If one were to base an administrative margin solely on this very conservative statistical analysis, an administrative margin of at most 0.03 is necessary to statistically justify the use of these benchmarks. This is significantly less than the 0.05 administrative margin used for the two AOAs. Note that the administrative margin is applied in addition to the calculated bias and uncertainty for each AOA. This means that the proposed 0.05 administrative margin is still more conservative than that determined in the 95/99.9 statistical treatment and is justified in the MFFF.

7.1.3 Summary of Administrative Margin Practice

This effort involves the validation of the code to applications within one or more specific areas of applicability. There is no intent to account for or to address the uncertainties and unknowns involved in the actual design applications. This approach is consistent with NUREG/CR-6698 which states “*the subcritical margin is not intended to account for process upset conditions or for uncertainties associated with a process.*” These issues are properly addressed in the nuclear criticality safety evaluations (NCSEs). These evaluations will demonstrate that the design application falls within the required AOA, that design uncertainties and unknowns are properly and conservatively addressed, that sensitivity to controlled parameters is adequately addressed, and that the criticality models themselves are suitably conservative representations of the actual physical phenomena. In cases where calculated k_{eff} values are shown to be sensitive to controlled parameters, the NCSE will demonstrate the adequacy of the control. In conclusion, an administrative margin of 0.05, selected on the basis of NRC guidance and conservative comparison with applicable precedent, and substantiated through statistical methods, is justified, and is sufficiently conservative to provide for an adequate margin of subcriticality.

Table 7–1 Fuel Cycle and Industry Practice

Facility	Process/Application	Material	Administrative Margin
Framatome Cogema Fuels	Fuel assembly manufacture	Low enriched U	0.05
Westinghouse Columbia Site	Fuel assembly manufacture	Low enriched U	0.02
Nuclear Fuel Services	Fuel processing (solutions, powder, pellets, etc.)	Various U enrichments	0.03 LEU 0.05 HEU
Paducah Uranium Enrichment Plant	Uranium enrichment	Low enriched U	0.02
Rocky Flats	Weapons material processing	Plutonium	0.03
BWXT	Fuel assembly manufacture	Low to high enriched U	0.03 LEU 0.05 HEU
Savannah River Site	a) MTR fuel assemblies b) Pipe overpack material storage c) Mark 42 tube dissolution d) Ion exchange columns with fissile solutions e) DDF-1 package	a) High enriched U b) ^{239}Pu c) ^{239}Pu d) ^{239}Pu solution e) Pu metal and oxide	a) 0.02 b) 0.02 c) 0.05 d) 0.04 e) 0.05
Y-12	Weapons material processing	High enriched U	0.02 – 0.05 ¹
Idaho National Engineering and Environmental Lab	Solutions/spent fuel/powders/pieces	Low to high enriched U, including ^{233}U ; some Pu	0.02 – 0.05 0.05 typical
Hanford Site	Waste tanks packaging and transportation	Various	0.05

¹ Pending final approval of validation document.

Table 7–2 USLSTATS Method 2 Analysis Results

Area of Applicability	Maximum USL-2 Minimum Margin of Subcriticality	Administrative Margin
AOA(5)	0.0239	0.05

8. References

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ATTACHMENT NUMBER 1

Sensitivity Study Results

Table A1-1 Critical experiment with PuO₂-polystyrene with plexiglas reflector at H/Pu=15, cf. Table A4-1b

Case	C (Pu) [g/cm ³]	wt. % ²⁴⁰ Pu	H/Pu	k _{eff}	σ	GEN	NPG	NSK	EALF [eV]
10	1.12	2.2	15	1.0314	0.0007	1500	1000	30	4.12
11	1.12	2.2	15	1.0293	0.0008	1500	1000	7	4.55
12	1.12	2.2	15	1.0270	0.0008	1500	1000	21	5.14
13	1.12	2.2	15	1.0259	0.0007	1500	1000	20	5.44
14	1.12	2.2	15	1.0285	0.0008	1500	1000	7	5.57
15	1.12	2.2	15	1.0271	0.0008	1500	1000	21	5.57
16	1.12	2.2	15	1.0232	0.0008	1500	1000	14	5.15
17	1.05	8.06	15	1.0064	0.0007	1500	1000	3	4.93
18	1.05	8.06	15	1.0114	0.0008	1500	1000	4	6.19
19	1.05	8.06	15	1.0086	0.0007	1500	1000	29	6.47
20	1.05	8.06	15	1.0096	0.0008	1500	1000	176	6.67
21	1.05	8.06	15	1.0088	0.0008	1500	1000	42	6.68
22	1.05	8.06	15	1.0130	0.0007	1500	1000	5	6.42

Table A1-2 PuO₂+ H₂O mixture at H/Pu=15 in the same experimental configuration of Table A1-1

Case	C (Pu) [g/cm ³]	wt. % ²⁴⁰ Pu	H/Pu	k _{eff}	σ	GEN	NPG	NSK	EALF [eV]
10	1.5059	4	15	1.0932	0.0007	1500	1000	7	6.39
11	1.5059	4	15	1.0942	0.0008	1500	1000	17	6.98
12	1.5059	4	15	1.0975	0.0008	1500	1000	73	7.88
13	1.5059	4	15	1.0968	0.0007	1500	1000	13	8.30
14	1.5059	4	15	1.1002	0.0008	1500	1000	75	8.48
15	1.5059	4	15	1.0994	0.0008	1500	1000	8	8.44
16	1.5059	4	15	1.0926	0.0007	1500	1000	11	7.82
17	1.5059	4	15	1.1602	0.0007	1500	1000	21	7.47
18	1.5059	4	15	1.1749	0.0008	1500	1000	23	9.18
19	1.5059	4	15	1.1785	0.0008	1500	1000	64	9.50
20	1.5059	4	15	1.1785	0.0008	1500	1000	16	9.77
21	1.5059	4	15	1.1798	0.0007	1500	1000	37	9.77
22	1.5059	4	15	1.1807	0.0008	1500	1000	29	9.51

Table A1–3 PuO₂F₂+H₂O mixture at H/Pu=15 in the same experimental of
Table A1-1

Case	C (Pu) [g/cm ³]	wt. % ²⁴⁰ Pu	H/Pu	k _{eff}	σ	GEN	NPG	NSK	EALF [eV]
10	1.1842	4	15	1.0085	0.0007	1500	1000	5	4.59
11	1.1842	4	15	1.0052	0.0007	1500	1000	50	5.02
12	1.1842	4	15	1.0020	0.0007	1500	1000	13	5.64
13	1.1842	4	15	0.9987	0.0008	1500	1000	48	5.98
14	1.1842	4	15	1.0017	0.0007	1500	1000	3	6.15
15	1.1842	4	15	0.9994	0.0007	1500	1000	6	6.10
16	1.1842	4	15	0.9977	0.0007	1500	1000	44	5.69
17	1.1842	4	15	1.0763	0.0007	1500	1000	40	5.51
18	1.1842	4	15	1.0826	0.0008	1500	1000	102	6.77
19	1.1842	4	15	1.0822	0.0007	1500	1000	17	7.09
20	1.1842	4	15	1.0810	0.0008	1500	1000	23	7.29
21	1.1842	4	15	1.0817	0.0008	1500	1000	37	7.29
22	1.1842	4	15	1.0853	0.0008	1500	1000	3	7.05

Table A1–4 Pu-oxalate+H₂O mixture at H/Pu=15 in the same experimental configuration of
Table A1-1

