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10 October 2003  
DCS-NRC-000159

Subject: Docket Number 070-03098  
Duke Cogema Stone & Webster  
Mixed Oxide (MOX) Fuel Fabrication Facility  
Criticality Validation Report – Revision 3 of Part II  
Response to DSER Open Item NCS-04

- References:
- 1) R. C. Pierson (NRC) to P. S. Hastings, *Draft Safety Evaluation Report on Construction of Proposed Mixed Oxide Fuel Fabrication Facility, Revision 1*, Dated 30 April 2003
  - 2) A. Persinko (NRC) to B. Smith (NRC) Memorandum, *September 11, 2003 Meeting Summary: Meeting with Duke Cogema Stone & Webster to Discuss Nuclear Criticality Safety Related to Mixed Oxide Fuel Fabrication Facility Revised Construction Authorization Request*, dated 11 October 2003

As part of the review of Duke Cogema Stone & Webster's (DCS') Mixed Oxide Fuel Fabrication Facility (MFFF) Construction Authorization Request (CAR) documented in the Draft Safety Evaluation Report (Reference 1), NRC Staff identified Open Item NCS-04 related to Nuclear Criticality Safety. NRC clarified their requests in discussions described in References 2 and 3.

Enclosure 1 to this letter discusses the response to the open item. Revision 3 of Part II of the MFFF Criticality Code Validation Report supports this response, and is transmitted as Enclosure 2 to this letter.

The Criticality Validation Report documents the validation of the nuclear criticality safety codes to be used in the design of the MFFF, and are being transmitted at this time to provide justification for selection of administrative margin for construction authorization.

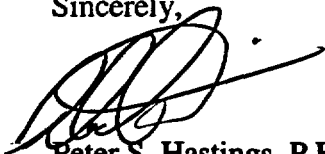
As indicated in the original transmittal of Part I, the MOX Standard Review Plan states that the validation report should be maintained at DCS' facility, the implication being that, should the NRC Staff wish to review it, the review would take place at DCS' facility. However, DCS presumes that the Staff's review of the validation report will be facilitated by making the report available directly. DCS considers the attached Criticality Validation Report to be a technical report that backs up conclusions in the Construction Authorization Request (CAR), but does not consider it to be part of the CAR.

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If I can provide any additional information, please feel free to contact me at (704) 373-7820.

Sincerely,



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Enclosures: (1) DSER Open Item NCS-04 Response  
(2) MFFF Criticality Validation Report, Part II, Revision 3

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Enclosure 1  
DSER Open Item NCS-04 Response

**Open Item NCS-04 – Nuclear Criticality Safety**

**Determination of Design Basis USLs for each process type, and determination of normal condition subcritical margin. Clarification of DCS' commitment to the preferred use of dual parameter control. (DSER Section 6.1.3.4.2 and 6.1.3.5.1)**

**Per the discussion at the September 11, 2003, meeting, DCS will consider revising Part II of the validation report using traditional methods to select benchmarks for AOA(3) and AOA(4).**

**Response:**

Revision 3 of the "Mixed Oxide Fuel Fabrication Facility Criticality Code Validation Part II," is enclosed for your review.

As was presented during the 11 September 2003 meeting on this topic, the Oak Ridge National Laboratory (ORNL) sensitivity/uncertainty (S/U) methodology for identifying benchmark experiments has been replaced by a "traditional" methodology based on NUREG/CR-6698, "Guide for Validation of Nuclear Criticality Safety Calculational Methodology," for AOAs 3 and 4.

The enclosed update provides the results of the application of NUREG/CR-6698 methodology to AOAs 3 and 4. The update provides a definition of the selection criteria through the review of the applicable benchmark experiments. NUREG/CR-6698 provides guidance on the selection process and evaluation processes (e.g., the statistical evaluation tools and the ANSI/ANS standards to be used).

Consistent with NUREG/CR-6698, the enclosed report defines the criteria that are used in the selection of the applicable experiments and defines the primary and secondary nuclear parameters for selection of the appropriate benchmark cases. In defining the process for identifying applicable experiments, NUREG/CR-6698 observes that there are parameters of each benchmark that are more important than other parameters, e.g., the nuclear characteristics of the experiments vs. the explicit configuration.

Based on the guidance in NUREG/CR-6698 appropriate benchmark experiments were selected for AOAs 3 and 4. Subsequently, statistical evaluations were performed to determine if the experiments would be considered normal or non-normal. NUREG/CR-6698 references the applicable ANSI/ANS standards that were applied to the computational results of the benchmark evaluations. From this exercise, the Upper Safety limit (USL) was determined for AOAs 3 and 4.

The resulting USLs, as noted in Section 7 of the update, are the 0.9345 for AOA 3 and 0.9349 for AOA 4. DCS concludes that the process of demonstrating that the tools used to evaluate nuclear criticality are appropriate and the definition of the USL for AOAs 3 and 4 can be considered closed.

**Enclosure 1**  
**DSER Open Item NCS-04 Response**

**As noted in our 11 September 2003 conference call, DCS intends to continue to work with ORNL to monitor the improvement of the S/U process for possible future use.**

**Enclosure 2**  
**MFFF Criticality Code Validation Report**  
**Part II**  
**Revision 3**



DUKE COGEMA  
STONE & WEBSTER

# **Mixed Oxide Fuel Fabrication Facility**

## **Criticality Code Validation**

### **Part II**

**Revision 3**

**Docket Number 070-03098**

**Prepared by  
Duke Cogema Stone & Webster**

**October 2003**

**Under  
U.S. Department of Energy  
Contract DE-AC02-99-CH10888**

**REVISION DESCRIPTION SHEET**

REVISION NUMBER	DESCRIPTION
0	Initial Issue October 2001
1	Incorporate benchmark experiments identified using ORNL sensitivity and uncertainty analysis. Affected pages: 8, 18-19, 24-34, 38-56. Editorial and typographical corrections: various pages.
2	Define area of applicability based on key parameter ranges of input design applications used in sensitivity and uncertainty analysis. Remove waste store and laboratory from typical design applications for AOA(3) since these units can be analyzed using ANSI-ANS-8.1 limits. Affected pages: 36-38, 42-44. Editorial and typographical corrections: various pages.
3	General revision to implement NUREG/CR-6698 experiment selection methodology. Affected sections: 1. Introduction; 3.6 Identification of Benchmark Experiments; 4.3 Physical Parameters for AOA (3); 4.4 Physical Parameters for AOA (4); 5. Benchmark Experiments; 6. Analysis of Validation Results; 7. Conclusions

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## LIST OF ACRONYMS

ANS	American Nuclear Society
ANSI	American National Standards Institute
AOA	area of applicability
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

## EXECUTIVE SUMMARY

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 packages [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  $k_{\text{eff}}$  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) PuO<sub>2</sub> powders, (4) MOX powders, and (5) aqueous solutions of Pu compounds (Pu-oxalate solutions). The first two AOAs are validated in the validation report Part I [16]. The present report addresses the third and fourth AOAs: (3) PuO<sub>2</sub> powders (homogeneous systems), and (4) MOX powders (homogeneous systems). The AOA(5) will be addressed in the Part III [17].

The report concludes that the upper safety limit (USL) for the third design AOA (i.e., PuO<sub>2</sub> powder) is 0.9345, and the USL for the fourth design AOA (i.e., MOX powder) is 0.9349. The USL accounts for the computational bias, uncertainties, and a 0.05 administrative margin.

## **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 packages [1] with the 238 energy group cross-section library 238GROUPNDF5 on the PC platform 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 and fissile materials in the MFFF:

- Pu-nitrate aqueous solutions
- MOX pellets, fuel rods, and fuel assemblies
- PuO<sub>2</sub> powders
- MOX powders
- Aqueous solutions of Pu compounds (e.g., Pu-oxalate solutions).

This report addresses the third and fourth AOAs:

- PuO<sub>2</sub> powder mixture (homogeneous systems),
- MOX powder mixture (homogeneous systems).

## **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 at 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 (from the Pit Disassembly and Conversion Facility) 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 margin of subcriticality for safety.*” In order to comply with this requirement, NUREG 1718 [3] and ANSI/ANS-8.1 [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  $k_{\text{eff}}$  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 [4].

SCALE 4.4a is a collection of modules designed to perform nuclear criticality, shielding, and thermal calculations. Each SCALE functional module may be run individually, or a sequence of functional modules may be executed using a special module referred to as a control module. For criticality analyses, various criticality safety analysis sequence (CSAS) control modules are available which differ in the specific functional modules executed and in the processing of cross-sections used as input. In general, MFFF criticality analyses are performed using the CSAS26 control module and the 238 energy group cross-section library 238GROUPNDF5, based on ENDF/B-V data. These modules perform cross-section processing using the BONAMI and NITAWL-II functional modules, and the calculation of  $k_{\text{eff}}$  is performed using the KENO VI Monte Carlo transport code.

Recent KENO-VI updates, up to and including Update 3 available from the SCALE Download web site, have been applied to SCALE 4.4a used for calculations presented here. Comparison between patched and unpatched SCALE 4.4a versions do not indicate statistically significant differences [15].

### 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 packages has been procured, installed, and verified on the SGN 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  $k_{\text{eff}}$  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 3-2 lists some of the key parameters for the MFFF.

The second step involves several substeps. First, based on the key parameters, the AOA and expected range of the 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) PuO<sub>2</sub> powders; (4) MOX powders; and (5) aqueous solutions of Pu compounds. 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 AOAs are selected from the references listed in the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* [5], the *Guide to Verification and Validation of the SCALE-4 Criticality Safety Software* [6], and the *Neutronics Benchmarks for the Utilization of Mixed-Oxide Fuel* [7]. 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  $k_{\text{eff}}$  values of the selected critical benchmark experiments<sup>1</sup>.

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.

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<sup>1</sup> Note that these models contain simplifications of critical experiments geometry. These simplifications lead to additional uncertainties, 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, ( $k_{\text{eff}}$ ) of the design application (system)
- $k_c$  = the mean  $k_{\text{eff}}$  value resulting from the calculation of benchmark critical experiments using a specific calculation method and data
- $\Delta k_s$  = the uncertainty in the value of  $k_s$
- $\Delta k_c$  = the uncertainty in the value of  $k_c$
- $\Delta k_m$  = the administrative margin to ensure subcriticality.

Sources of uncertainty that determine  $\Delta k_s$  include:

- statistical and/or convergence uncertainties
- material and fabrication tolerances
- limitations in the geometric and/or material representations used.

Sources of uncertainty that determine  $\Delta k_c$  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 ( $\beta$ ) 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.  $\beta$  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  $k_{\text{eff}}$  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.

$\beta$  is related to system parameters and may not be constant over the range of a parameter of interest. If  $k_{\text{eff}}$  values for benchmark experiments vary as a function of a system parameter, such as enrichment or degree of moderation, then  $\beta$  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  $\beta$  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 0).

One or two calculations are insufficient to determine calculational 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.

### 3.2 USL DETERMINATION METHODS

NUREG/CR-6361 [9] describes two parametric 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].

The parametric statistical methods described in NUREG/CR-6361 require the benchmark data to be normally distributed. In cases where the data fails a test for normality, a nonparametric technique is described which is based on rank order statistics. In this analysis, the nonparametric technique described in NUREG/CR-6361 [9] is employed.

#### 3.2.1 USL Method 1: Confidence Band with Administrative Margin

This method applies a statistical calculation of the bias ( $\beta$ ) and its uncertainty ( $\Delta\beta$ ) plus an administrative safety margin ( $\Delta k_m$ ) 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  $\beta$ .  $W$  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

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

and

$n$  = the number of critical calculations used in establishing  $k_c(x)$

$t_{1-\gamma, s_p}$  = the Student - t distribution for  $1 - \gamma$  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  $\sigma_i$  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,  $\Delta k_m$  is given an arbitrary administrative value. NUREG-1718 [3] states that a “minimum subcritical margin ( $\Delta k_m$ ) 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 0 provides further justification for 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:

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

### **3.2.2 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,  $\Delta k_m$  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  $\alpha$  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  $\alpha$  that an additional calculation of  $k_{eff}$  for a critical system will lie within the band. For example, a  $C_{95/99.5}$  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:

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

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

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

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

$A$ ,  $\rho$ , 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,  $\Delta k_m$  which can be determined as the difference  $(C_{\alpha P} \cdot s_p) - W$ . 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.

### 3.2.3 Non-Normal Distributions

In cases where the benchmark results fail the  $\chi^2$  test for normality, the nonparametric technique described in NUREG-6698 [18] is applied to the data. This statistical technique is based on a rank order analysis of the data. The USL is established according to

$$\text{USL} = \text{Smallest } k_{\text{eff}} \text{ value} - \text{Uncertainty for smallest } k_{\text{eff}} - \text{Nonparametric margin} - \Delta k_m \quad (\text{Eq. 3.1})$$

Where the nonparametric margin is an additional margin intended to account for small sample size, and  $\Delta k_m$  is the administrative margin. Recommended values for the nonparametric margin



as a function of the degree of confidence are obtained from Table 2.2 of NUREG-6698, which is reproduced in Table 3-1.

The degree of confidence  $\beta$  that a fraction  $q$  of the population is greater than the lowest observed value is established for a given sample size  $n$  according to

$$\beta = 1 - q^n \quad (\text{Eq. 3.2})$$

For a desired population fraction of 95%, this becomes

$$\beta = 1 - 0.95^n \quad (\text{Eq. 3.3})$$

In order to obtain a 95% confidence that 95% of the population is larger than the smallest observed sample, at least 59 critical experiments are required.

Table 3-1 Recommended Non-Parametric Margin Values from NUREG-6698

Degree of Confidence for 95% of the Population	Non-parametric Margin (NPM)
>90%	0.00
>80%	0.01
>70%	0.02
>60%	0.03
>50%	0.04
>40%	0.05
≤40%	Additional data needed. (This corresponds to less than 10 data points.)

### 3.3 UNCERTAINTIES

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

Experimental uncertainty ( $\sigma_e$ ) – 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 ( $\sigma_s$ ) – Monte Carlo calculation techniques result in a statistical uncertainty associated with the actual calculation. This type of uncertainty is dependent upon many factors, including number of neutron generations performed, variance reduction techniques employed, and problem geometry. For this document,  $\sigma_s$  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.

### 3.4 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  $k_{eff} = 1.0$ . 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:

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

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,  $\sigma_i$ , is made.