Case	C (Pu) [g/cm ³]	wt. % ²⁴⁰ Pu	H/Pu	k _{eff}	σ	GEN	NPG	NSK	EALF [eV]
10	1.0829	4	15	0.9917	0.0008	1500	1000	33	4.14
11	1.0829	4	15	0.9915	0.0007	1500	1000	111	4.56
12	1.0829	4	15	0.9881	0.0007	1500	1000	34	5.15
13	1.0829	4	15	0.9878	0.0007	1500	1000	3	5.45
14	1.0829	4	15	0.9911	0.0007	1500	1000	17	5.62
15	1.0829	4	15	0.9889	0.0007	1500	1000	17	5.66
16	1.0829	4	15	0.9838	0.0008	1500	1000	7	5.17
17	1.0829	4	15	1.0612	0.0009	1500	1000	5	4.99
18	1.0829	4	15	1.0713	0.0008	1500	1000	12	6.28
19	1.0829	4	15	1.0710	0.0007	1500	1000	33	6.59
20	1.0829	4	15	1.0715	0.0007	1500	1000	9	6.76
21	1.0829	4	15	1.0709	0.0007	1500	1000	7	6.78
22	1.0829	4	15	1.0747	0.0008	1500	1000	19	6.49

Figure A1-1 Normalized flux in an infinite full water reflected slab for two dry Pu compounds (H/Pu=0.04) in the range of 1.E02 eV < Energy < 1.E07 eV

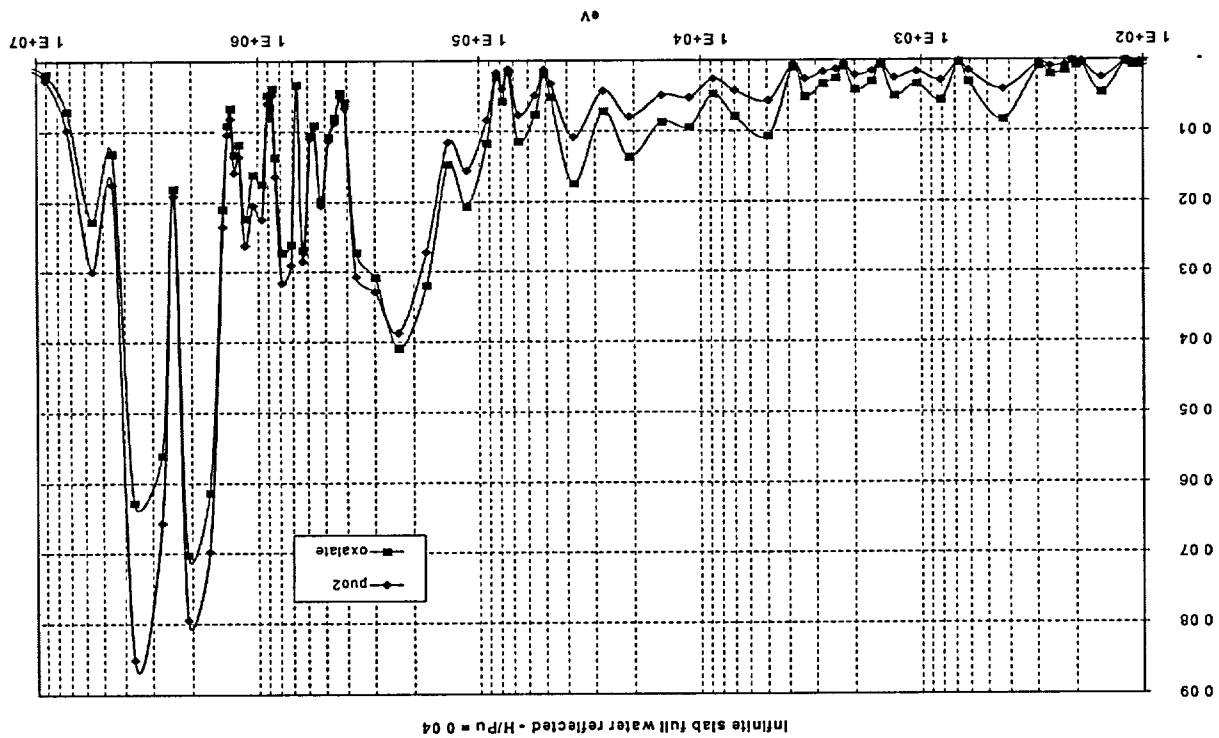
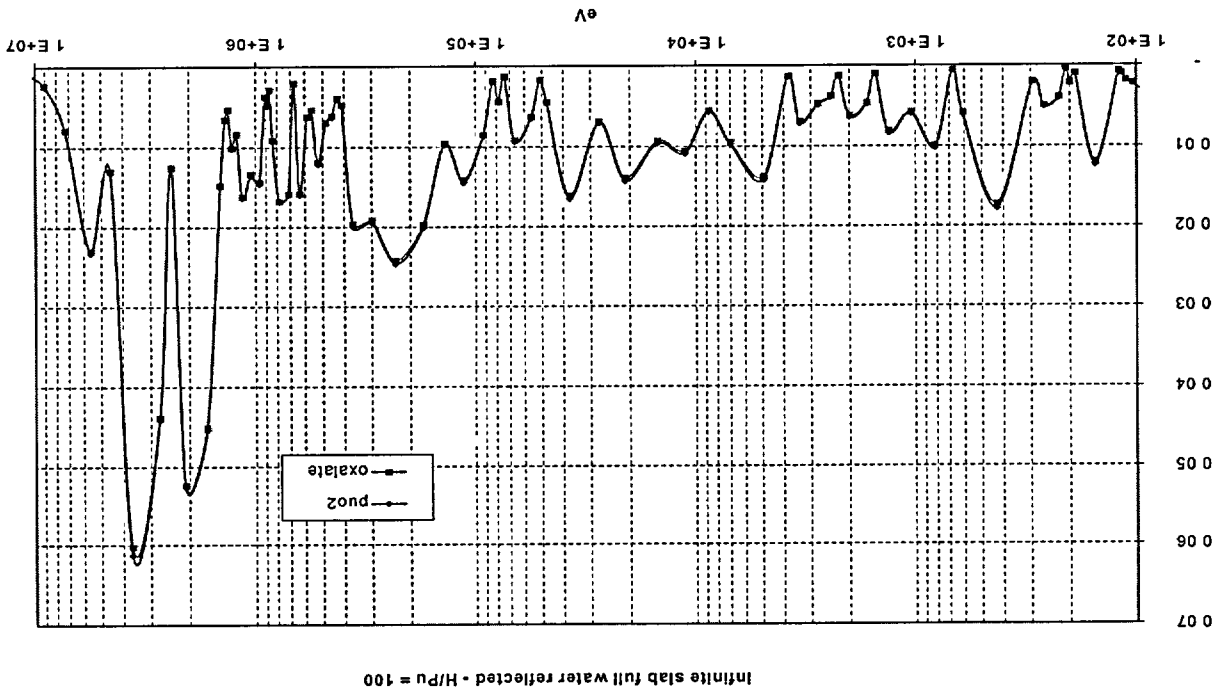


Figure A1-2 Normalized flux in an infinite full water reflected slab for two Pu compounds in water (H/Pu=100) in the range of 1.E02 eV < Energy < 1.E07 eV



**ATTACHMENT NUMBER 2
REACTIVITY BOUNDING FISSILE MEDIUM RESULTS**

Table A2–1 k_{eff} -values of an infinite slab 6 cm thick, full water reflected, filled with Pu compounds of MFFF versus H/Pu ratio – XSDRNPM calculations

H/Pu	PuO ₂ powder 11.46 g/cm ³	PuO ₂ F ₂ « standard salt » 4.187 g/cm ³	Pu-oxalate. 6H ₂ O (*) 2.70 g/cm ³	Pu-oxalate. 2H ₂ O (*) 3.05 g/cm ³	Pu-oxalate. 0H ₂ O 3.50 g/cm ³	Pu(III)-nitrate. 5H ₂ O (*) 2.15 g/cm ³
0.01	1.4724	0.9912	-	-	0.8605	-
0.05	1.4641	0.9905	-	-	0.8606	-
0.1	1.4540	0.9895	-	-	0.8608	-
0.5	1.3875	0.9826	-	-	0.8628	-
1	1.3289	0.9757	-	-	0.8655	-
1.674	1.2735	0.9684	-	-	0.8691	-
3	1.2030	0.9579	-	-	0.8759	-
4	1.1676	0.9556	-	0.8914	0.8804	-
5	1.1407	0.9538	-	0.8949	0.8844	-
5.973	1.1202	0.9556	-	0.8979	0.8878	-
10	1.0676	0.9617	-	0.9073	0.8989	0.9018
12	1.0521	0.9642	0.9456	0.9109	0.9031	0.9057
15	1.0356	0.9676	0.9462	0.9155	0.9084	0.9104
20	1.0185	0.9776	0.9476	0.9216	0.9155	0.9171
30	1.0013	0.9858	0.9506	0.9306	0.9258	0.9265
40	0.9933	0.9817	0.9534	0.9369	0.9329	0.9331
50	0.9887	0.9796	0.9556	0.9415	0.9380	0.9378
60	0.9856	0.9782	0.9572	0.9448	0.9418	0.9413
70	0.9832	0.9770	0.9582	0.9472	0.9445	0.9437
80	0.9811	0.9758	0.9588	0.9488	0.9463	0.9453
90	0.9791	0.9746	0.9589	0.9498	0.9475	0.9463
100	0.9772	0.9733	0.9586	0.9502	0.9481	0.9468
125	0.9721	0.9693	0.9567	0.9496	0.9479	0.9462
150	0.9665	0.9644	0.9533	0.9471	0.9456	0.9438
200	0.9537	0.9528	0.9434	0.9386	0.9373	0.9352
300	0.9248	0.9249	0.9175	0.9141	0.9132	0.9108
500	0.8635	0.8618	0.8590	0.8568	0.8562	0.8538
700	0.8057	0.8045	0.8024	0.8009	0.8005	0.7982
900	0.7536	0.7526	0.7510	0.7498	0.7495	0.7475
1000	0.7296	0.7288	0.7274	0.7263	0.7260	0.7240
1300	0.6655	0.6649	0.6638	0.6630	0.6628	0.6612
1500	0.6284	0.6279	0.6269	0.6263	0.6261	0.6246

(*) No values below the minimum H/Pu corresponding to the number of crystalline water in these Pu compounds

ATTACHMENT NUMBER 3

BENCHMARKS USED - AOA(5)

ICSBEP PUO₂ POWDER BENCHMARKS

The ICSBEP Handbook [5] includes a number of experiments relevant to PuO₂ powder applications. The list below provides the reasoning for inclusion of each candidate experiment.

- PU-COMP-MIX-001:** All the experiments are selected. The input files are directly obtained from the Handbook and translated to a CSAS26 input file using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-COMP-MIX-002:** All the experiments are selected. The input files are directly obtained from the Handbook and translated to a CSAS26 input file using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-001:** All the experiments are selected. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-008:** All the experiments are selected. The ICSBEP calculated keff are not in good agreement with the experimental keff but this benchmark is interesting because of the concrete reflection. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-014:** All the experiments are selected. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-015:** All the experiments are selected. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-016:** All the experiments are selected. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.
- PU-SOL-THERM-017:** All the experiments are selected. The input file are directly obtained from the Handbook and translated to CSAS26 using the c5toc6 program. The 27 group library is replaced by the 238 group library.

ATTACHMENT NUMBER 4

CRITICALITY CALCULATION RESULTS FOR AOA(5)

Table A4-1: SCALE 4.4a calculations on PC

Experiment	H/Pu	²⁴⁰ Pu	Exp. k_{eff}	Exp. Uncertainty	CSAS26 238GROUP k_{eff}	σ	EALF	GEN	NPG	NSK
PU-COMP-MIXED-001										
Case 2	5	11.46	1	0.0033	1.0204	0.0007	1.75E+03	1503	1000	15
Case 3	15	2.2	0.999	0.0047	1.0163	0.0009	3.27E+01	1503	1000	5
Case 5	49.6	18.35	0.9989	0.0053	1.0077	0.0009	1.55E+00	1503	1000	44
PU-COMP-MIXED-002										
Case 1	0.04	18.35	0.999	0.0045	1.0334	0.0007	4.90E+03	1503	1000	3
Case 2	0.04	18.35	0.999	0.0045	1.0302	0.0007	4.20E+03	1503	1000	51
Case 3	0.04	18.35	0.999	0.0045	1.0266	0.0008	3.46E+03	1503	1000	42
Case 4	0.04	18.35	0.999	0.0045	1.0207	0.0007	2.60E+03	1503	1000	7
Case 5	0.04	18.35	0.999	0.0045	1.0163	0.0007	1.87E+03	1503	1000	78
Case 6	5	11.46	1	0.0043	1.0237	0.0007	9.21E+01	1503	1000	7
Case 7	5	11.46	1	0.0043	1.0212	0.0008	8.42E+01	1503	1000	11
Case 8	5	11.46	1	0.0043	1.0214	0.0008	6.79E+01	1503	1000	8
Case 9	5	11.46	1	0.0043	1.0223	0.0007	5.70E+01	1503	1000	3
Case 10	15	2.2	1	0.0043	1.0314	0.0007	4.12E+00	1503	1000	30
Case 11	15	2.2	1	0.0043	1.0293	0.0008	4.55E+00	1503	1000	7
Case 12	15	2.2	1	0.0043	1.027	0.0008	5.14E+00	1503	1000	21
Case 13	15	2.2	1	0.0043	1.0259	0.0007	5.44E+00	1503	1000	20
Case 14	15	2.2	1	0.0043	1.0285	0.0008	5.57E+00	1503	1000	7
Case 15	15	2.2	1	0.0043	1.0271	0.0008	5.57E+00	1503	1000	21
Case 16	15	2.2	1	0.0043	1.0232	0.0008	5.15E+00	1503	1000	14
Case 17	15	8.06	0.9988	0.0043	1.0064	0.0007	4.93E+00	1503	1000	3
Case 18	15	8.06	0.9988	0.0043	1.0114	0.0008	6.19E+00	1503	1000	4
Case 19	15	8.06	0.9988	0.0043	1.0086	0.0007	6.47E+00	1503	1000	29
Case 20	15	8.06	0.9988	0.0043	1.0096	0.0008	6.67E+00	1503	1000	176
Case 21	15	8.06	0.9988	0.0043	1.0088	0.0008	6.68E+00	1503	1000	42
Case 22	15	8.06	0.9988	0.0043	1.0130	0.0007	6.42E+00	1503	1000	5
Case 23	49.6	18.35	1	0.0045	1.0079	0.0007	6.86E-01	1503	1000	7
Case 24	49.6	18.35	1	0.0045	1.0100	0.0008	6.97E-01	1503	1000	9
Case 25	49.6	18.35	1	0.0045	1.0086	0.0008	7.06E-01	1503	1000	42
Case 26	49.6	18.35	1	0.0045	1.0101	0.0007	7.13E-01	1503	1000	66
Case 27	49.6	18.35	1	0.0045	1.0105	0.0007	7.23E-01	1503	1000	14
Case 28	49.6	18.35	1	0.0045	1.0101	0.0008	7.29E-01	1503	1000	49
Case 29	49.6	18.35	1	0.0045	1.0124	0.0008	7.36E-01	1503	1000	5

GEN : = Number of generations

NPG : = Number of neutrons per generation

NSK : = Number of generations skipped prior to collecting data



Table A4-2: SCALE 4.4a calculations on PC

Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k _{eff}	Exp. Uncertainty	CSAS26 238GROUP k _{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-001											
Case 3	119.00	205.14	4.67	1.0000	0.005	1.0115	0.0008	1.35E-01	1503	1000	17
Case 4	132.00	180.97	4.67	1.0000	0.005	1.0059	0.0008	1.51E-01	1503	1000	48
Case 5	140.00	171.21	4.67	1.0000	0.005	1.0092	0.0008	1.60E-01	1503	1000	42
Case 6	268.70	86.66	4.67	1.0000	0.005	1.0087	0.0008	3.47E-01	1503	1000	61

Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k _{eff}	Exp. Uncertainty	CSAS26 238GROUP k _{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-008											
Case 9	232	85.03	4.67	1.0000	0.0061	1.0071	0.0008	5.49E-01	1503	1000	24
Case 22	232	88.43	4.67	1.0000	0.0061	0.9948	0.0008	5.20E-01	1503	1000	10