### 3.5 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.

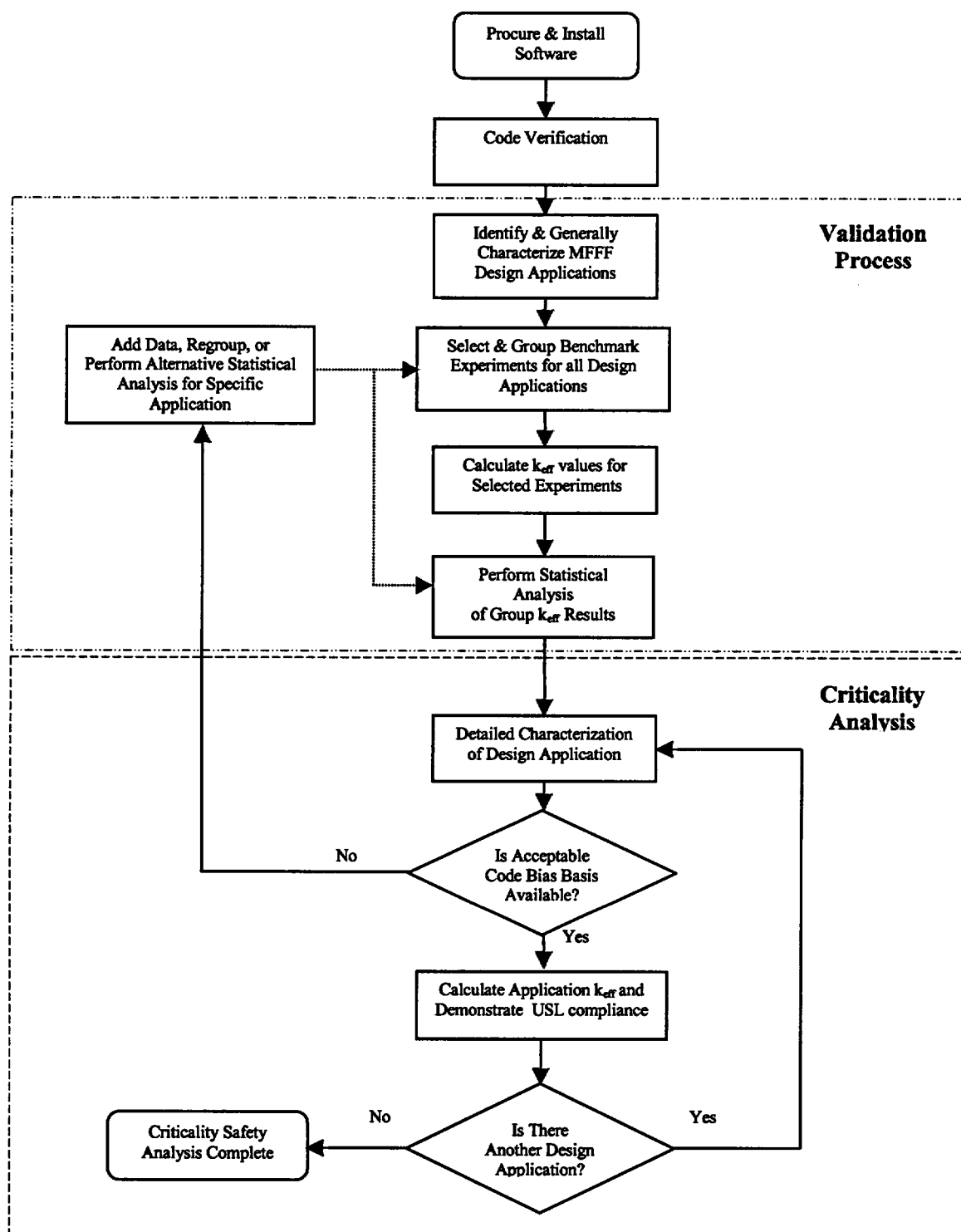


Figure 3-1 Overview of the Criticality Analysis Process of the MFFF

Table 3-2 Characteristics of the MFFF Application Areas\*

Parameter	Pu-nitrate solution	MOX pellets, fuel rods, FAs	PuO <sub>2</sub> 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 <sub>2</sub> powder	MOX powder	(a) Pu-oxalate (b) PuO <sub>2</sub> F <sub>2</sub>
Isotopic composition of fissile material **	96% <sup>239</sup> Pu 4% <sup>240</sup> Pu	96% <sup>239</sup> Pu 4% <sup>240</sup> Pu depleted U	96% <sup>239</sup> Pu 4% <sup>240</sup> Pu	96% <sup>239</sup> Pu 4% <sup>240</sup> Pu depleted U	96% <sup>239</sup> Pu 4% <sup>240</sup> Pu
PuO <sub>2</sub> /(UO <sub>2</sub> +PuO <sub>2</sub> )	100 %	≤ 6.3 %	100 %	6.3% – 22%	100 %
Maximum oxide density [g/cm <sup>3</sup> ]	–	7.0, 11.0	3.5, 7.0, 11.46	4.1, 5.5	–
Pu concentration [g/liter]	125 – 237	–	–	–	(a) 242 (b) 696
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 and 700 – 1900	H/Pu=1.6 – 291	(a) H/Pu=100 (b) H/Pu=30
Low density moderation [wt.% H <sub>2</sub> 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 AOAs

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

\*\*\* Per calculation

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

### 3.6 IDENTIFICATION OF BENCHMARK EXPERIMENTS

Benchmark experiments applicable to the validation of SCALE 4.4a for the areas of applicability covered in this report are identified in accord with the guidance in NUREG/CR-6698 [18]. The suggested methodology in this report is the following:

“The first step in performing a validation is to identify the range of parameters for which the validation will apply. Critical experiments should be selected that span the range of parameters. This initially defines the areas of applicability for the validation. An iterative process is required to finally establish the area of applicability. The number of available experiments and the results of the statistical evaluation may necessitate some changes to the boundaries of the area(s) of applicability.”

The report also notes that

“When initially determining the range of parameters for the validation, consideration should be given to the needs of subsequent analyses that will evaluate both normal and credible upset conditions.”

In summary, the process is

- (1) Review areas of applications, identify key parameters and identify key parameter ranges based upon both the established current analyses and the needs of potential subsequent analyses,
- (2) Develop an initial screening criteria based upon extension of the parameter ranges identified in step (1) by the suggested factors cited in Table 2.3 (in Ref. [18]),
- (3) Identify the applicable experiments in the database of benchmark experiments that meet the initial screening criteria in step (2), and
- (4) Verify that the identified experiments bound the parameter ranges identified in Step (1) for the area(s) of applicability (AOAs). If one or more parameter range(s) in the AOA(s) identified in Step 1 is not bounded by available benchmark experiments, iterate the selection process (one time only) by the following:
  - (a) Extend the unbounded parameter range in the preliminary screening criteria,
  - (b) Identify additional benchmark experiments that are now within the (revised) screening criteria range, and
  - (c) Revise the parameter range(s) of the AOA(s), if necessary, in conformance with the suggested factors in Table 2.3.

Since NUREG/CR-6698 does not propose factors for extending parameter ranges in step (4)(a), the following guidelines have been adopted:

- (4)(a)(i) Neutron energy ranges (e.g. EALFs) and the ranges of other parameters whose importance in the physics of neutron transport is logarithmic may be extended by a factor of 5, and
- (4)(a)(ii) Ranges of other quantitative parameters not logarithmic in nature (e.g., isotopic composition) may be extended by a factor of 2.

Use of these extension factors for screening is justified based upon the slow variation in bias with the parameters of interest. For example, Figure 3-3 and Figure 3-4, which are discussed in Section 3.6.3, show plots of the KENO V  $k_{eff}$  values of all candidate benchmarks in the current MFFF database as a function of EALF and  $H/(Pu + U)$ . Additionally, shown on each figure is a trend line based upon a linear ( $y = Ax + B$ ) least squares fit to the data. As can be seen from the data shown on Figure 3-3 in the region of primary interest (intermediate energy range), there is no discernable trend as a function of the logarithmically important parameter EALF in the range of 0.01 to 100,000 eV. Thus a variation in a portion of this range of a factor of five such as from 100 eV to 500 eV appears to be very small and thus use of a factor of five for screening is justified.

Similarly, Figure 3-4 shows  $k_{eff}$  as a function of the non-logarithmically important parameter  $H/(Pu + U)$ . Again, there is no discernible trend over the region of interest. Thus, a variation in a portion of this range by a factor of two, such as from 10 to 20 or 20 to 40, represents a very small variation in  $k_{eff}$  and thus use of a factor of two for screening is justified.

Therefore, as shown above, changes in the logarithmically important parameters such as EALF by a factor of five and changes in non-logarithmically important parameters such as  $H/(Pu + U)$  by a factor of two, result in very small changes in  $k_{eff}$ . Accordingly, using factors of five for logarithmically important parameters and two for non-logarithmically important parameters for one-time extension of the screening ranges in accordance with the iterative process in NUREG-6698 is justified since the changes in the data over this range is small.

After the revised screening criteria, identified benchmarks and Area(s) of Applicability are determined, the benchmark database may be evaluated for other applicable experiments. Additional cases from this evaluation may be added to the set of validation benchmarks if they satisfy one or more of the following:

- A. The parameter(s) that is/are not within the screening criteria range(s) are not considered to be of primary importance in the determination of the Scale 4.4a bias and uncertainty (for example, the fissile material concentration of an added benchmark is close to, but outside of the screening range),
- B. The parameter(s) in question is/are in the same cross-section range (i.e., thermal, intermediate or high) as the screening range (for example, the H/X range of an added benchmark is outside of the screening range, but it is still within the same moderation range [thermal, intermediate or high]),
- C. The parameter(s) in question is/are close to the screening range and other key parameters are within the range and its/their inclusion help(s) to reduce the gaps between benchmark cases within the range (for example, the physical form of the fissile material in an added benchmark is not exactly the same as the screening range, but the EALF is within the screening criteria EALF range and provides a value not previously covered by the within-range benchmarks), or
- D. The added case(s) has/have (a) similar fission spectra in the fuel region to one or more design applications that lie within the designated AOA.

### 3.6.1 Guidelines for Physical Parameter Ranges of Areas of Applicability and Screening Criteria

Table 3-3 summarizes the general guidelines for relating ranges of physical parameters in the AOAs covered in this report and the corresponding screening criteria for selection of benchmark experiments. Parameters are listed in two categories based on their relative importance in the validation of the Scale 4.4a code. Primary parameters are those (usually quantitative) parameters such as EALF that are the most important and which are expected to have a major and direct impact on the calculated  $k_{\text{eff}}$  values of the benchmarks. Secondary parameters such as physical form are those that are well modeled by the Scale 4.4a code, which tend to be more qualitative in nature and which are not expected to have a significant impact on the  $k_{\text{eff}}$  values of the benchmarks. For example, the  $\text{O}_2$  in  $\text{PuO}_2$  is not considered to be a major factor, and Pu metal is considered to be an acceptable alternative. Physical parameter ranges for selecting benchmarks are only applicable to the primary parameters.

### 3.6.2 Parameter Correlations

In the areas of applicability covered in this report, two pairs of the primary parameters listed in the above table are not independent but are highly correlated due to the types of fuel and fuel moderator models. The first pair is the  $^{239}\text{Pu}$  and  $^{240}\text{Pu}$  isotopic content, which is related by

$$\text{Pu} = {}^{239}\text{Pu} + {}^{240}\text{Pu}$$

Thus if the screening criteria range for the  $^{239}\text{Pu}$  concentration is 86% to 100%, the corresponding range for the  $^{240}\text{Pu}$  concentration is 0% to 14%.

The second correlated pair is the  $\text{H}/(\text{Pu} + \text{U})$  ratio and the neutron energy EALF. These are correlated because the  $\text{H}/(\text{Pu} + \text{U})$  ratio is a measure of the hydrogenous moderation in the fuel mixture and the amount of moderation in the fuel is related to the average energy of the neutrons causing fission. This is illustrated in the Figure 3-2, which shows plots of the  $\text{H}/\text{X}$  atomic ratio (X is the  $\text{Pu} + \text{U}$  number density, or Pu only if the fuel does not contain uranium) versus the EALF for KENO VI k-infinite calculations for  $\text{PuO}_2$  (100% Pu content) and MOX (22% and 6.3%  $\text{PuO}_2$ ) powder homogeneously saturated with  $\text{H}_2\text{O}$ . The correlation between  $\text{H}/\text{X}$  and EALF can also depend on the degree and type of reflection, and the degree and type of interstitial moderator, but the curves for the k-infinities are representative of the relationships for single units that are either unreflected or that are fully reflected by water. Thus,  $\text{H}/\text{X}$  and EALF are not independent.

Table 3-3 Physical Parameters and Screening Criteria Guidelines

Application Parameter	Potential Application Parameter Range	Allowable Screening Criteria Range	Allowable Extension Factor for Screening Criteria Range to AOA Range
<b>Primary Parameters</b>			
<b>Fuel</b>			
Fissile Isotope $^{239}\text{Pu}$	5 – 10 wt. % 20 – 80 wt. % 80 – 100 wt. %	$\pm 2.5$ wt. % $\pm 15$ wt. % $\pm 10$ wt. %	$\pm 5$ wt. %  $\pm 20$ wt. %
Fissionable Isotopes $^{240}\text{Pu}$ $^{238}\text{U}$	0 – 32 wt. % 0 – 98 wt. %	$\pm 4$ wt. % $\pm 4$ wt. %	1 – $^{239}\text{Pu}$ Content Based on $\text{PuO}_2 + \text{UO}_2 = 100\%$
<b>Fuel Moderator</b>			
Moderating Element Hydrogen	N/A	N/A	NA
H/X Atomic Ratio (X is Pu for Metal or $\text{PuO}_2$ , Pu + U for MOX)	0 – Max Value	$\pm 20$ %	Factor of 2
Neutron Energy EALF	$0.022 - 10^6$ ev	Same Energy Range (Thermal, Intermediate or Fast)	Factor of 5 (May exceed Range)



Table 3-3 Physical Parameters and Screening Criteria Guidelines – Continued

Application Parameter	ApplicationParameter Range	Allowable Screening Criteria Range	Allowable Extension for Screening Criteria Range to AOA Range
<b>Secondary Parameters</b>			
<u><b>Fuel</b></u>			
Physical Form: PuO <sub>2</sub> powder, MOX powder	N/A	N/A	Pu Metal, in lieu of PuO <sub>2</sub> powder, since O <sub>2</sub> total neutron cross-sections in the energy ranges of interest are less than 4 barns compared to the 100s -1000s of barns for <sup>239</sup> Pu cross-sections
Maximum Density	11.46 gm/cm <sup>3</sup> for Oxide 19.8 for Metal	N/A	
Fuel Temperature	Room Temperature	273°K ± 25°K	N/A
			N/A
<u><b>Fuel Moderator</b></u>			
Physical Form: Water or Plastic	N/A	N/A	Low amount of Carbon (e.g., < 5 wt. %) permitted since the C moderating effect with hydrogen is not important at this level.
Moderator Density	0 – Max	N/A	N/A
<u><b>Interstitial Moderator and External Reflectors</b></u>			
Physical Form: None, hydrogenous, Neutron Absorbers (inc. <sup>238</sup> U)	N/A 0 – Max	N/A	N/A [Note: Worth of neutron absorbers in hydrogenous reflectors is not high]
<u><b>Geometry</b></u> Region types	Infhommedium, lattice cell or multiregion	Same region type	Same region type

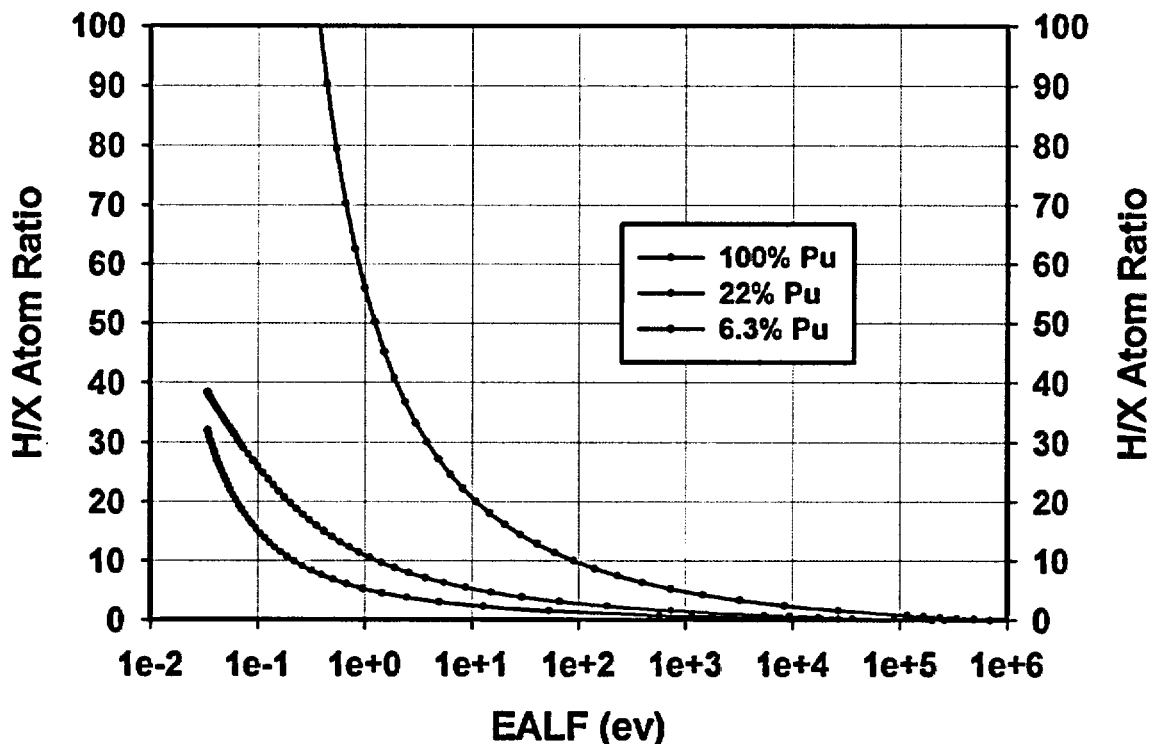


Figure 3-2 Relationship of H/X and EALF for pure  $\text{PuO}_2$  and MOX powders

Figure 3-2 shows a monotonically decreasing relationship between H/X and EALF as the EALF increases. Also, the relationships for 22% and 6.3% Pu MOX is much less extreme in the thermal (low EALF) region.

### 3.6.3 Database of Benchmark Experiments

Figure 3-3 and Figure 3-4 show plots of the KENO V  $k_{\text{eff}}$  values of the 318 candidate benchmark experiments in the current MFFF database as functions of EALF and  $H/(\text{Pu} + \text{U})$ . The plot in Figure 3-4 goes from 0 to 125 and therefore shows only the 308 benchmark cases that have  $H/(\text{Pu} + \text{U})$ s below the upper value. Illustrated by these plots are the following points:

- Although all of the candidate benchmark experiments would not be expected to meet the screening criteria or to be otherwise applicable, they nevertheless show that all KENO results are clearly bounded by 0.93 (and essentially by 0.98).
- The behavior of  $k_{\text{eff}}$  (i.e., the factor “1.0 + bias”) as calculated by the code, is slightly above 1.0. Thus, on average, KENO calculates conservative k-effectives.
- There are no visually apparent trends in the calculated  $k_{\text{eff}}$  as a function of EALF or  $H/(\text{Pu} + \text{U})$  in the regions of interest
- There is a large margin between all data points and the proposed USL (approximately 0.93).

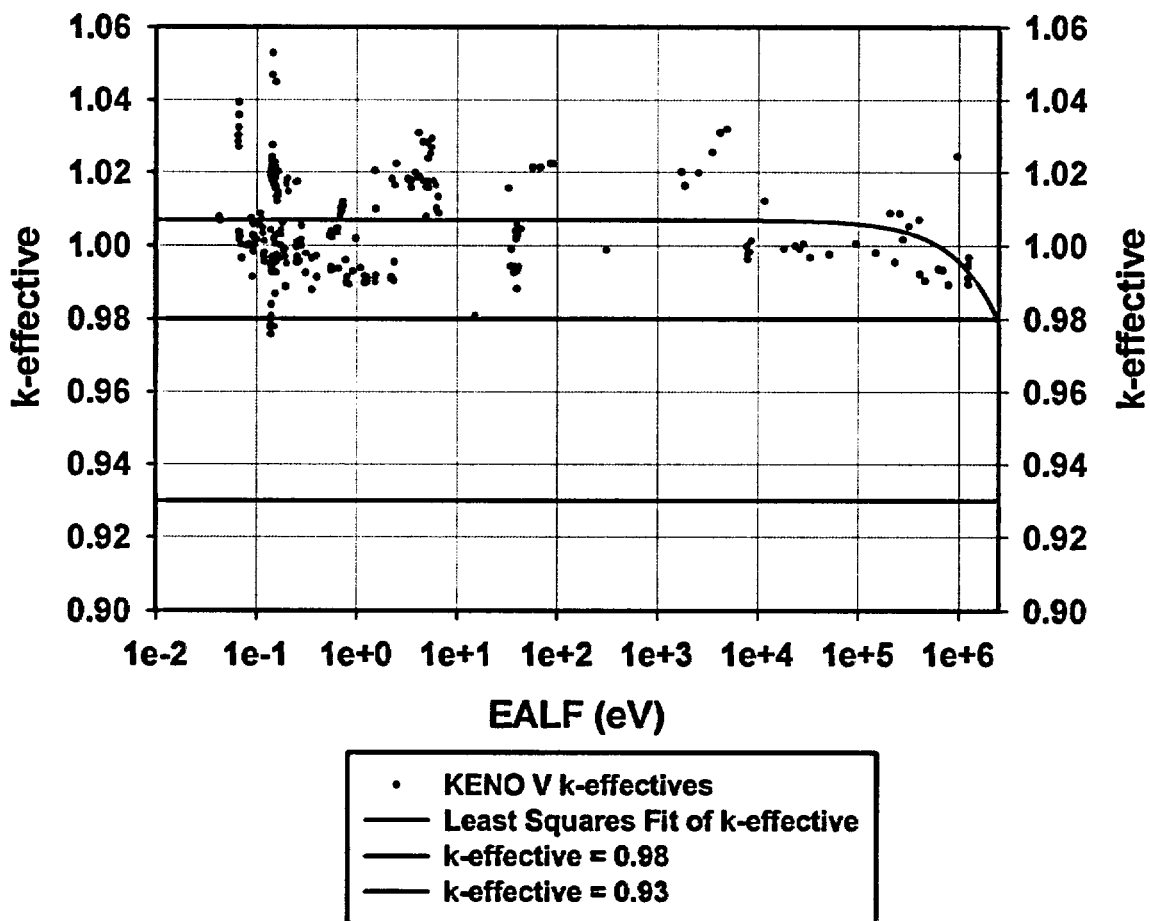


Figure 3-3 KENO-V  $k$ -effectives of Pu Candidate Benchmark Set vs. EALF

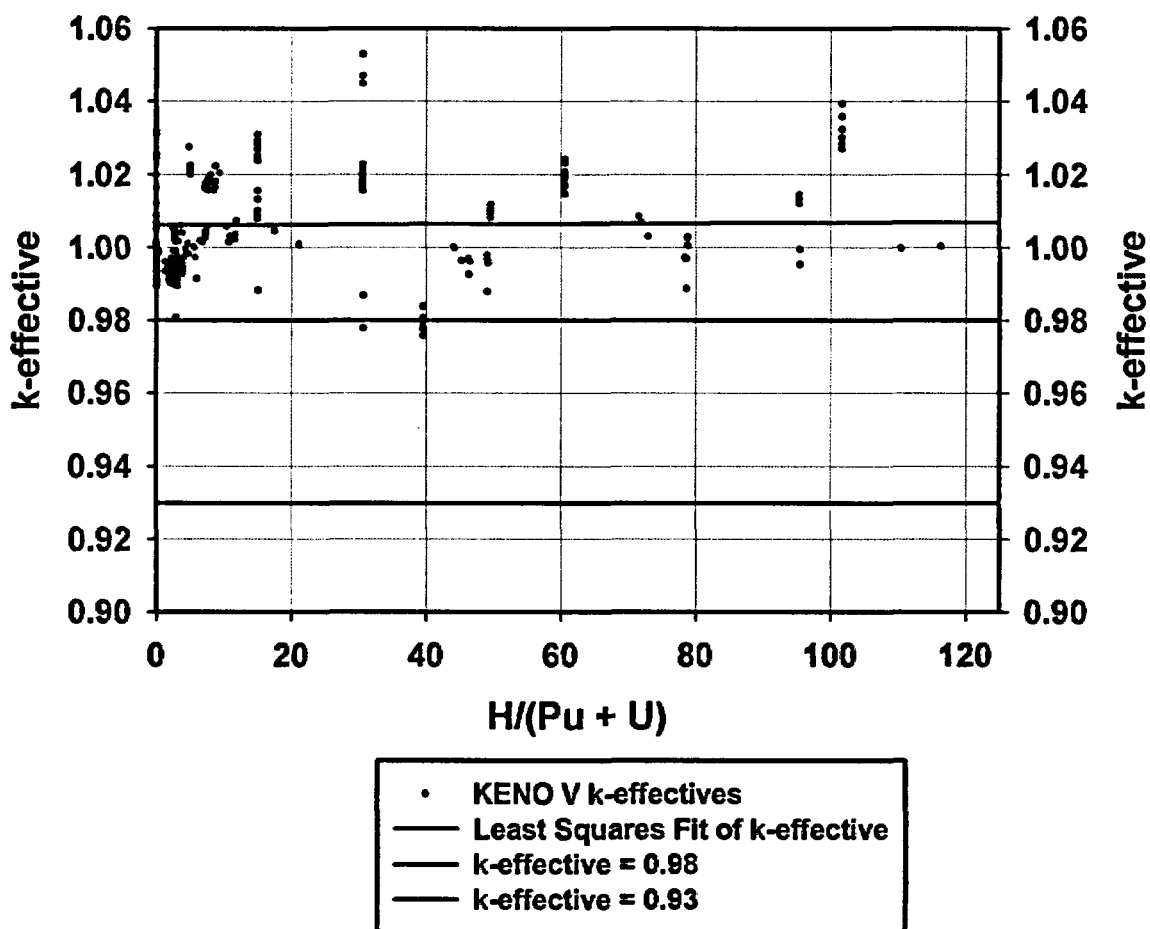


Figure 3-4 KENO-V k-effectives of Pu Candidate Benchmark Set vs.  $H/(Pu + U)$

#### **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 3-2):

- Pu-nitrate aqueous solution
- MOX pellets, fuel rods, and fuel assemblies (FA)
- PuO<sub>2</sub> powders
- MOX powders
- Aqueous solutions of Pu compounds (e.g., Pu-oxalate solution).

##### **4.1 DESIGN APPLICATION (3) – PuO<sub>2</sub> POWDER**

Table 4-1 summarizes the anticipated criticality calculations to be performed for the design of the MFFF in which PuO<sub>2</sub> will be processed. The table provides the relevant parameters (i.e., chemical form, isotopic vector, moderator to fuel atomic ratio (H/Pu), and EALF) for each criticality design application.

For some applications, geometry control is used and the calculations are performed at optimum moderation taking into account full water reflection. In these cases a thermal neutron spectrum will be found. In other applications (e.g., jar store and the can receiving and emptying unit) where mass and moderation control are used and the fissile materials are reflected by borated concrete materials, or the concrete reflector is far from the fuel, the neutron spectrum will be intermediate to fast.

**Table 4-1 Anticipated Criticality Calculation Derived Characteristics for Design Applications Involving PuO<sub>2</sub> Powder**

Fuel Configuration	Reflector Conditions	Chemical Form	Pu-Isotopic Composition	Max $\rho(\text{PuO}_2)$ [g/cm <sup>3</sup> ]	H/Pu	EALF [eV]
<b>AP: Decanning</b>						
PuO <sub>2</sub> dosing hopper	Water	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	7.0	0 - 4	1,640 – 119,000
Buffer Store	Water	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	7.0	0 – 2	45,000 – 135,000
<b>AP: Dissolution</b>						
Electrolyzer	Water <sup>1</sup> /Cd <sup>2</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	7.0	1 – 9.5	10,500 – 18,000
Filter glove box	Water <sup>1</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	7.0	1 – 2.5	270 – 1,050
Tanks in cell	Water <sup>1</sup> /Cd <sup>2</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	7.0	1 - 2	15,600 – 19,200
<b>AP: Oxalic Precipitation Conversion</b>						
Furnace GB	Water <sup>1</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	5 – 7	40 - 97
<b>AP: Homogenization</b>						
Homogenizer	Water	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	5 - 10	93 - 775
PuO <sub>2</sub> Canning GB	Water	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	4 - 9	70 - 656
<b>MP: Powder Area</b>						
MFFF Receiving	Water	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	11.46	0-10	22 – 44,000
PuO <sub>2</sub> 3013 can store	Concrete reflected water or bare array	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	11.46	0 – 0.3	1,330 – 266,000
PuO <sub>2</sub> can buffer store	Concrete <sup>3</sup> reflected array	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	0.93-16.5	3 – 177,000
PuO <sub>2</sub> decanning unit	Water <sup>1</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	0.3-0.93	30 - 60
Primary dosing unit	Water <sup>1</sup>	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5	0.30 - 6	50 – 20,000
Ball Milling	Water <sup>1</sup>	PuO <sub>2</sub> powder <sup>4</sup>	4% <sup>240</sup> Pu	3.5	0.93 – 1.1	5,000 – 16,000
Scrap Processing	Water <sup>1</sup>	PuO <sub>2</sub> powder <sup>4</sup>	4% <sup>240</sup> Pu	3.5	0.93 – 1.1	5,000 – 16,000
Range of Design Application	Various	PuO <sub>2</sub> powder	4% <sup>240</sup> Pu	3.5 – 11.46	0 – 16.5	3 to 266,000

<sup>1</sup> The concrete walls are conservatively modeled. However, the presence of a close fitting water reflector effectively eliminates its effect.

<sup>2</sup> Cadmium sheet of 0.05 cm thickness (clad in 0.1 cm stainless steel).

<sup>3</sup> Boron is actually present in the concrete, but no credit is required in the safety analysis of the unit.

<sup>4</sup> Bounding material

## 4.2 DESIGN APPLICATION (4) – MOX POWDER

Table 4-2 summarizes the anticipated criticality calculations to be performed for the design of the MOX powder process. In addition, the table provides the relevant parameters (i.e., chemical form, moderator to fuel atomic ratio (H/Pu), and EALF) for each criticality design application.

Table 4-2 Anticipated Criticality Calculation Derived Characteristics for Design Applications Involving MOX Powder

Fuel Configuration	Reflector Condition	Chemical Form	Pu/(U+Pu)	Pu-isotopic Composition	Max $\rho(\text{MOX})$ [g/cm <sup>3</sup> ]	H/(U+Pu)	EALF [eV]
<b>MP: Powder area</b>							
Jar store unit	Water <sup>1</sup>	MOX powder	6.3%, 22%	4% <sup>240</sup> Pu	5.5	1.6	0.28 – 0.79
Final dosing unit	Water	MOX powder	6.3%, 22%	4% <sup>240</sup> Pu	5.5	1.1 – 1.6	50 - 850
Final mix homogenization and press station unit	Water	MOX powder	6.3%, 22%	4% <sup>240</sup> Pu	5.5	1.1 – 1.6	3 - 6
Auxiliary powder unit	Water	MOX powder	6.3%, 22%	4% <sup>240</sup> Pu	5.5	1.1 – 1.6	50 - 850
Expected Range of Application	Water	MOX powder	6.3%, 22 %	4% <sup>240</sup> Pu	5.5	1.1 – 1.6	0.28 - 850

<sup>1</sup> The concrete walls are conservatively modeled. However, the presence of a close fitting water reflector effectively eliminates its effect.