GEN : = Number of generations

NPG : = Number of neutrons per generation

NSK : = Number of generations skipped prior to collecting data



Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k_{eff}	Exp. Uncertainty	CSAS26 238GROUP k_{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-014											
Case 1	115.10	210.18	4.23	0.9980	0.0032	1.0071	0.0008	1.68E-01	1503	1000	31
Case 2	115.10	210.18	4.23	0.9980	0.0032	1.0059	0.0009	1.67E-01	1503	1000	28
Case 3	115.10	210.18	4.23	0.9980	0.0032	1.0080	0.0009	1.67E-01	1503	1000	11
Case 4	115.10	210.18	4.23	0.9980	0.0032	1.0060	0.0008	1.67E-01	1503	1000	22
Case 5	115.10	210.18	4.23	0.9980	0.0032	1.0074	0.0009	1.67E-01	1503	1000	35
Case 6	115.10	210.18	4.23	0.9980	0.0032	1.0060	0.0009	1.67E-01	1503	1000	4
Case 7	115.10	210.18	4.23	0.9980	0.0032	1.0059	0.0009	1.68E-01	1503	1000	29
Case 8	115.10	210.18	4.23	0.9980	0.0032	1.0055	0.0008	1.68E-01	1503	1000	23
Case 9	115.10	210.18	4.23	0.9980	0.0032	1.0052	0.0008	1.67E-01	1503	1000	9
Case 10	115.10	210.18	4.23	0.9980	0.0032	1.0038	0.0009	1.67E-01	1503	1000	9
Case 11	115.10	210.18	4.23	0.9980	0.0032	1.0053	0.0008	1.67E-01	1503	1000	7
Case 12	115.10	210.18	4.23	0.9980	0.0032	1.0070	0.0009	1.67E-01	1503	1000	58
Case 13	115.10	210.18	4.23	0.9980	0.0043	1.0077	0.0008	1.68E-01	1503	1000	3
Case 14	115.10	210.18	4.23	0.9980	0.0043	1.0043	0.0009	1.68E-01	1503	1000	99
Case 15	115.10	210.18	4.23	0.9980	0.0043	1.0070	0.0008	1.67E-01	1503	1000	10
Case 16	115.10	210.18	4.23	0.9980	0.0043	1.0057	0.0009	1.67E-01	1503	1000	7
Case 17	115.10	210.18	4.23	0.9980	0.0043	1.0055	0.0009	1.67E-01	1503	1000	5
Case 18	115.10	210.18	4.23	0.9980	0.0043	1.0080	0.0009	1.68E-01	1503	1000	7
Case 19	115.10	210.18	4.23	0.9980	0.0043	1.0049	0.0010	1.68E-01	1503	1000	9
Case 20	115.10	210.18	4.23	0.9980	0.0043	1.0068	0.0009	1.67E-01	1503	1000	114
Case 21	115.10	210.18	4.23	0.9980	0.0043	1.0063	0.0008	1.67E-01	1503	1000	22
Case 22	115.10	210.18	4.23	0.9980	0.0043	1.0060	0.0009	1.67E-01	1503	1000	4
Case 23	115.10	210.18	4.23	0.9980	0.0043	1.0053	0.0009	1.67E-01	1503	1000	28
Case 24	115.10	210.18	4.23	0.9980	0.0043	1.0082	0.0008	1.69E-01	1503	1000	36
Case 25	115.10	210.18	4.23	0.9980	0.0043	1.0042	0.0009	1.68E-01	1503	1000	65
Case 26	115.10	210.18	4.23	0.9980	0.0043	1.0068	0.0009	1.67E-01	1503	1000	20
Case 27	115.10	210.18	4.23	0.9980	0.0043	1.0059	0.0009	1.67E-01	1503	1000	70
Case 28	115.10	210.18	4.23	0.9980	0.0043	1.0053	0.0009	1.67E-01	1503	1000	15
Case 29	115.10	210.18	4.23	0.9980	0.0043	1.0057	0.0009	1.67E-01	1503	1000	5
Case 30	115.10	210.18	4.23	0.9980	0.0043	1.0051	0.0008	1.68E-01	1503	1000	32
Case 31	115.10	210.18	4.23	0.9980	0.0043	1.0039	0.0009	1.68E-01	1503	1000	5
Case 32	115.10	210.18	4.23	0.9980	0.0043	1.0045	0.0009	1.68E-01	1503	1000	23
Case 33	115.10	210.18	4.23	0.9980	0.0043	1.0063	0.0008	1.67E-01	1503	1000	10
Case 34	115.10	210.18	4.23	0.9980	0.0043	1.0043	0.0010	1.68E-01	1503	1000	44
Case 35	115.10	210.18	4.23	0.9980	0.0043	1.0050	0.0010	1.67E-01	1503	1000	12



Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k_{eff}	Exp. Uncertainty	CSAS26 238GROUP k_{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-015											
Case 1	152.50	155.21	4.23	0.9980	0.0038	1.0073	0.0009	2.38E-01	1503	1000	61
Case 2	152.50	155.27	4.23	0.9980	0.0038	1.0080	0.0008	2.37E-01	1503	1000	5
Case 3	152.50	155.27	4.23	0.9980	0.0038	1.0059	0.0009	2.37E-01	1503	1000	3
Case 4	152.50	155.27	4.23	0.9980	0.0038	1.0063	0.0009	2.37E-01	1503	1000	38
Case 5	152.50	155.27	4.23	0.9980	0.0038	1.0047	0.0009	2.37E-01	1503	1000	231
Case 6	152.50	155.27	4.23	0.9980	0.0038	1.0073	0.0008	2.36E-01	1503	1000	40
Case 7	152.50	155.27	4.23	0.9971	0.0047	1.0075	0.0009	2.38E-01	1503	1000	71
Case 8	152.50	155.27	4.23	0.9971	0.0047	1.0070	0.0009	2.37E-01	1503	1000	19
Case 9	152.50	155.27	4.23	0.9971	0.0047	1.0068	0.0008	2.37E-01	1503	1000	15
Case 10	152.50	155.27	4.23	0.9971	0.0047	1.0055	0.0009	2.36E-01	1503	1000	6
Case 11	152.50	155.27	4.23	0.9971	0.0047	1.0040	0.0009	2.38E-01	1503	1000	150
Case 12	152.50	155.27	4.23	0.9971	0.0047	1.0036	0.0008	2.38E-01	1503	1000	4
Case 13	152.50	155.27	4.23	0.9971	0.0047	1.0060	0.0009	2.37E-01	1503	1000	6
Case 14	152.50	155.27	4.23	0.9971	0.0047	1.0067	0.0009	2.36E-01	1503	1000	19
Case 15	152.50	155.27	4.23	0.9971	0.0047	1.0071	0.0008	2.39E-01	1503	1000	22
Case 16	152.50	155.27	4.23	0.9971	0.0047	1.0053	0.0009	2.38E-01	1503	1000	53
Case 17	152.50	155.27	4.23	0.9971	0.0047	1.0062	0.0009	2.37E-01	1503	1000	4

Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k_{eff}	Exp. Uncertainty	CSAS26 238GROUP k_{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-016											
Case 1	152.50	155.27	4.23	0.9980	0.0043	1.0061	0.0009	2.37E-01	1503	1000	3
Case 2	152.50	155.27	4.23	0.9980	0.0043	1.0053	0.0009	2.37E-01	1503	1000	14
Case 3	152.50	155.27	4.23	0.9980	0.0043	1.0071	0.0009	2.37E-01	1503	1000	10
Case 4	152.50	155.27	4.23	0.9980	0.0043	1.0068	0.0009	2.36E-01	1503	1000	16
Case 5	115.10	210.18	4.23	0.9969	0.0038	1.0043	0.0009	1.68E-01	1503	1000	11
Case 6	115.10	210.17	4.23	0.9969	0.0038	1.0044	0.0009	1.67E-01	1503	1000	6
Case 7	115.10	210.17	4.23	0.9969	0.0038	1.0070	0.0009	1.67E-01	1503	1000	13
Case 8	115.10	210.17	4.23	0.9969	0.0038	1.0077	0.0009	1.67E-01	1503	1000	35
Case 9	115.10	210.17	4.23	0.9963	0.0033	1.0059	0.0009	1.66E-01	1503	1000	34
Case 10	115.10	210.17	4.23	0.9963	0.0033	1.0050	0.0010	1.66E-01	1503	1000	6
Case 11	115.10	210.17	4.23	0.9963	0.0033	1.0064	0.0009	1.67E-01	1503	1000	10