## 4.3 PHYSICAL PARAMETERS FOR AOA(3)

AOA(3) covers the areas in the design of the MFFF in which PuO<sub>2</sub> powder will be processed. The bases of the design in these areas is Pu with the properties in Table 4-3:

Table 4-3 Physical Parameter for AOA(3)

Parameter	Design Basis
Fissile Material Physical/Chemical Form	PuO <sub>2</sub> Powder
Isotopic Composition of Fissile Material	96 % <sup>239</sup> Pu 4% <sup>240</sup> Pu 0% <sup>238</sup> U
Maximum Density	11.46 g/cm <sup>3</sup> for Pu Oxide
Type of Moderation	Hydrogenous (Homogeneous Fuel Mixtures)

The following sections summarize the determination of the screening range used in the validation of SCALE 4.4a for this AOA.

#### **4.3.1 AOA(3) Applications and Parameter Ranges**

Table 4-1 presents a review of the unit criticality safety analyses currently in process for the PuO<sub>2</sub> powder operations in the MFFF. The last row in this table summarizes the key parameters and ranges in the current and anticipated calculations.

In accordance with the process as described in NUREG-6698, the benchmark experiments are to be “selected which span the range of parameters.” However, the MFFF calculations are often performed in the vicinity of the worst case condition. As a result, parameter ranges of some parameters as shown in Table 4-1 for AOA(3) are correspondingly narrow. Selection of benchmarks according to these worst case ranges – even with the extensions suggested by NUREG-6698, Table 2.3 – would result in benchmarks that would not span the range of parameters as recommended by NUREG-6698. Thus, the one-time iteration of parameters as described in Section 3.6 is warranted.

Following the process as recommended by NUREG-6698 and described in Section 3.6, a comparison of the anticipated MFFF application parameter ranges and the screening criteria for AOA(3) is shown in Table 4-4.

**Table 4-4 Summary of Screening Criteria for AOA(3)**

<b>Parameter</b>	<b>Application Range</b>	<b>Screening Range</b>
<b>Pu Physical Form</b>	<b>PuO<sub>2</sub> Powder</b>	<b>PuO<sub>2</sub> Powder or Pu Metal</b>
<b>Wt. % <sup>239</sup>Pu</b>	<b>96</b>	<b>86 – 100</b>
<b>Wt. % <sup>240</sup>Pu</b>	<b>4</b>	<b>0 – 14*</b>
<b>H/Pu</b>	<b>0 – 16.5</b>	<b>0 – 39.6</b>
<b>EALF (ev)</b>	<b>3 – 100,000</b> <b>100,000 – 266,000</b>	<b>1 – 100,000**</b> <b>100,000 - 10<sup>7**</sup></b>

\*Range based on <sup>239</sup>Pu range

\*\* Intermediate and fast energy ranges as defined in NUREG-6698, Table 2.3

#### **4.4 PHYSICAL PARAMETERS FOR AOA(4)**

AOA(4) covers the areas in the design of the MFFF in which MOX powder will be processed. The bases of the design in these areas is MOX powder with the properties shown in Table 4-5.



**Table 4-5 Physical Parameters for AOA(4)**

<b>Parameter</b>	<b>Design Basis</b>
<b>Fissile Material Physical/Chemical Form</b>	<b>PuO<sub>2</sub> + UO<sub>2</sub> Powder (MOX)</b>
<b>Isotopic Composition of Fissile Material</b>	<b>96 % <sup>239</sup>Pu 4% <sup>240</sup>Pu</b>
<b>Isotopic Composition Of UO<sub>2</sub></b>	<b>99.7% <sup>238</sup>U 0.3% <sup>235</sup>U</b>
<b>Pu Content in MOX</b>	<b>6.3% and 22%</b>
<b>Maximum Density [gm/cm<sup>3</sup>]</b>	<b>11.46 for PuO<sub>2</sub> 10.96 for UO<sub>2</sub></b>
<b>Type of Moderation</b>	<b>Hydrogenous</b>

The following sections summarize the determination of the screening range used in the validation of SCALE 4.4a for this AOA.

#### **4.4.1 AOA(4) Applications and Parameter Ranges**

Table 4-2 presents a review of the unit criticality safety analyses currently in process for the MOX powder operations in the MFFF. The last row in this table summarizes the key parameters and ranges in the current and anticipated calculations.

In accordance with the process as described in NUREG-6698, the benchmark experiments are to be “selected which span the range of parameters.” However, the MFFF calculations are often performed in the vicinity of the worst case condition. As a result, parameter ranges of some parameters as shown in Table 4-2 for AOA(4) are correspondingly narrow. Selection of benchmarks according to these worst case ranges – even with the extensions suggested by NUREG-6698, Table 2.3 – would result in benchmarks that would not span the range of parameters as recommended by NUREG-6698. Thus, the one-time iteration of parameters as described in Section 3.6 is warranted.

Following the process as recommended by NUREG-6698 and described in Section 3.6, a comparison of the anticipated MFFF application parameter ranges and the screening criteria for AOA(4) is shown in Table 4-6.

Table 4-6 Summary of Screening Criteria for AOA(4)

Parameter	Application Range	Screening Range
Pu Physical Form	MOX Powder	MOX Powder
Wt. % <sup>239</sup> Pu	96	86 – 100
Wt. % <sup>240</sup> Pu	4	0 – 14*
Wt. % <sup>238</sup> U in U	99.7	80 – 100
Wt. % <sup>235</sup> U in U	0.3	0 – 20*
Wt. % Pu in MOX	6.3 and 22	1.2 – 52**
H/(Pu + U)	1.1 – 1.6	0.44 – 3.84
EALF (ev)	0.28 – 850	0.022 – 1.0*** 1.0 – 100,000

\*Ranges based on <sup>239</sup>Pu or <sup>238</sup>U Ranges

\*\* 0 – 52 [2×26]% Pu.

\*\*\* Same thermal and intermediate energy ranges

## 5. BENCHMARK EXPERIMENTS

The final validation experiment sets for AOA(3) and AOA(4) are presented in Table 5-1 and Table 5-3, respectively. Descriptions of the critical experiments comprising the final validation experiment sets for AOA(3) and AOA(4) in the following sections. Comparisons of the selected benchmark experiments and the design applications with respect to key design parameters are shown in Table 5-2 and Table 5-4 for AOA(3) and AOA(4), respectively.

**Table 5-1 Critical Experiments Selected for AOA(3)**

Case ID	Exp.	Pu Content	H/Pu	EALF [eV]	<sup>240</sup> Pu wt. %	Description
PU-COMP-MIXED-001	2 - 4	100%	5 - 15	33 – 1,740	2.2 - 11.5%	Bare PuO <sub>2</sub> moderated compacts
PU-COMP-MIXED-002	1 - 22	100%	0 - 15	5 – 4,920	2.2 - 18.4%	Reflected PuO <sub>2</sub> moderated compacts
PU-MET-FAST-001	1	100%	0	1,240,000	4.5%	Pu metal sphere
PU-MET-FAST-003	1 - 5	100%	0	628,000-1,250,000	6%	Pu metal buttons, bare and reflected
PU-MET-FAST-016	1 - 6	100%	0	7,800-11,700	6%	Flooded Pu metal cylinders
PU-MET-FAST-017	1 - 5	100%	0	93,800-783,000	6%	Moderated Pu metal cylinders
PU-MET-FAST-033	1	52.5%	0	400,000	5.9%	Graphite reflected Pu Cylinders
PU-MET-FAST-037	1,5,7,10,12,15,16	100%	0	18,300-146,000	6	Flooded Pu metal cylinders
BNWL2129T4	1	29%	9	6	11.5%	Reflected MOX moderated compacts
NSE55T5	1 - 10	30%	10	39-44	11.5%	Reflected MOX moderated compacts
PU-29 (NSE61)	1 - 9	29%	9	34-42	11.5%	Reflected MOX moderated compacts

**Table 5-2 AOA(3) Comparison of Key Parameters and Definition of Validated AOA**

Parameter	Design Application (cf. Table 4-1)	Benchmarks (cf. Table 5-1)	Validated AOA
Geometric shape	Parallelepipeds Arrays of cylinders Spheres	Parallelepipeds Arrays of cylinders Spheres	Parallelepipeds Arrays of cylinders Spheres
Absorber/reflector	Water, Cd, Concrete	Plexiglas, air, water	Water
Chemical form	PuO <sub>2</sub> powder	PuO <sub>2</sub> in polystyrene (C <sub>8</sub> H <sub>8</sub> ) Pu-metal in air/water	PuO <sub>2</sub> powder
Isotopic composition	4 wt. % <sup>240</sup> Pu	2.2 wt. % to 18.4 wt. % <sup>240</sup> Pu	4 wt. % <sup>240</sup> Pu
H/Pu	0 to 16.5	0 to 15	0 to 15
EALF [eV]	3 to 266,000	5 to 1,250,000	5 to 266,000

**Table 5-3 Critical Experiments Selected for AOA(4)**

Case ID	Exp.	Pu Content	H/(Pu+U)	EALF [eV]	<sup>240</sup> Pu wt. %	Description
NSE55T5	1 - 10	29%	2.8	39-44	11.5%	Reflected MOX moderated compacts
PU-29 (NSE61)	1 - 9	29%	2.8	34-42	11.5%	Reflected MOX moderated compacts
PU-COMP-MIXED-002	6 - 22	100%	5 - 15	5 - 93	2.2 - 11.5%	Reflected PuO <sub>2</sub> moderated compacts
BNWL2129T4	1 - 19	29%	2.8	1 - 6	11.5%	Reflected MOX moderated compacts
PU-8 (NSE61)	1 - 4	8%	7.3	0.6	11.6%	Reflected MOX moderated compacts

**Table 5-4 AOA(4) Comparison of Key Parameters and Definition of Validated AOA**

Parameter	Design Application (cf. Table 4-2)	Benchmark (cf. Table 5-3)	Validated AOA
Geometrical shape	Parallelepipeds Spheres	Parallelepipeds	Parallelepipeds Spheres
Absorber/reflector	Water	Plexiglas	Water Depleted Uranium
Chemical form	MOX powder	MOX and PuO <sub>2</sub> powder in polystyrene	MOX powder
Pu/(U+Pu) composition	6.3 or 22 wt. %	8 to 100% wt. %	8 to 22 wt. % <sup>1</sup>
Isotopic composition	4 wt. % <sup>240</sup> Pu	2.2 to 11.50 wt. % <sup>240</sup> Pu	4 wt. % <sup>240</sup> Pu
H/(U+Pu)	1.1 to 1.6	2.8 to 15	2.8 to 15 <sup>2</sup>
EALF [eV]	0.28 to 850	0.63 to 92.6	0.63 to 92.6 <sup>3</sup>

<sup>1</sup> 6.3 wt. % will be treated as out of AOA.

<sup>2</sup> H/(U+Pu) of 1.1 to 1.6 will be treated as out of AOA.

<sup>3</sup> EALF below 0.63 and above 92.6 will be treated as out of AOA.

## 5.1 AOA(3) PuO<sub>2</sub> POWDER MIXTURE

Seventy plutonium benchmarks are included in the AOA(3) experiment set. These include both metal systems and oxide systems. Justification for the inclusion of each of the benchmark sets is provided below

### 5.1.1 PU-COMP-MIXED-001

PU-COMP-MIXED-001 is a set of five unreflected benchmark cases utilizing plutonium oxide mixed with various quantities of polystyrene and compacted into cubes. These cubes are stacked in arrays to form critical configurations without Plexiglas reflection. Cases 2, 3, and 4 are taken from this set.

This experiment set is within the screening range for AOA(3). For the three experiments included, H/Pu varies from 5 to 15, Pu content is 100%, <sup>240</sup>Pu content is 2.2% to 11.46% and EALF varies from 32.6 to 1740 eV.

As noted above, the fissionable material in this set is plutonium oxide exactly matching the AOA(3) fissile material. Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(3) MFFF design applications.

The lack of reflector in this set is consistent with the range of configurations analyzed for AOA(3) which includes unreflected situations.

Since this experiment is within the screening range and has similar characteristics to the design application, it is included. The omitted cases within this experiment set have key parameters that fall outside the screening criteria and have been excluded.

### **5.1.2 PU-COMP-MIXED-002**

PU-COMP-MIXED-002 is a set of 29 experiments similar to PU-COMP-MIXED-001 involving plutonium oxide mixed with various quantities of polystyrene, and then compacted into cubes. For PU-COMP-MIXED-002, these cubes are stacked in array configurations with full reflection by Plexiglas. Twenty two of these reflected experiments are taken from this set for AOA(3). These are cases 01 through 22.

Cases 06 through 22 of this set are within the AOA(3) screening range. For these 17 experiments, H/Pu varies from 5 to 15, Pu content is 100%, <sup>240</sup>Pu content is 2.2% to 11.46% and EALF varies from 4.14 to 92.6 eV.

Experiments 01 through 05 of the PU-COMP-MIXED-002 set have primary parameter ranges that meet the AOA(3) screening range limits for all except the wt. % <sup>239</sup>Pu and <sup>240</sup>Pu. These five cases have 81.65% of <sup>239</sup>Pu (18.35 wt. % of <sup>240</sup>Pu), which is just below the 86.0% lower limit. The corresponding H/Pu for all five cases is 0.04, and EALF ranges from 1870 to 4920 eV. These five cases have been included in the AOA(3) benchmark set because the 81.65% <sup>239</sup>Pu content is close to the 86.0% screening range, which is considered to be an insignificant deviation, and the inclusion of these experiments adds EALF values that are important in filling gaps within the desired EALF validation range.

Further justification of the similar physical characteristics for these five cases is provided by a comparison of the fission spectra between this experiment and that of a typical AOA(3) design application (fully reflected PuO<sub>2</sub> sphere, density 3.25, 5% internal water) as shown in Figure 5-1.

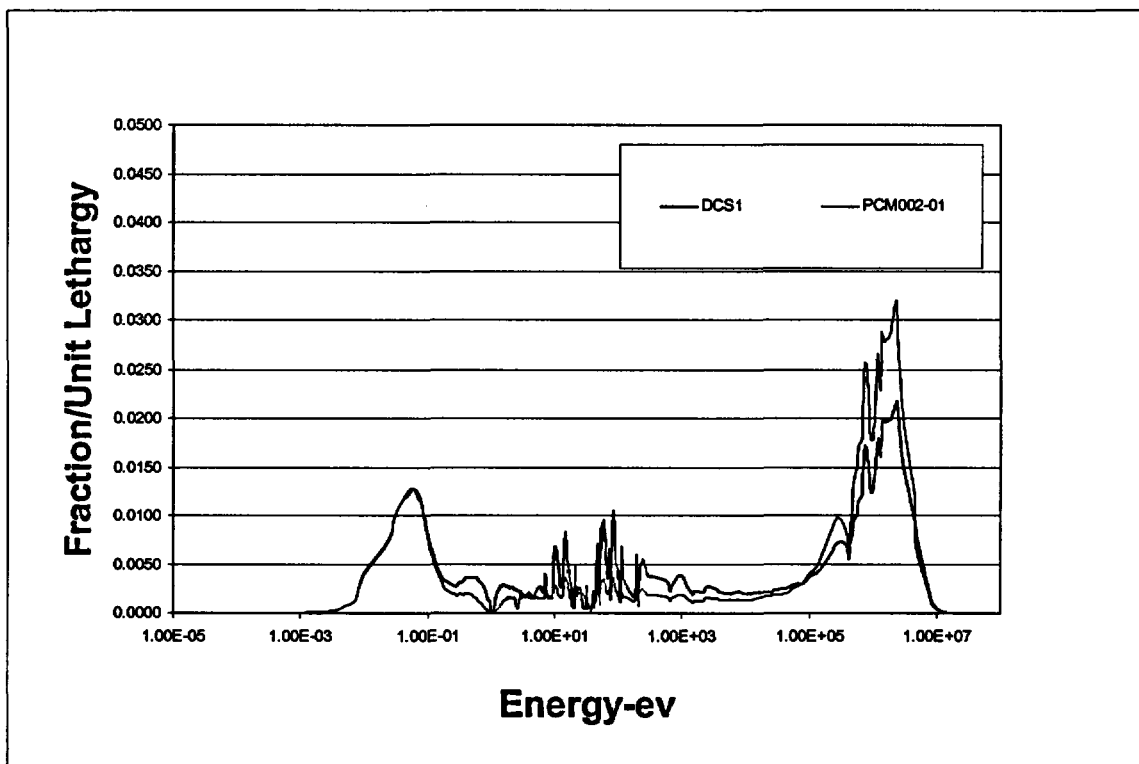


Figure 5-1 Neutron spectra comparison between PCM002-01 and MFFF typical design application

As can be seen from Figure 5-1 in both cases, the neutron spectra causing fissions are essentially identical with similar fissions occurring in both the low and high energy ranges providing additional justification for the applicability of this experiment to AOA(3).

As noted above, the fissionable materials in this set is plutonium oxide exactly matching the AOA(3) materials. Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(3) MFFF materials.

The presence of reflector in this set is consistent with the range of configurations analyzed for AOA(3) which includes reflected situations.

This experiment is included since it is within the screening range and has similar characteristics to the design application.

### 5.1.3 PU-MET-FAST-001

One plutonium metal experiment is included from this benchmark set. This is a bare metal sphere with a low  $^{240}\text{Pu}$  content, designated PU-MET-FAST-001.

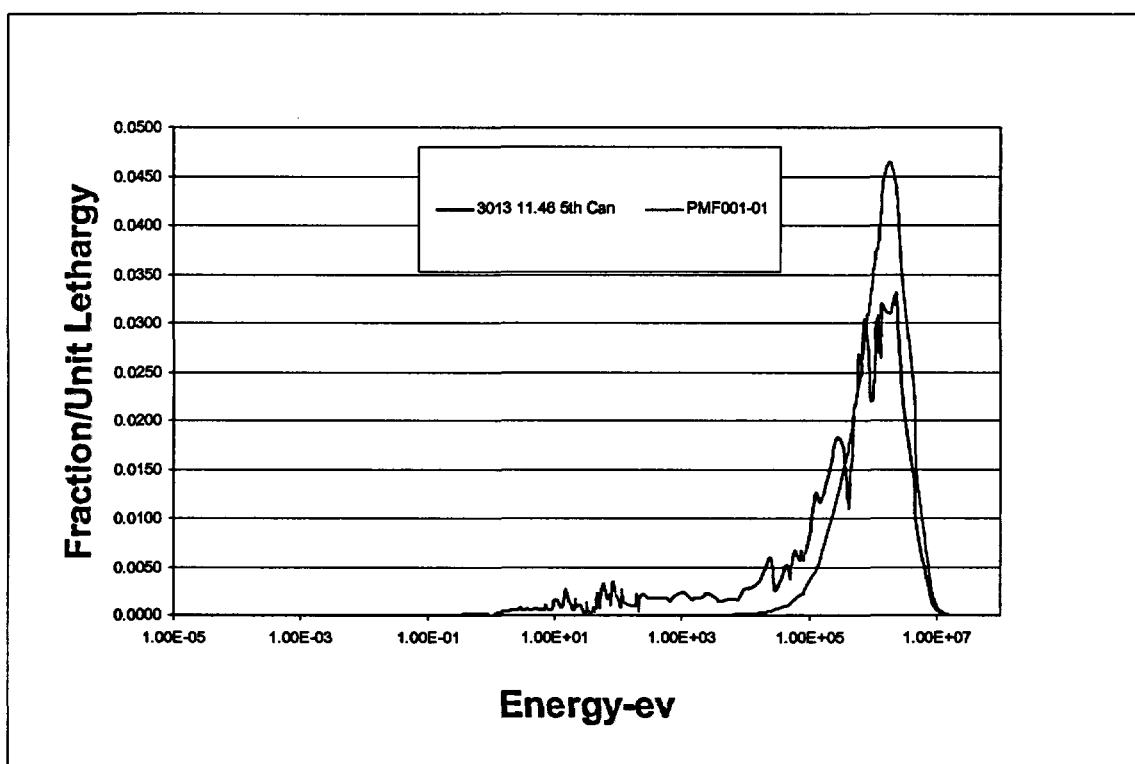
This experiment is within the screening range for AOA(3). For this experiment, H/Pu is 0,  $^{240}\text{Pu}$  content is 4.5%, EALF is 1,240,000 eV.

This experiment is Pu metal. It has physics characteristics similar to full theoretical density (11.46 g/cc) PuO<sub>2</sub> powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator, and thus H/Pu are 0 for both and both are unreflected. The limiting case of the MFFF storage area is sometimes unreflected, thus comparing some benchmarks which are also unreflected is appropriate.

The <sup>240</sup>Pu content of 4.5% is in excellent agreement with the analyzed value in the MFFF of 4%.

While the EALF of the experiment is higher than found in the MFFF, it is within the fast energy range consistent with the models developed for the MFFF storage area.

Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of the MFFF 3013 can storage area as shown in Figure 5-2.



**Figure 5-2 Neutron spectra comparison between PMF001-01 and MFFF typical design application**

As can be seen from Figure 5-2, in both cases, essentially all fissions occur in the fast energy region providing additional justification for the applicability of this experiment to AOA(3).

#### **5.1.4 PU-MET-FAST-003**

A set of five experiments using arrays of unmoderated plutonium metal buttons, either bare or with one side reflected by polyethylene, are included (PU-MET-FAST-003 Cases 1 through 5).

These experiments are within the screening range for AOA(3). For these experiments, H/Pu is 0,  $^{240}\text{Pu}$  content is 6%, EALF varies from 628,000 to 1,250,000 eV.

This experiment set is Pu metal. It has physics characteristics similar to full theoretical density (11.46 g/cc)  $\text{PuO}_2$  powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator. Some experiments are unreflected and some have a hydrogenous reflector. This is consistent with the MFFF storage area analysis which considers both reflected and unreflected configurations.

The  $^{240}\text{Pu}$  content of 6% is in good agreement with the analyzed value in the MFFF of 4%.

While the EALF of the experiment is higher than found in the MFFF, it is within the fast energy range consistent with the models developed for the MFFF storage area.

Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of the MFFF 3013 can storage area as shown in Figure 5-3.

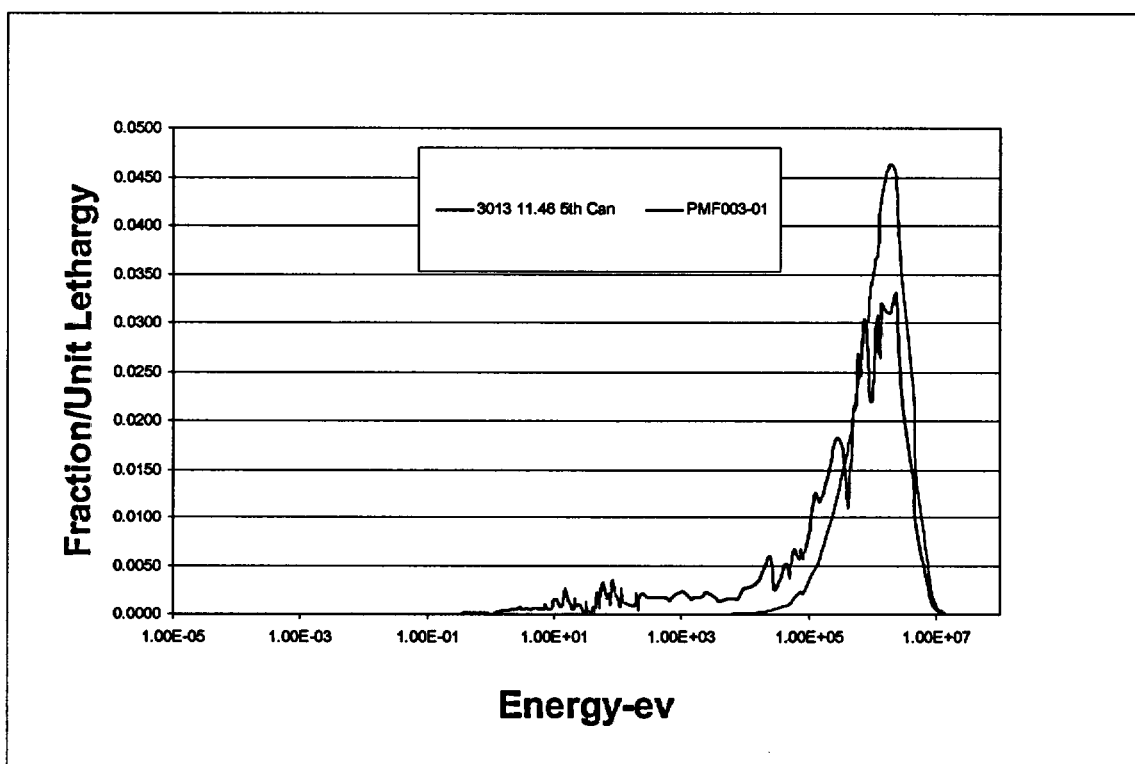


Figure 5-3 Neutron spectra comparison between PMF003-01 and MFFF typical design application

As can be seen from Figure 5-3, in both cases essentially all fissions occur in the fast energy region providing additional justification for the applicability of this experiment to AOA(3).



### 5.1.5 PU-MET-FAST-016

A group of six experiments using plutonium metal in cans placed in  $3 \times 3 \times 3$  arrays with water moderation and reflection are taken from PU-MET-FAST-016.

This experiment set is within the screening range for AOA(3). For these experiments, H/Pu is 0,  $^{240}\text{Pu}$  content is 6%, EALF varies from 7,800 to 11,700 eV.

This experiment set is Pu metal. It has physical characteristics similar to full theoretical density (11.46 g/cc)  $\text{PuO}_2$  powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator. The experiments are flooded with water and thus have a hydrogenous reflector. This is similar to the MFFF storage area which is analyzed in both reflected and unreflected configurations.

The  $^{240}\text{Pu}$  content of 6% is in good agreement with the analyzed value in the MFFF of 4%.

The range of EALF found in this experiment set is in the intermediate range and is in good agreement with that found in analyses of the MFFF storage area.

Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of a typical analyzed configuration of the MFFF 3013 can storage area with interspersed water as shown in Figure 5-4.

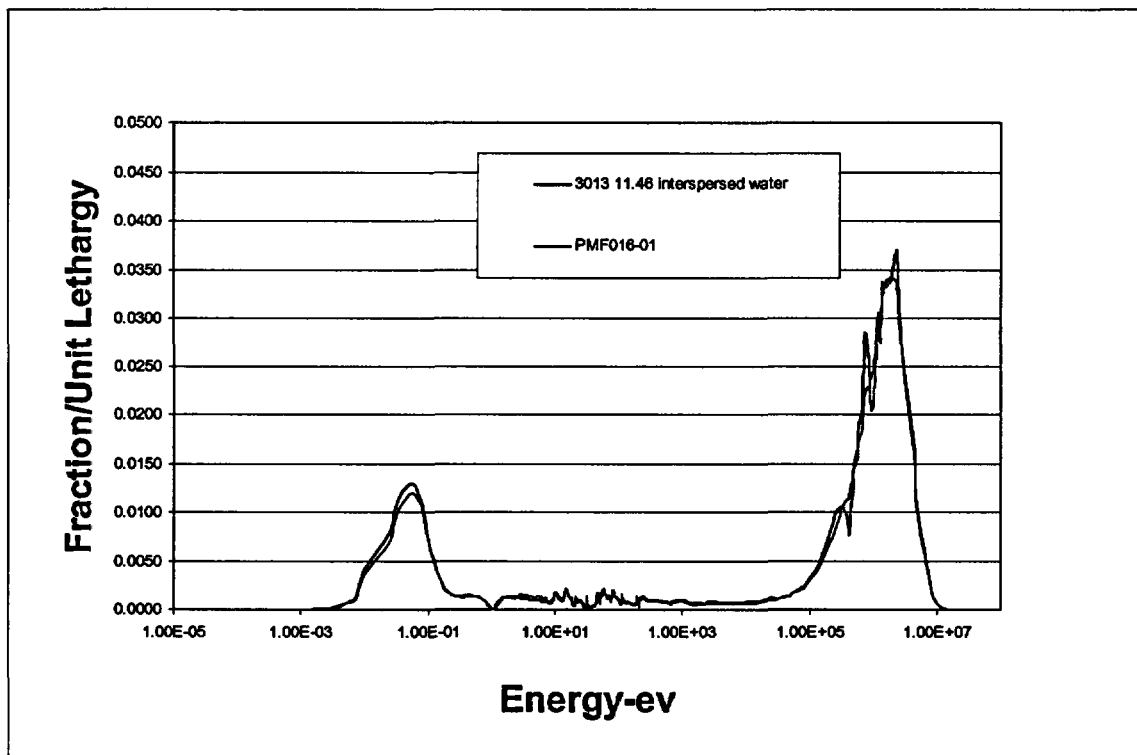


Figure 5-4 Neutron spectra comparison between PMF016-01 and MFFF typical design application

As can be seen from Figure 5-4, in both cases the neutron spectra causing fissions are essentially identical with similar fissions occurring in both the low and high energy ranges providing additional justification for the applicability of this experiment to AOA(3).

#### **5.1.6 PU-MET-FAST-017**

A group of five experiments using moderated arrays of plutonium metal cylinders are included from PU-MET-FAST-017.

This experiment set is within the screening range for AOA(3). For these experiments, H/Pu is 0,  $^{240}\text{Pu}$  content is 6.0%, EALF varies from 93,800 to 783,000 eV.

This experiment set is Pu metal. It has physics characteristics similar to full theoretical density (11.46 g/cc)  $\text{PuO}_2$  powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator. The experiments have some interspersed hydrogenous material between metal cans. This is similar to the MFFF storage area which is analyzed in both reflected and unreflected configurations.

The  $^{240}\text{Pu}$  content of 6.0% is in good agreement with the analyzed value in the MFFF of 4%.

The range of EALF found in this experiment set is primarily in the fast range and in good agreement with that found in analyses of the MFFF storage area.

Further justification of the similar physical characteristics is provided by a comparison of the neutron spectra causing fissions between this experiment and that of a typical analyzed configuration of the MFFF 3013 can storage area with interspersed water as shown in Figure 5-5.