Experiment	C(Pu)	H/X	²⁴⁰ Pu [wt. %]	Exp. k_{eff}	Exp. Uncertainty	CSAS26 238GROUP k_{eff}	σ	EALF	GEN	NPG	NSK
PU-SOL-THERM-017											
Case 1	115.10	210.18	4.23	0.9969	0.0038	1.0042	0.0009	1.67E-01	1503	1000	72
Case 2	115.10	210.18	4.23	0.9969	0.0038	1.0057	0.0009	1.67E-01	1503	1000	12
Case 3	115.10	210.18	4.23	0.9969	0.0038	1.0052	0.0009	1.67E-01	1503	1000	27
Case 4	115.10	210.18	4.23	0.9969	0.0038	1.0049	0.0008	1.67E-01	1503	1000	20
Case 5	115.10	210.18	4.23	0.9969	0.0038	1.0062	0.0009	1.67E-01	1503	1000	15
Case 6	115.10	210.18	4.23	0.9969	0.0038	1.0056	0.0009	1.67E-01	1503	1000	8
Case 7	115.10	210.18	4.23	0.9969	0.0038	1.0038	0.0010	1.67E-01	1503	1000	86
Case 8	115.10	210.18	4.23	0.9969	0.0038	1.0052	0.0010	1.67E-01	1503	1000	25
Case 9	115.10	210.18	4.23	0.9969	0.0038	1.0059	0.0010	1.67E-01	1503	1000	17
Case 10	115.10	210.18	4.23	0.9969	0.0038	1.0047	0.0009	1.68E-01	1503	1000	20
Case 11	115.10	210.18	4.23	0.9969	0.0038	1.0058	0.0009	1.67E-01	1503	1000	36
Case 12	115.10	210.18	4.23	0.9969	0.0038	1.0056	0.0010	1.67E-01	1503	1000	25
Case 13	115.10	210.18	4.23	0.9969	0.0038	1.0060	0.0009	1.67E-01	1503	1000	17
Case 14	115.10	210.18	4.23	0.9969	0.0038	1.0061	0.0009	1.67E-01	1503	1000	71
Case 15	115.10	210.18	4.23	0.9969	0.0038	1.0071	0.0008	1.67E-01	1503	1000	61
Case 16	115.10	210.18	4.23	0.9969	0.0038	1.0070	0.0009	1.67E-01	1503	1000	52
Case 17	115.10	210.18	4.23	0.9969	0.0038	1.0057	0.0009	1.67E-01	1503	1000	39
Case 18	115.10	210.18	4.23	0.9969	0.0038	1.0064	0.0009	1.67E-01	1503	1000	14

ATTACHMENT NUMBER 5

**OUTPUT LISTING OF USLSTATS V1.0
FOR PC CALCULATIONS**



Figure A5-1: USLSTATS output listing for AOA(5) Group 1: PuO₂ powder k_{eff} versus EALF as trending parameter, SCALE 4.4a on PC

uslstats: a utility to calculate upper subcritical
limits for criticality safety applications

Version 1.3.7, May 18, 1999
Oak Ridge National Laboratory

Input to statistical treatment from file:ealf.in

Title: PuO2 powder EALF

Proportion of the population = .999
Confidence of fit = .950
Confidence on proportion = .950
Number of observations = 32
Minimum value of closed band = 0.00
Maximum value of closed band = 0.00
Administrative margin = 0.05

independent variable - x	dependent variable - y	deviation in y	independent variable - x	dependent variable - y	deviation in y
4.90213E+03	1.03443E+00	4.65296E-03	4.92600E+00	1.00761E+00	4.45533E-03
4.20132E+03	1.03123E+00	4.65296E-03	6.19100E+00	1.01262E+00	4.47214E-03
3.46319E+03	1.02763E+00	4.66905E-03	6.46700E+00	1.00981E+00	4.45533E-03
2.60173E+03	1.02172E+00	4.65296E-03	6.67400E+00	1.01081E+00	4.47214E-03
1.87477E+03	1.01732E+00	4.65296E-03	6.68200E+00	1.01001E+00	4.47214E-03
9.20880E+01	1.02370E+00	4.45533E-03	6.42000E+00	1.01422E+00	4.45533E-03
8.42160E+01	1.02120E+00	4.47214E-03	6.86000E-01	1.00790E+00	4.65296E-03
6.78560E+01	1.02140E+00	4.47214E-03	6.97000E-01	1.01000E+00	4.66905E-03
5.69610E+01	1.02230E+00	4.45533E-03	7.06000E-01	1.00860E+00	4.66905E-03
4.12300E+00	1.03140E+00	4.45533E-03	7.13000E-01	1.01010E+00	4.65296E-03
4.55400E+00	1.02930E+00	4.47214E-03	7.23000E-01	1.01050E+00	4.65296E-03
5.13800E+00	1.02700E+00	4.47214E-03	7.29000E-01	1.01010E+00	4.66905E-03
5.43700E+00	1.02590E+00	4.45533E-03	7.36000E-01	1.01240E+00	4.66905E-03
5.57000E+00	1.02850E+00	4.47214E-03	1.74727E+03	1.02040E+00	3.37343E-03
5.57100E+00	1.02710E+00	4.47214E-03	3.26850E+01	1.01732E+00	4.78539E-03
5.15100E+00	1.02320E+00	4.47214E-03	1.54800E+00	1.00881E+00	5.37587E-03

WARNING *** the test for normal may be unreliable due to insufficient data.

chi = 8.0000 (upper bound = 9.49). The data tests normal.

Output from statistical treatment

PuO2 powder EALF

Number of data points (n)	32
Linear regression, k(X)	1.0167 + (3.1025E-06)*X
Confidence on fit (1-gamma) [input]	95.0%
Confidence on proportion (alpha) [input]	95.0%
Proportion of population falling above	
lower tolerance interval (rho) [input]	99.9%
Minimum value of X	0.6860
Maximum value of X	4902.1300
Average value of X	600.11431
Average value of k	1.01858
Minimum value of k	1.00761
Variance of fit, s(k,X)^2	5.4730E-05
Within variance, s(w)^2	2.0709E-05
Pooled variance, s(p)^2	7.5439E-05
Pooled std deviation, s(p)	8.6855E-03
C(alpha,rho)*s(p)	4.6595E-02
student-t @ (n-2,1-gamma)	1.69700E+00
Confidence band width, W	1.7218E-02
Minimum margin of subcriticality, C*s(p)-W	2.9376E-02

Upper subcritical limits: (0.68600 <= X <= 4902.1)



USL Method 1 (Confidence Band with
Administrative Margin) USL1 = 0.9328 (0.68600 < X < 4902.1)

USL Method 2 (Single-Sided Uniform
Width Closed Interval Approach) USL2 = 0.9534 (0.68600 < X < 4902.1)

USLs Evaluated Over Range of Parameter X.

**** ***** ** ***** **

X	6.86E-1	7.01E+2	1.40E+3	2.10E+3	2.80E+3	3.50E+3	4.20E+3	4.90E+3
USL-1:	0.9328	0.9328	0.9328	0.9328	0.9328	0.9328	0.9328	0.9328
USL-2:	0.9534	0.9534	0.9534	0.9534	0.9534	0.9534	0.9534	0.9534

Thus spake USLSTATS
Finis.