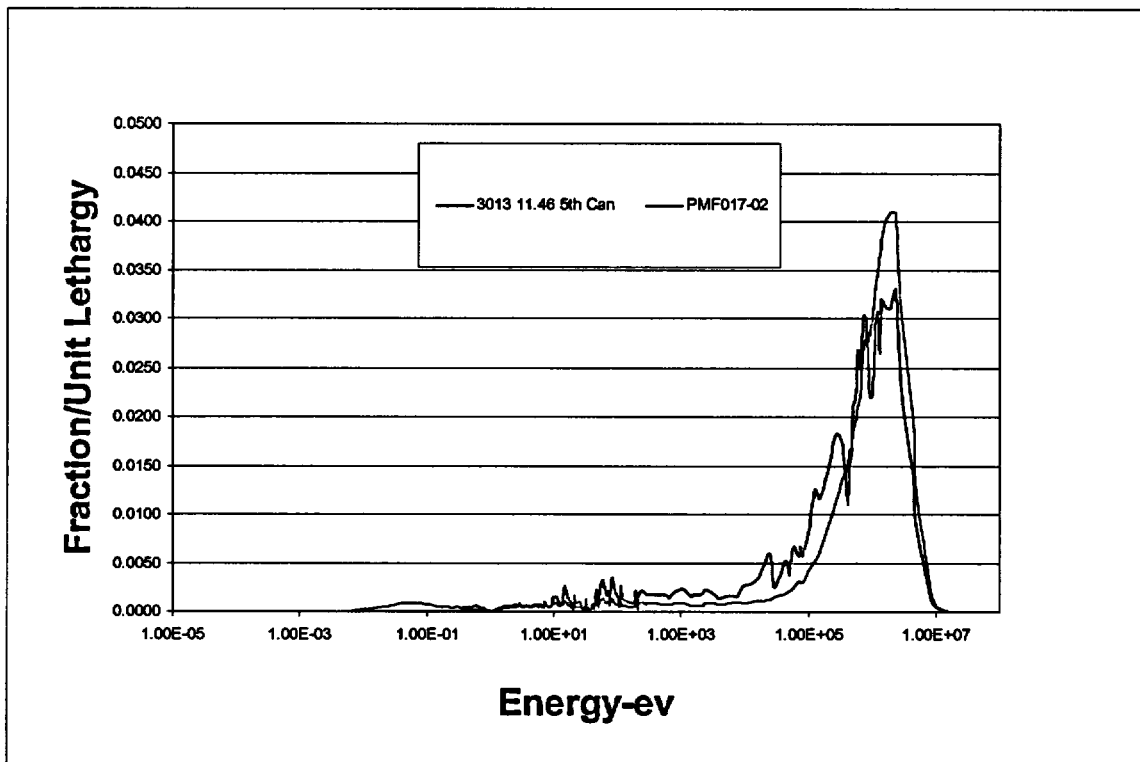


Figure 5-5 Neutron spectra comparison between PMF017-02 and MFFF typical design application

As can be seen from Figure 5-5, in both cases essentially all fissions occur in the fast energy region providing additional justification for the applicability of this experiment to AOA(3).

### 5.1.7 PU-MET-FAST-033

One plutonium metal experiment is included from this benchmark set. This is a cylindrical assembly of Pu metal with a low  $^{240}\text{Pu}$  content, designated PU-MET-FAST-033.

This experiment is within the screening range for AOA(3). For this experiment, H/Pu is 0,  $^{240}\text{Pu}$  content is 5.9%, EALF is 400,000.

This experiment is Pu and depleted U metal. It has physical characteristics similar to full theoretical density (11.46 g/cc)  $\text{PuO}_2$  powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator; hence H/Pu is 0 for both, and both are unreflected by hydrogen. (The limiting case of the MFFF storage area is sometimes unreflected.) The experiment is reflected by graphite, but, as discussed below, this material provides little impact on the neutron spectra causing fissions.

The  $^{240}\text{Pu}$  content of 5.9% is in good agreement with the analyzed value in the MFFF of 4%.

While the EALF of the experiment is slightly higher than found in the MFFF, it is within the fast energy range, just as the MFFF storage area is.

The experiment falls outside the screening criteria for AOA(3) due to the Pu content (52.5%) of the fissile material. However, the H/Pu ratio (0),  $^{240}\text{Pu}$  content (5.9 wt. %) and EALF (400,000 eV) are consistent with the screening criteria for AOA(3).

Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of the MFFF 3013 can storage area as shown in Figure 5-6.

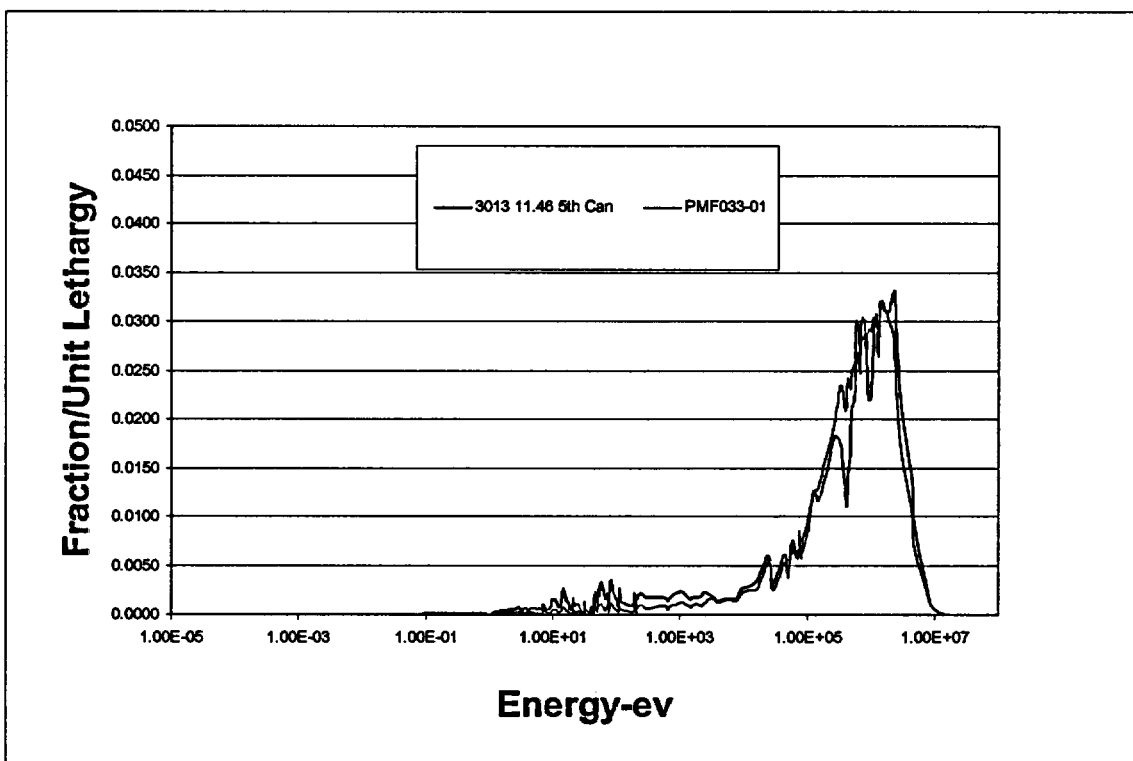


Figure 5-6 Neutron spectra comparison between PMF033-01 and MFFF typical design application

As can be seen from Figure 5-6, there is excellent agreement in the neutron spectra causing fissions between both cases. As noted previously, in spite of the presence of the graphite reflector the agreement with the MFFF 3013 can storage area design application is excellent. In both cases, essentially all fissions occur in the fast energy region providing additional justification for the applicability of this experiment to AOA(3).

### 5.1.8 PU-MET-FAST-037

A group of seven experiments using moderated arrays of plutonium metal cylinders are included from PU-MET-FAST-037.

This experiment set is within the screening range for AOA(3). For these experiments, H/Pu is 0,  $^{240}\text{Pu}$  content is 6.0%, EALF varies between 18,300 and 146,000 eV.

This experiment is Pu metal. It has physics characteristics similar to full theoretical density (11.46 g/cc)  $\text{PuO}_2$  powder modeled in the MFFF storage area. Both applications have no internal hydrogen moderator. The experiments have some interspersed hydrogenous material between metal cans. This is similar to the MFFF storage area which is analyzed in both reflected and unreflected configurations.

The  $^{240}\text{Pu}$  content of 6.0% is in good agreement with the analyzed value in the MFFF of 4%.

The range of EALF found in this experiment set is in both the intermediate and the fast range and in good agreement with that found in analyses of the MFFF storage area.

Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of a typical analyzed configuration of the MFFF 3013 can storage area with interspersed water as shown in Figure 5-7.

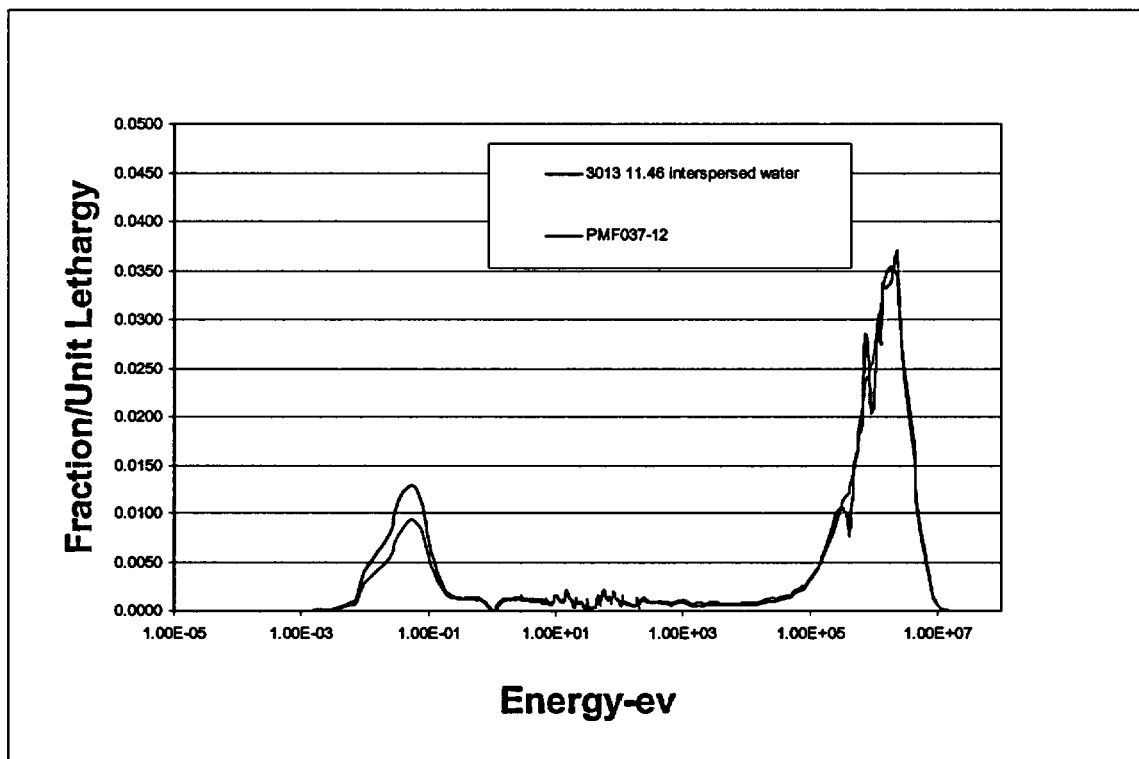


Figure 5-7 Neutron spectra comparison between PMF037-12 and MFFF typical design application

As can be seen from Figure 5-7, there is excellent agreement in the neutron spectra causing fissions between both cases. In both cases, most fissions occur in the fast energy region with some in the thermal region providing additional justification for the applicability of this experiment to AOA(3).

### 5.1.9 BNWL2129T4

This experiment set is based on the Bierman MOX polystyrene compact experiment described in [24]. Although the experiment involves a mixed oxide material, the predominant fissile contribution is made by  $^{239}\text{Pu}$ . Of the 19 cases described in Table IV of the report, only Case 1 is included in the AOA(3) experiment set, since the remaining cases involve absorber materials, and the inclusion of cases combining both uranium and an additional absorber material is deemed to be too far outside the desired experiment criteria.

The experiment falls outside the screening criteria for AOA(3) due to the mixed oxide nature of the fissile material. The H/Pu (9.47),  $^{240}\text{Pu}$  content (11.5 wt. %) and EALF value (6.14 eV) are consistent with the screening criteria for AOA(3).

The presence of fissionable uranium in the system does not significantly perturb the fission spectrum in comparison to that of a typical MFFF design application model, as shown in Figure 5-8. Here, the fission spectrum for the modeled MFFF Pu Buffer Store shows close agreement with that of Case 1 over the entire spectrum of neutron energies.

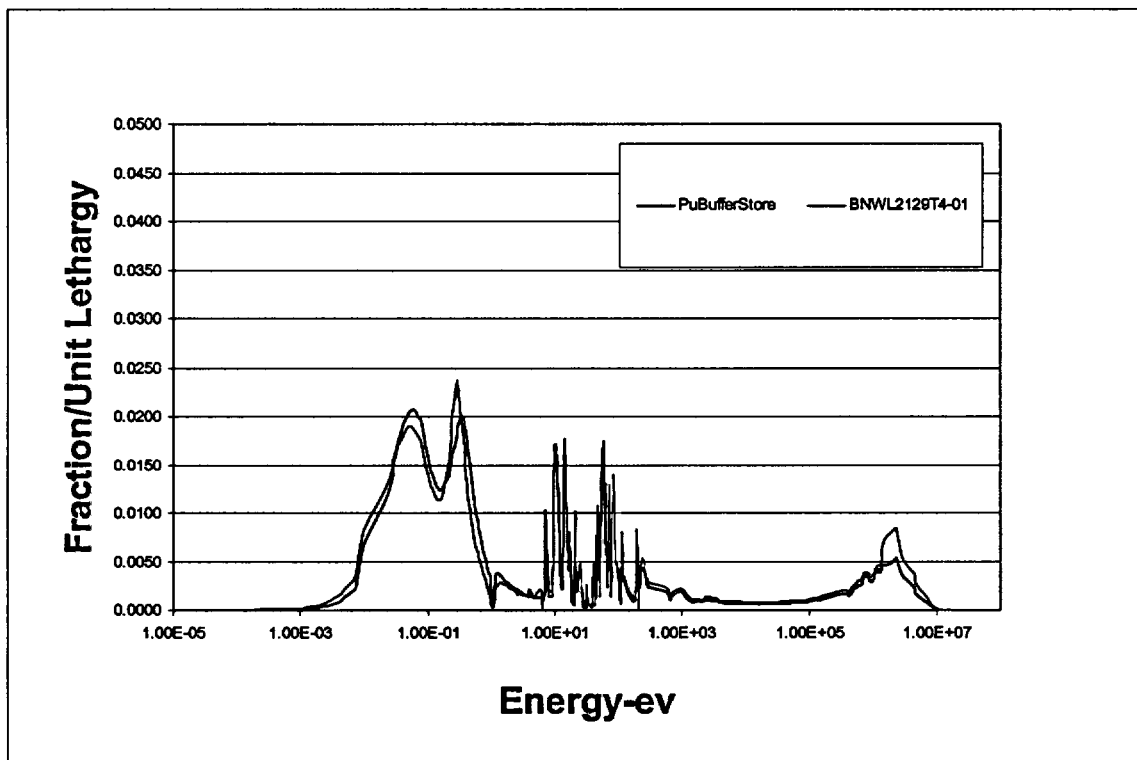


Figure 5-8 Neutron spectra comparison between BNWL2129T4-01 and MFFF typical design application

#### 5.1.10 NSE55T5

The ten cases shown in Table 5 of NSE55 [22] are included in the experiment set for AOA(3). These cases are comprised of the same MOX and polystyrene compacts employed in the BNWL2129 experiment discussed above. Although the experiment involves a mixed oxide material, the predominant fissile contribution is made by  $^{239}\text{Pu}$ .

The experiment falls outside the screening criteria for AOA(3) due to the mixed oxide nature of the fissile material. However, the H/Pu ratio (9.55),  $^{240}\text{Pu}$  content (11.5 wt. %) and EALF range (39-44 eV) are consistent with the screening criteria for AOA(3). The fissile material contains a relatively high Pu content (29.3 wt. %) which dominates the relatively minor neutronic contribution from  $^{238}\text{U}$  in the system.

The presence of fissionable uranium in the system does not significantly perturb the fission spectrum in comparison to that of a typical MFFF design application model, as shown in Figure 5-9. Here, the fission spectrum for a representative AOA(3) design application shows close agreement with that of Case 1 over the entire spectrum of neutron energies.

Additionally, although the experimental configurations contain extraneous absorbers such as copper, copper-cadmium and aluminum sheets, the neutronic influence of these materials does not significantly impact the neutron spectra causing fissions. Cadmium is a strong absorber of neutrons at energies near its resonance at 0.18 eV, but the experimental configuration consists of relatively low H/(U+Pu) fissile material, with EALF ranging from 34 to 42 eV well above the active cadmium resonance region. Hence, the presence of the cadmium in three experimental cases is not expected to significantly impact the results. Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of the typical MFFF AOA(3) design application (fully reflected  $\text{PuO}_2$  sphere, density  $2.9 \text{ g/cm}^3$ , 16.6% internal water) as shown in Figure 5-9.

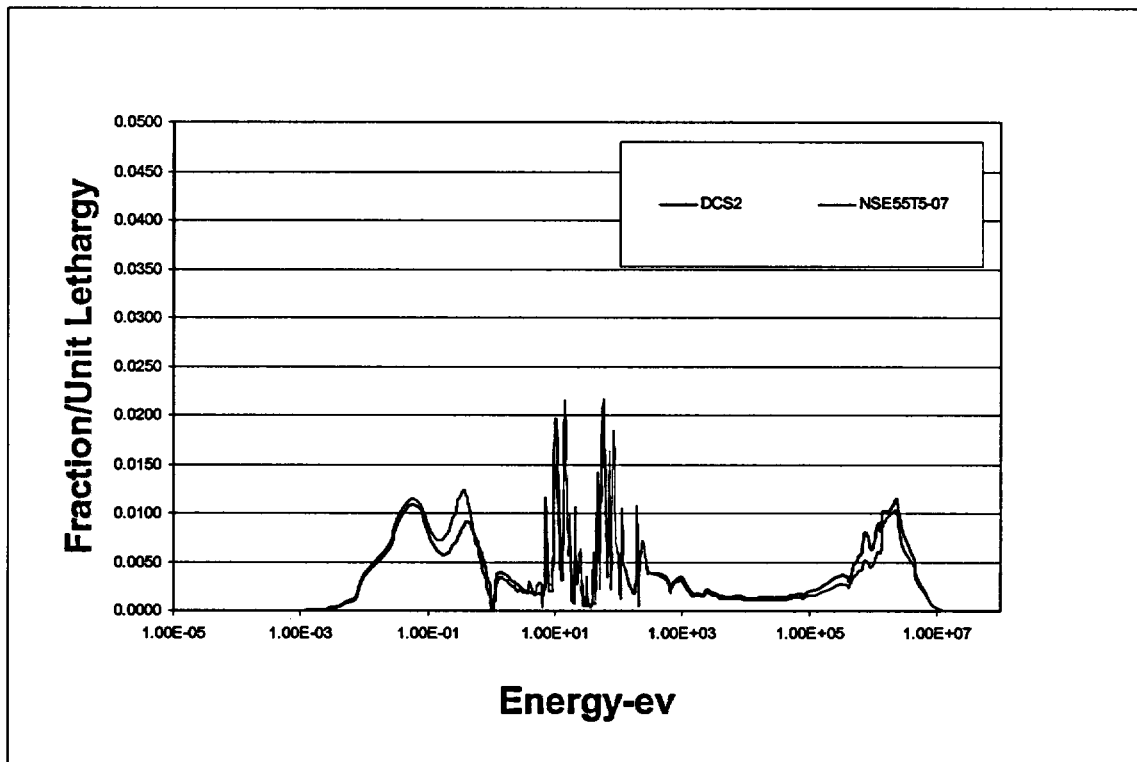


Figure 5-9 Neutron spectra comparison between NSE55T5-07 and MFFF typical design application

#### 5.1.11 PU-29 (NSE61)

The nine Pu-29-1 cases shown in NSE61 [23] are included in the experiment set for AOA(3). This experiment set is based on the Bierman MOX polystyrene compact experiment described in [23]. PU-29-1 is a set of nine reflected benchmark cases utilizing a mixture of plutonium oxide and depleted uranium oxide mixed with polystyrene and compacted into cubes. These cubes are stacked in arrays to form critical configurations with Plexiglas reflection. These cases are comprised of the same MOX and polystyrene compacts employed in the BNWL2129 experiment discussed above. Although the experiment involves a mixed oxide material, the predominant fissile contribution is made by  $^{239}\text{Pu}$ .

The experiment falls outside the screening criteria for AOA(3) due to the mixed oxide nature of the fissile material. However, the H/Pu ratio (9.47),  $^{240}\text{Pu}$  content (11.5 wt. %) and EALF range (34-41 eV) are consistent with the screening criteria for AOA(3). The fissile material contains a relatively high Pu content (29.3 wt. %) which dominates the relatively minor neutronic contribution from  $^{238}\text{U}$  in the system.

The presence of reflector in this set is consistent with the range of configurations analyzed for AOA(3) which includes reflected situations.



The presence of fissionable uranium in the system does not significantly perturb the fission spectrum in comparison to that of a typical MFFF design application model, as shown in Figure 5-10. Here, the fission spectrum for a representative AOA(3) design application shows close agreement with that of Case 1 over the entire spectrum of neutron energies.

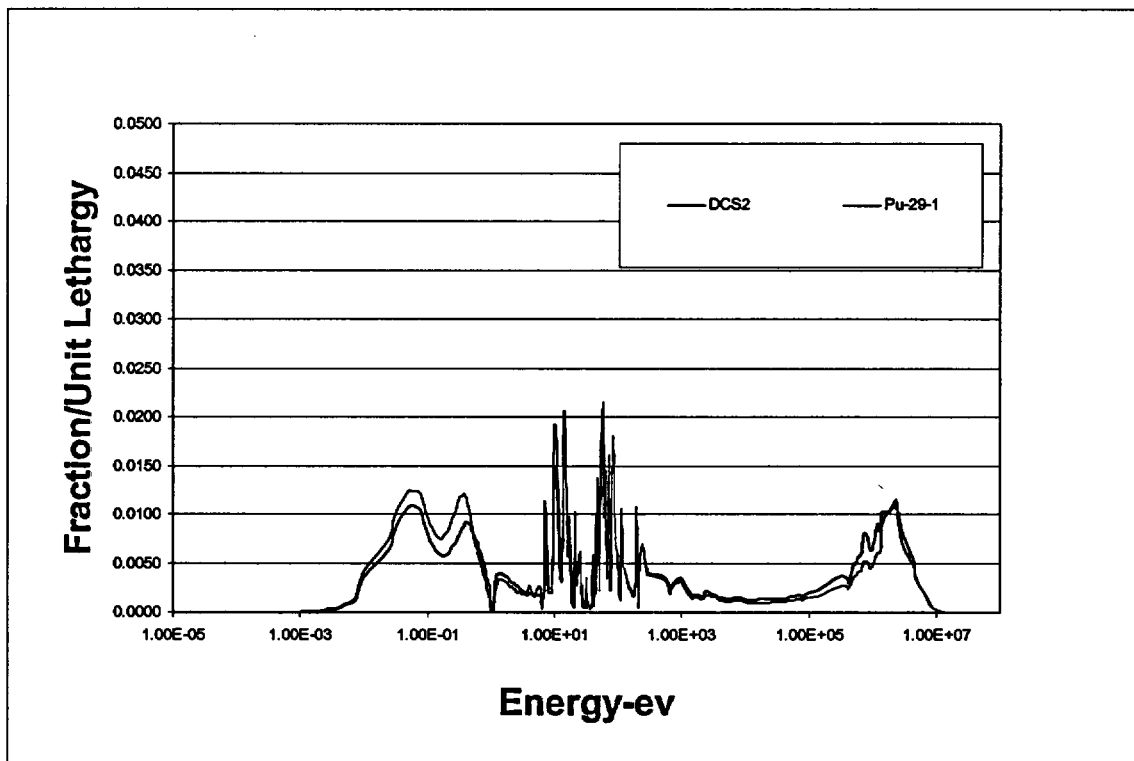


Figure 5-10 Neutron spectra comparison between Pu-29-1 and MFFF typical design application

## 5.2 AOA (4) MOX POWDER MIXTURE

Fifty-nine plutonium benchmarks are included in the validation experiment set for AOA(4). These include hydrogenous moderated and reflected oxide systems. Justification for the inclusion of each of the benchmark sets is provided below.

### 5.2.1 NSE55T5

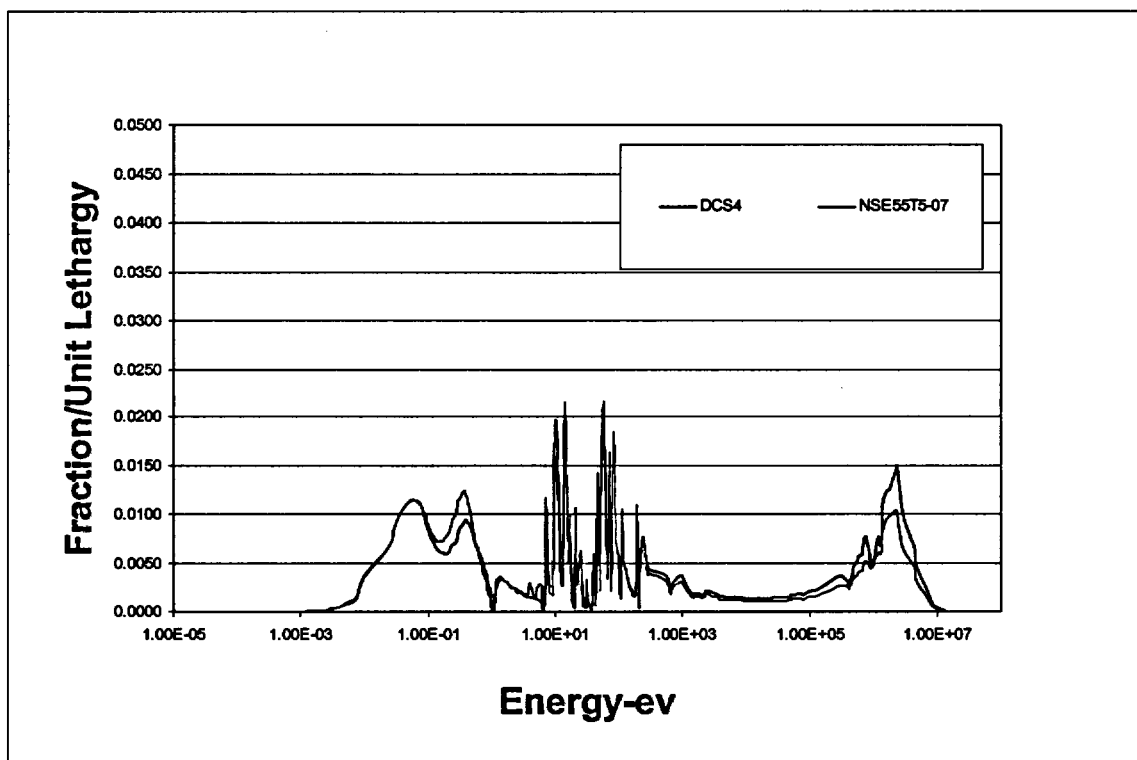
Ten experiments described in Table 5 of the NSE55 [22] paper are included in the experiment set for AOA(4). These cases are comprised of the same MOX and polystyrene compacts employed in the BNWL2129 [24] experiment discussed previously.

These cases are in very close agreement with the screening criteria. The H/(U+Pu) ratio for the cases is 2.79 and EALF ranges from 39 to 44 indicating good agreement with the moderation and energy spectrum parameters of the desired validation range. <sup>240</sup>Pu content is 11.5 wt. % and is within the screening range of 0 to 16 wt. %. The Pu content of the fissile material is 29.3 wt. %, again falling within the desired screening range of 1.2 to 52 wt. %.

As noted above, the fissionable material in this set is a mixture of plutonium oxide and depleted uranium oxide within the screening range for the AOA(4) fissile material and very similar to the MFFF primary blend. Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(4) MFFF design applications.

The presence of reflector in this set is consistent with the range of configurations analyzed for AOA(4) which includes reflected situations.

Although the experimental configurations contain extraneous absorbers such as copper, copper-cadmium and aluminum sheets, the neutronic influence of these materials does not significantly impact the neutron spectra causing fissions. Cadmium is a strong absorber of neutrons at energies near its resonance at 0.18 eV, but the experimental configuration consists of relatively low H/(U+Pu) fissile material, with EALF ranging from 39 to 44 eV well above the active cadmium resonance region. Hence, the presence of the cadmium in three experimental cases is not expected to significantly impact the results. Further justification of the similar physical characteristics is a comparison of the neutron spectra causing fissions between this experiment and that of a typical AOA(4) design application (primary blend sphere, 5% water moderation, full reflection) as shown in Figure 5-11.



**Figure 5-11 Neutron spectra comparison between NSE55T5-07 and MFFF typical design application**



As can be seen from Figure 5-11, there is excellent agreement in the neutron spectra causing fissions between both cases. In both cases, fissions occur in both the intermediate and the fast energy region with some in the thermal region providing additional justification for the applicability of this experiment to AOA(3).

Since this experiment is within the screening range and has similar characteristics to the design application, it is included.

### **5.2.2 Pu-29-1 (NSE61)**

The nine Pu-29-1 cases shown in NSE61 [23] are included in the experiment set for AOA(4). These nine reflected benchmark cases utilize plutonium oxide mixed with polystyrene and compacted into cubes. These cubes are stacked in arrays to form critical configurations with Plexiglas reflection.

This experiment set is within the screening range for AOA(4). For the nine experiments, H/(Pu+U) is 2.8, Pu content is 29.3%, <sup>240</sup>Pu content is 11.50% and EALF varies from 34 to 42 eV.

As noted above, the fissionable material in this set is a mixture of plutonium oxide and depleted uranium oxide within the screening range for the AOA(4) fissile material and very similar to the MFFF primary blend. Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(4) MFFF design applications.

The presence of reflector in this set is consistent with the range of configurations analyzed for AOA(4) which includes reflected situations.

Since this experiment is within the screening range and has similar characteristics to the design application, it is included.