Figure A5-2: USLSTATS output listing for AOA(5) Group 1: PuO₂ powder k_{eff} versus H/Pu as trending parameter, SCALE 4.4a on PC

```

uslstats: a utility to calculate upper subcritical
          limits for criticality safety applications

*****
                          Version 1.3.7, May 18, 1999
                          Oak Ridge National Laboratory
*****

Input to statistical treatment from file:hpu.in

Title: PuO2 powder H/Pu

Proportion of the population = .999
Confidence of fit             = .950
Confidence on proportion     = .950
Number of observations       = 32
Minimum value of closed band = 0.00
Maximum value of closed band = 0.00
Administrative margin        = 0.05


independent   dependent   deviation   independent   dependent   deviation
variable - x   variable - y   in y        variable - x   variable - y   in y

4.00000E-02    1.03443E+00    4.65296E-03    1.50000E+01    1.00761E+00    4.45533E-03
4.00000E-02    1.03123E+00    4.65296E-03    1.50000E+01    1.01262E+00    4.47214E-03
4.00000E-02    1.02763E+00    4.66905E-03    1.50000E+01    1.00981E+00    4.45533E-03
4.00000E-02    1.02172E+00    4.65296E-03    1.50000E+01    1.01081E+00    4.47214E-03
4.00000E-02    1.01732E+00    4.65296E-03    1.50000E+01    1.01001E+00    4.47214E-03
5.00000E+00    1.02370E+00    4.45533E-03    1.50000E+01    1.01422E+00    4.45533E-03
5.00000E+00    1.02120E+00    4.47214E-03    4.96000E+01    1.00790E+00    4.65296E-03
5.00000E+00    1.02140E+00    4.47214E-03    4.96000E+01    1.01000E+00    4.66905E-03
5.00000E+00    1.02230E+00    4.45533E-03    4.96000E+01    1.00860E+00    4.66905E-03
1.50000E+01    1.03140E+00    4.45533E-03    4.96000E+01    1.01010E+00    4.65296E-03
1.50000E+01    1.02930E+00    4.47214E-03    4.96000E+01    1.01050E+00    4.65296E-03
1.50000E+01    1.02700E+00    4.47214E-03    4.96000E+01    1.01010E+00    4.66905E-03
1.50000E+01    1.02590E+00    4.45533E-03    4.96000E+01    1.01240E+00    4.66905E-03
1.50000E+01    1.02850E+00    4.47214E-03    5.00000E+00    1.02040E+00    3.37343E-03
1.50000E+01    1.02710E+00    4.47214E-03    1.50000E+01    1.01732E+00    4.78539E-03
1.50000E+01    1.02320E+00    4.47214E-03    4.96000E+01    1.00881E+00    5.37587E-03


WARNING *** the test for normal may be unreliable due to insufficient data.

chi = 8.0000 (upper bound = 9.49). The data tests normal.


Output from statistical treatment

PuO2 powder H/Pu

Number of data points (n)                32
Linear regression, k(X)                   1.0246 + (-3.0367E-04)*X
Confidence on fit (1-gamma) [input]       95.0%
Confidence on proportion (alpha) [input]   95.0%
Proportion of population falling above
lower tolerance interval (rho) [input]     99.9%
Minimum value of X                        0.0400
Maximum value of X                        49.6000
Average value of X                        19.75000
Average value of k                        1.01858
Minimum value of k                        1.00761
Variance of fit, s(k,X)^2                 4.0344E-05
Within variance, s(w)^2                   2.0709E-05
Pooled variance, s(p)^2                   6.1053E-05
Pooled std. deviation, s(p)               7.8136E-03
C(alpha,rho)*s(p)                         3.7933E-02
student-t @ (n-2,1-gamma)                 1.69700E+00
Confidence band width, W                  1.4010E-02
Minimum margin of subcriticality, C*s(p)-W 2.3923E-02

Upper subcritical limits: ( 4.00000E-02 <= X <= 49.600 )
*****

```

USL Method 1 (Confidence Band with
Administrative Margin) USL1 = 0.9360 (4.00000E-2< X < 49.600)

USL Method 2 (Single-Sided Uniform
Width Closed Interval Approach) USL2 = 0.9621 (4.00000E-2< X < 49.600)

USLs Evaluated Over Range of Parameter X:
**** ***** **

X	4.00E-2	7.12E+0	1.42E+1	2.13E+1	2.84E+1	3.54E+1	4.25E+1	4.96E+1
USL-1:	0.9360	0.9360	0.9360	0.9360	0.9360	0.9360	0.9360	0.9360
USL-2:	0.9621	0.9621	0.9621	0.9621	0.9621	0.9621	0.9621	0.9621

Thus spake USLSTATS
Finis.

Figure A5-3: USLSTATS output listing for AOA(5) Group 1: PuO₂ powder k_{eff} versus ²⁴⁰Pu as trending parameter, SCALE 4.4a on PC

uslstats a utility to calculate upper subcritical
limits for criticality safety applications

Version 1.3.7, May 18, 1999
Oak Ridge National Laboratory

Input to statistical treatment from file: %pu.in

Title: PuO2 powder %Pu

Proportion of the population = .999
Confidence of fit = .950
Confidence on proportion = .950
Number of observations = 32
Minimum value of closed band = 0.00
Maximum value of closed band = 0.00
Administrative margin = 0.05

independent variable - x	dependent variable - y	deviation in y	independent variable - x	dependent variable - y	deviation in y
1.83500E+01	1.03443E+00	4.65296E-03	8.06000E+00	1.00761E+00	4.45533E-03
1.83500E+01	1.03123E+00	4.65296E-03	8.06000E+00	1.01262E+00	4.47214E-03
1.83500E+01	1.02763E+00	4.66905E-03	8.06000E+00	1.00981E+00	4.45533E-03
1.83500E+01	1.02172E+00	4.65296E-03	8.06000E+00	1.01081E+00	4.47214E-03
1.83500E+01	1.01732E+00	4.65296E-03	8.06000E+00	1.01001E+00	4.47214E-03
1.14600E+01	1.02370E+00	4.45533E-03	8.06000E+00	1.01422E+00	4.45533E-03
1.14600E+01	1.02120E+00	4.47214E-03	1.83500E+01	1.00790E+00	4.65296E-03
1.14600E+01	1.02140E+00	4.47214E-03	1.83500E+01	1.01000E+00	4.66905E-03
1.14600E+01	1.02230E+00	4.45533E-03	1.83500E+01	1.00860E+00	4.66905E-03
2.20000E+00	1.03140E+00	4.45533E-03	1.83500E+01	1.01010E+00	4.65296E-03
2.20000E+00	1.02930E+00	4.47214E-03	1.83500E+01	1.01050E+00	4.65296E-03
2.20000E+00	1.02700E+00	4.47214E-03	1.83500E+01	1.01010E+00	4.66905E-03
2.20000E+00	1.02590E+00	4.45533E-03	1.83500E+01	1.01240E+00	4.66905E-03
2.20000E+00	1.02850E+00	4.47214E-03	1.14600E+01	1.02040E+00	3.37343E-03
2.20000E+00	1.02710E+00	4.47214E-03	2.20000E+00	1.01732E+00	4.78539E-03
2.20000E+00	1.02320E+00	4.47214E-03	1.83500E+01	1.00881E+00	5.37587E-03

WARNING *** the test for normal may be unreliable due to insufficient data.

chi = 8.0000 (upper bound = 9.49). The data tests normal.

Output from statistical treatment

PuO2 powder %Pu

Number of data points (n) 32
Linear regression, k(X) 1.0237 + (-4.5199E-04)*X
Confidence on fit (1-gamma) [input] 95.0%
Confidence on proportion (alpha) [input] 95.0%
Proportion of population falling above
lower tolerance interval (rho) [input] 99.9%
Minimum value of X 2.2000
Maximum value of X 18.3500
Average value of X 11.30656
Average value of k 1.01858
Minimum value of k 1.00761
Variance of fit, s(k,X)^2 6.3200E-05
Within variance, s(w)^2 2.0709E-05
Pooled variance, s(p)^2 8.3909E-05
Pooled std. deviation, s(p) 9.1602E-03
C(alpha,rho)*s(p) 4.3914E-02
student-t @ (n-2,1-gamma) 1.69700E+00
Confidence band width, W 1.6242E-02
Minimum margin of subcriticality, C*s(p)-W 2.7672E-02

Upper subcritical limits: (2.2000 <= X <= 18.350)

USL Method 1 (Confidence Band with
Administrative Margin) USL1 = 0.9338 (2.2000 < X < 18.350)

USL Method 2 (Single-Sided Uniform
Width Closed Interval Approach) USL2 = 0.9561 (2.2000 < X < 18.350)

USLs Evaluated Over Range of Parameter X

**** ***** ** ***** **

X:	2.20E+0	4.51E+0	6.81E+0	9.12E+0	1.14E+1	1.37E+1	1.60E+1	1.84E+1
USL-1:	0.9338	0.9338	0.9338	0.9338	0.9338	0.9338	0.9338	0.9338
USL-2:	0.9561	0.9561	0.9561	0.9561	0.9561	0.9561	0.9561	0.9561

Thus spake USLSTATS
Finis.

Figure A5-4: USLSTATS output listing for AOA(5) Group 2: Pu Nitrate k_{eff} versus EALF as trending parameter, SCALE 4.4a on PC

uslstats: a utility to calculate upper subcritical
limits for criticality safety applications

Version 1.3.7, May 18, 1999
Oak Ridge National Laboratory

Input to statistical treatment from file ealfPC

Title: gr2 PC EALF

Proportion of the population = .999
Confidence of fit = .950
Confidence on proportion = .950
Number of observations = 87
Minimum value of closed band = 0.00
Maximum value of closed band = 0.00
Administrative margin = 0.05

independent variable - x	dependent variable - y	deviation in y	independent variable - x	dependent variable - y	deviation in y
1.34839E-01	1.01150E+00	5.06360E-03	2.36831E-01	1.00830E+00	3.90513E-03
1.50757E-01	1.00590E+00	5.06360E-03	2.36587E-01	1.00670E+00	3.90513E-03
1.59544E-01	1.00920E+00	5.06360E-03	2.36202E-01	1.00930E+00	3.88330E-03
3.46678E-01	1.00870E+00	5.06360E-03	2.38483E-01	1.01040E+00	4.78539E-03
5.48519E-01	1.00710E+00	6.15224E-03	2.37274E-01	1.00990E+00	4.78539E-03
5.20183E-01	9.94800E-01	6.15224E-03	2.36695E-01	1.00970E+00	4.76760E-03
1.67812E-01	1.00910E+00	3.29849E-03	2.36058E-01	1.00840E+00	4.78539E-03
1.67457E-01	1.00790E+00	3.32415E-03	2.38161E-01	1.00690E+00	4.78539E-03
1.66807E-01	1.01000E+00	3.32415E-03	2.37891E-01	1.00650E+00	4.76760E-03
1.67233E-01	1.00800E+00	3.29849E-03	2.36841E-01	1.00890E+00	4.78539E-03
1.66668E-01	1.00940E+00	3.32415E-03	2.36296E-01	1.00960E+00	4.78539E-03
1.66668E-01	1.00800E+00	3.32415E-03	2.38548E-01	1.01000E+00	4.76760E-03
1.68142E-01	1.00790E+00	3.32415E-03	2.38276E-01	1.00820E+00	4.78539E-03
1.67636E-01	1.00750E+00	3.29849E-03	2.37141E-01	1.00910E+00	4.78539E-03
1.67279E-01	1.00720E+00	3.29849E-03	2.37431E-01	1.00810E+00	4.39318E-03
1.67337E-01	1.00580E+00	3.32415E-03	2.36989E-01	1.00730E+00	4.39318E-03
1.66955E-01	1.00730E+00	3.29849E-03	2.36537E-01	1.00910E+00	4.39318E-03
1.66546E-01	1.00900E+00	3.32415E-03	2.36458E-01	1.00880E+00	4.39318E-03
1.68373E-01	1.00970E+00	4.37379E-03	1.67942E-01	1.00740E+00	3.90513E-03
1.67903E-01	1.00630E+00	4.39318E-03	1.67467E-01	1.00750E+00	3.90513E-03
1.67166E-01	1.00900E+00	4.37379E-03	1.67208E-01	1.01010E+00	3.90513E-03
1.66898E-01	1.00770E+00	4.39318E-03	1.66786E-01	1.01080E+00	3.90513E-03
1.66630E-01	1.00750E+00	4.39318E-03	1.65519E-01	1.00960E+00	3.42053E-03
1.68449E-01	1.01000E+00	4.39318E-03	1.66435E-01	1.00870E+00	3.44819E-03
1.67790E-01	1.00690E+00	4.41475E-03	1.67131E-01	1.01010E+00	3.42053E-03
1.66997E-01	1.00880E+00	4.39318E-03	1.66869E-01	1.00730E+00	3.90513E-03
1.66691E-01	1.00830E+00	4.37379E-03	1.66968E-01	1.00880E+00	3.90513E-03
1.66682E-01	1.00800E+00	4.39318E-03	1.67120E-01	1.00830E+00	3.90513E-03
1.66969E-01	1.00730E+00	4.39318E-03	1.67064E-01	1.00800E+00	3.88330E-03
1.68612E-01	1.01020E+00	4.37379E-03	1.67223E-01	1.00930E+00	3.90513E-03
1.67699E-01	1.00620E+00	4.39318E-03	1.67150E-01	1.00870E+00	3.90513E-03
1.67331E-01	1.00880E+00	4.39318E-03	1.67269E-01	1.00690E+00	3.92938E-03
1.66818E-01	1.00790E+00	4.39318E-03	1.67189E-01	1.00830E+00	3.92938E-03
1.66664E-01	1.00730E+00	4.39318E-03	1.67010E-01	1.00900E+00	3.92938E-03
1.66641E-01	1.00770E+00	4.39318E-03	1.67538E-01	1.00780E+00	3.90513E-03
1.68215E-01	1.00710E+00	4.37379E-03	1.66900E-01	1.00890E+00	3.90513E-03
1.68357E-01	1.00590E+00	4.39318E-03	1.66967E-01	1.00870E+00	3.92938E-03
1.67772E-01	1.00650E+00	4.39318E-03	1.67078E-01	1.00910E+00	3.90513E-03
1.67416E-01	1.00830E+00	4.37379E-03	1.67248E-01	1.00920E+00	3.90513E-03
1.67630E-01	1.00630E+00	4.41475E-03	1.66704E-01	1.01020E+00	3.88330E-03
1.67462E-01	1.00700E+00	4.41475E-03	1.66824E-01	1.01010E+00	3.90513E-03
2.37509E-01	1.00930E+00	3.90513E-03	1.66972E-01	1.00880E+00	3.90513E-03
2.36912E-01	1.01000E+00	3.88330E-03	1.66697E-01	1.00950E+00	3.90513E-03
2.36543E-01	1.00790E+00	3.90513E-03			

chi = 9.3793 (upper bound = 9.49). The data tests normal.

Output from statistical treatment



gr2 PC EALF

Number of data points (n)	87
Linear regression, k(X)	1.0108 + (-1.3126E-02)*X
Confidence on fit (1-gamma) [input]	95.0%
Confidence on proportion (alpha) [input]	95.0%
Proportion of population falling above lower tolerance interval (rho) [input]	99.9%
Minimum value of X	0.1348
Maximum value of X	0.5485
Average value of X	0.19394
Average value of k	1.00824
Minimum value of k	0.99480
Variance of fit, s(k,X)^2	3.0167E-06
Within variance, s(w)^2	1.7752E-05
Pooled variance, s(p)^2	2.0769E-05
Pooled std. deviation, s(p)	4.5573E-03
C(alpha,rho)*s(p)	2.2118E-02
student-t @ (n-2,1-gamma)	1.66558E+00
Confidence band width, W	8.9068E-03
Minimum margin of subcriticality, C*s(p)-W	1.3211E-02

Upper subcritical limits (0.13484 <= X <= 0.54852)

USL Method 1 (Confidence Band with Administrative Margin) USL1 = 0.9411 (0.13484 < X < 0.54852)

USL Method 2 (Single-Sided Uniform Width Closed Interval Approach) USL2 = 0.9779 (0.13484 < X < 0.54852)

USLs Evaluated Over Range of Parameter X:

	X: 1.35E-1	1.94E-1	2.53E-1	3.12E-1	3.71E-1	4.30E-1	4.89E-1	5.49E-1
USL-1:	0.9411	0.9411	0.9411	0.9411	0.9411	0.9411	0.9411	0.9411
USL-2:	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779	0.9779

Thus spake USLSTATS
Finis.

Figure A5-5: USLSTATS output listing for AOA(5) Group 2: Pu Nitrate k_{eff} versus H/Pu as trending parameter, SCALE 4.4a on PC

uslstats: a utility to calculate upper subcritical
limits for criticality safety applications

Version 1.3.7, May 18, 1999
Oak Ridge National Laboratory

Input to statistical treatment from file:hpupc

Title: gr2 PC HPU

Proportion of the population = .999
Confidence of fit = .950
Confidence on proportion = .950
Number of observations = 87
Minimum value of closed band = 0.00
Maximum value of closed band = 0.00
Administrative margin = 0.05

independent variable - x	dependent variable - y	deviation in y	independent variable - x	dependent variable - y	deviation in y
2.05140E+02	1.01150E+00	5.06360E-03	1.55270E+02	1.00830E+00	3.90513E-03
1.80970E+02	1.00590E+00	5.06360E-03	1.55270E+02	1.00670E+00	3.90513E-03
1.71210E+02	1.00920E+00	5.06360E-03	1.55270E+02	1.00930E+00	3.88330E-03
8.66600E+01	1.00870E+00	5.06360E-03	1.55270E+02	1.01040E+00	4.78539E-03
8.50300E+01	1.00710E+00	6.15224E-03	1.55270E+02	1.00990E+00	4.78539E-03
8.84300E+01	9.94800E-01	6.15224E-03	1.55270E+02	1.00970E+00	4.76760E-03
2.10180E+02	1.00910E+00	3.29849E-03	1.55270E+02	1.00840E+00	4.78539E-03
2.10180E+02	1.00790E+00	3.32415E-03	1.55270E+02	1.00690E+00	4.78539E-03
2.10180E+02	1.01000E+00	3.32415E-03	1.55270E+02	1.00650E+00	4.76760E-03
2.10180E+02	1.00800E+00	3.29849E-03	1.55270E+02	1.00890E+00	4.78539E-03
2.10180E+02	1.00940E+00	3.32415E-03	1.55270E+02	1.00960E+00	4.78539E-03
2.10180E+02	1.00800E+00	3.32415E-03	1.55270E+02	1.01000E+00	4.76760E-03
2.10180E+02	1.00790E+00	3.32415E-03	1.55270E+02	1.00820E+00	4.78539E-03
2.10180E+02	1.00750E+00	3.29849E-03	1.55270E+02	1.00910E+00	4.78539E-03
2.10180E+02	1.00720E+00	3.29849E-03	1.55270E+02	1.00810E+00	4.39318E-03
2.10180E+02	1.00580E+00	3.32415E-03	1.55270E+02	1.00730E+00	4.39318E-03
2.10180E+02	1.00730E+00	3.29849E-03	1.55270E+02	1.00910E+00	4.39318E-03
2.10180E+02	1.00900E+00	3.32415E-03	1.55270E+02	1.00880E+00	4.39318E-03
2.10180E+02	1.00970E+00	4.37379E-03	2.10180E+02	1.00740E+00	3.90513E-03
2.10180E+02	1.00630E+00	4.39318E-03	2.10170E+02	1.00750E+00	3.90513E-03
2.10180E+02	1.00900E+00	4.37379E-03	2.10170E+02	1.01010E+00	3.90513E-03
2.10180E+02	1.00770E+00	4.39318E-03	2.10170E+02	1.01080E+00	3.90513E-03
2.10180E+02	1.00750E+00	4.39318E-03	2.10170E+02	1.00960E+00	3.42053E-03
2.10180E+02	1.01000E+00	4.39318E-03	2.10170E+02	1.00870E+00	3.44819E-03
2.10180E+02	1.00690E+00	4.41475E-03	2.10170E+02	1.01010E+00	3.42053E-03
2.10180E+02	1.00880E+00	4.39318E-03	2.10180E+02	1.00730E+00	3.90513E-03
2.10180E+02	1.00830E+00	4.37379E-03	2.10180E+02	1.00880E+00	3.90513E-03
2.10180E+02	1.00800E+00	4.39318E-03	2.10180E+02	1.00830E+00	3.90513E-03
2.10180E+02	1.00730E+00	4.39318E-03	2.10180E+02	1.00800E+00	3.88330E-03
2.10180E+02	1.01020E+00	4.37379E-03	2.10180E+02	1.00930E+00	3.90513E-03
2.10180E+02	1.00620E+00	4.39318E-03	2.10180E+02	1.00870E+00	3.90513E-03
2.10180E+02	1.00880E+00	4.39318E-03	2.10180E+02	1.00690E+00	3.92938E-03
2.10180E+02	1.00790E+00	4.39318E-03	2.10180E+02	1.00830E+00	3.92938E-03
2.10180E+02	1.00730E+00	4.39318E-03	2.10180E+02	1.00900E+00	3.92938E-03
2.10180E+02	1.00770E+00	4.39318E-03	2.10180E+02	1.00780E+00	3.90513E-03
2.10180E+02	1.00710E+00	4.37379E-03	2.10180E+02	1.00890E+00	3.90513E-03
2.10180E+02	1.00590E+00	4.39318E-03	2.10180E+02	1.00870E+00	3.92938E-03
2.10180E+02	1.00650E+00	4.39318E-03	2.10180E+02	1.00910E+00	3.90513E-03
2.10180E+02	1.00830E+00	4.37379E-03	2.10180E+02	1.00920E+00	3.90513E-03
2.10180E+02	1.00630E+00	4.41475E-03	2.10180E+02	1.01020E+00	3.88330E-03
2.10180E+02	1.00700E+00	4.41475E-03	2.10180E+02	1.01010E+00	3.90513E-03
1.55210E+02	1.00930E+00	3.90513E-03	2.10180E+02	1.00880E+00	3.90513E-03
1.55270E+02	1.01000E+00	3.88330E-03	2.10180E+02	1.00950E+00	3.90513E-03
1.55270E+02	1.00790E+00	3.90513E-03			

chi = 9.3793 (upper bound = 9.49). The data tests normal.

Output from statistical treatment

gr2 PC HPU

```

Number of data points (n)                87
Linear regression, k(X)                  1.0054 + ( 1.4797E-05)*X
Confidence on fit (1-gamma) [input]      95.0%
Confidence on proportion (alpha) [input]  95.0%
Proportion of population falling above
lower tolerance interval (rho) [input]    99.9%
Minimum value of X                       85.0300
Maximum value of X                       210.1800
Average value of X                       191.82517
Average value of k                       1.00824
Minimum value of k                       0.99480
Variance of fit, s(k,X)^2                 3.5025E-06
Within variance, s(w)^2                  1.7752E-05
Pooled variance, s(p)^2                  2.1254E-05
Pooled std. deviation, s(p)              4.6103E-03
C(alpha,rho)*s(p)                        2.0310E-02
student-t @ (n-2,1-gamma)                1.66558E+00
Confidence band width, W                  8.2357E-03
Minimum margin of subcriticality, C*s(p)-W 1.2074E-02

```

Upper subcritical limits: (85.030 <= X <= 210.18)

USL Method 1 (Confidence Band with
Administrative Margin) USL1 = 0.9418 (85.030 < X < 210.18)

USL Method 2 (Single-Sided Uniform
Width Closed Interval Approach) USL2 = 0.9797 (85.030 < X < 210.18)

USLs Evaluated Over Range of Parameter X:

X	8 50E+1	1.03E+2	1.21E+2	1.39E+2	1.57E+2	1 74E+2	1.92E+2	2.10E+2
USL-1:	0.9418	0.9418	0.9418	0.9418	0.9418	0.9418	0.9418	0.9418
USL-2:	0.9797	0.9797	0.9797	0.9797	0.9797	0.9797	0.9797	0.9797

Thus spake USLSTATS
Finis.