### **5.2.3 PU-COMP-MIXED-002**

PU-COMP-MIXED-002 is a set of 29 experiments that involve 100% plutonium oxide (and no UO<sub>2</sub>) that has been mixed with various quantities of polystyrene and compacted into cubes. For PU-COMP-MIXED-002, these cubes are stacked in array configurations with full reflection by Plexiglas. For AOA(4), 17 of these reflected experiments are taken from this benchmark evaluation, Cases 06 through 22.

This experiment set is not within the screening range for AOA(4). For the experiments included, the deviating parameters are the H/Pu, which varies from 5 to 15, and the Pu content, which is 100%. However, both the <sup>239</sup>Pu content, which is 88.54% and 97.8%, and the EALF, which varies from 4.14 to 92.6 eV, are within the screening range.

This set of 17 experiments has been included in AOA(4) because, while the cases do not meet the H/(Pu + U) and wt. % PuO<sub>2</sub> ranges, they are neutronically very similar to AOA(4) design applications. This is illustrated not only by the similarity in EALF ranges but also by the illustration shown in Figure 5-12 which gives a comparison of the neutron spectra causing fissions for a typical AOA(4) design application and Case 06.

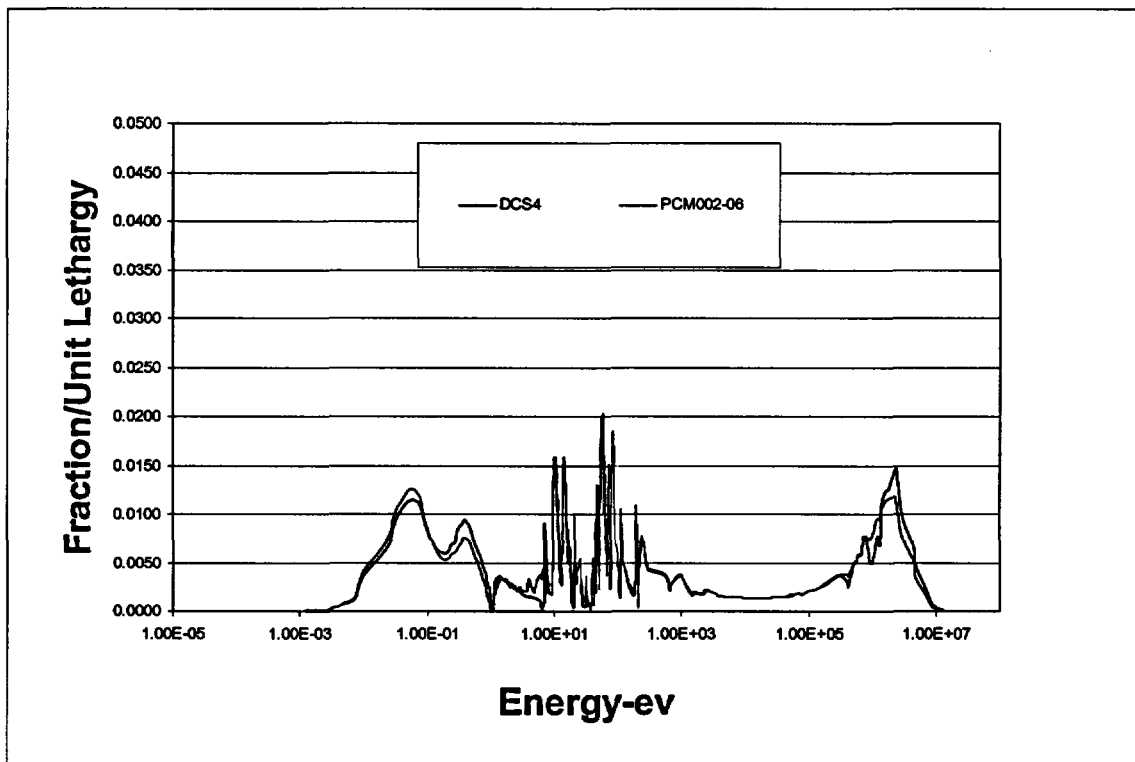


Figure 5-12 Neutron spectra comparison between PCM002-06 and MFFF typical design application

As can be seen from Figure 5-12, in both cases the neutron spectra causing fissions are essentially identical with similar fissions occurring throughout the low, intermediate and high energy ranges providing additional justification for the applicability of this experiment to AOA(4).

As noted above, the fissile material in this set is plutonium oxide that very closely matches the fissile material in AOA(4). Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(4) MFFF materials.

The presence of a reflector in this set is consistent with the range of configurations analyzed for AOA(4) which includes reflected situations.

Although these experiments do not contain  $^{238}\text{U}$  and fall outside the AOA(4) screening criteria, they have very similar neutronic characteristics to anticipated AOA(4) design applications, so they have been included to augment benchmarks in the 4 – 100 eV EALF range.

#### 5.2.4 BNWL2129T4

The 19 cases shown in Table IV of BNWL2129 [24] are included in the experiment set for AOA(4). The experiment involves a mixed oxide material with a Pu content of 29.3% within the

screening range for AOA(4). The H/X (2.8),  $^{240}\text{Pu}$  content (11.5 wt. %) and EALF values (1-6 eV) are consistent with the screening criteria for AOA(4).

The experiments in this series are comprised of fissile material contained polystyrene compacts with three differing concentrations of fissile material. Although the concentrations vary, in all cases one dominant material type contains at least 93% of all  $^{239}\text{Pu}$  atoms present in the system. Hence, the key parameters for the system, such as H/X and  $^{240}\text{Pu}$  content, are defined based in the corresponding parameters for this dominant material.

The experiment falls outside the screening criteria for AOA(4) because some cases contain potentially strong absorbers such as boron or cadmium. On the other hand, some cases contain no or weak absorbers such as steel, lead, and aluminum.

The presence of strong absorbers in the system does not significantly perturb the fission spectrum in comparison to that of a typical MFFF design application model, as shown in Figure 5-13. Here, the fission spectrum for the MFFF homogenizer/pelletizer unit containing additives shows close agreement with that of Case 12 over the entire spectrum of neutron energies. Even though this benchmark case contains BORAL poison plates, the neutron spectrum shows good agreement and provides justification that the neutron physics characteristics of the benchmark experiment are similar to that found in typical MFFF design applications.

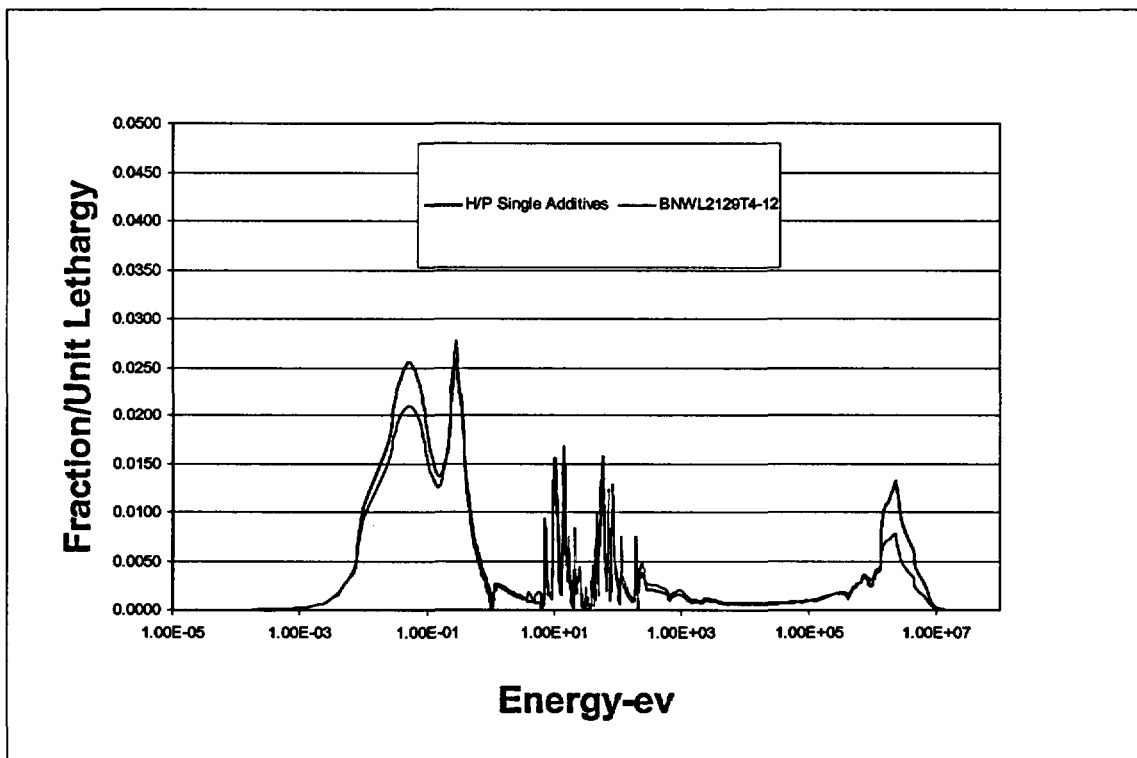


Figure 5-13 Neutron spectra comparison between BNWL2129T4-12 and MFFF typical design application

Examination of all other types of experiments in this set such as that for Case 10 which contains depleted uranium also show good agreement as illustrated in Figure 5-14.

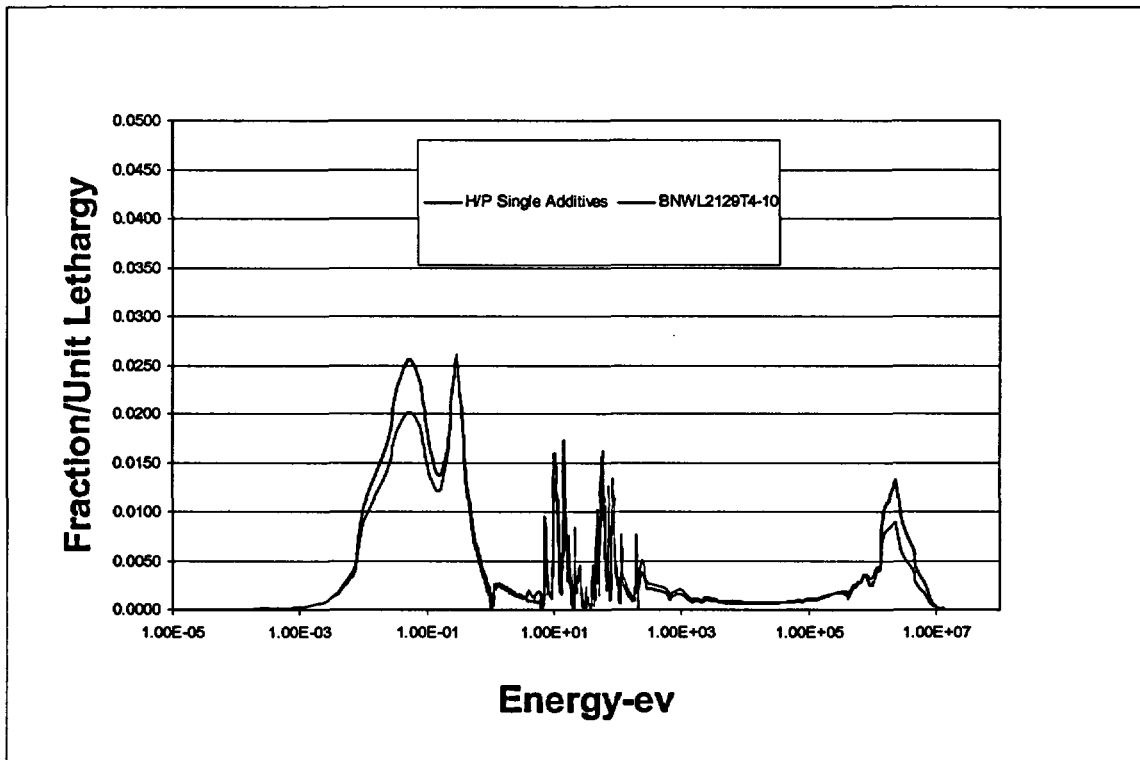


Figure 5-14 Neutron spectra comparison between BNWL2129T4-10 and MFFF typical design application

Similarly, the presence of the potentially strong absorber cadmium, as in Case 15, shows good agreement in the fission spectrum with that of the typical MFFF design application as shown in Figure 5-15.

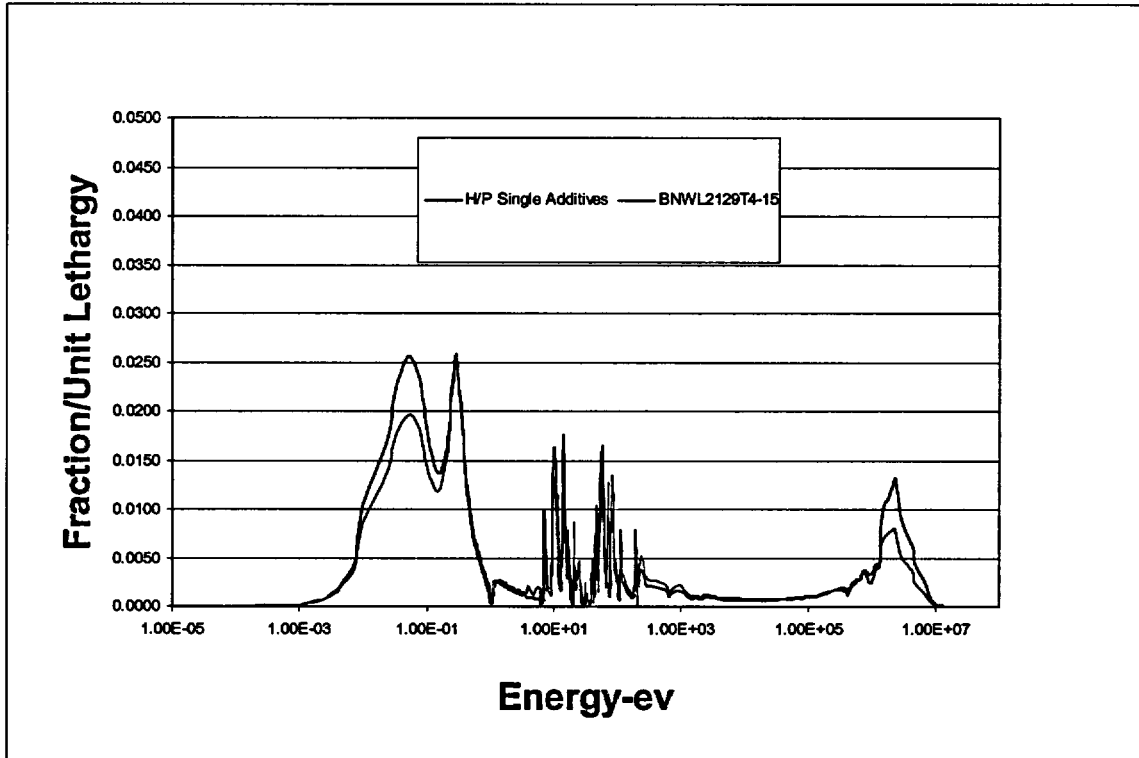


Figure 5-15 Neutron spectra comparison between BNWL2129T4-15 and MFFF typical design application

The presence of the relatively weak neutron absorber (lead), as in Case 17, continues to show good agreement in the fission spectrum with that of the typical MFFF design application as shown in Figure 5-16.

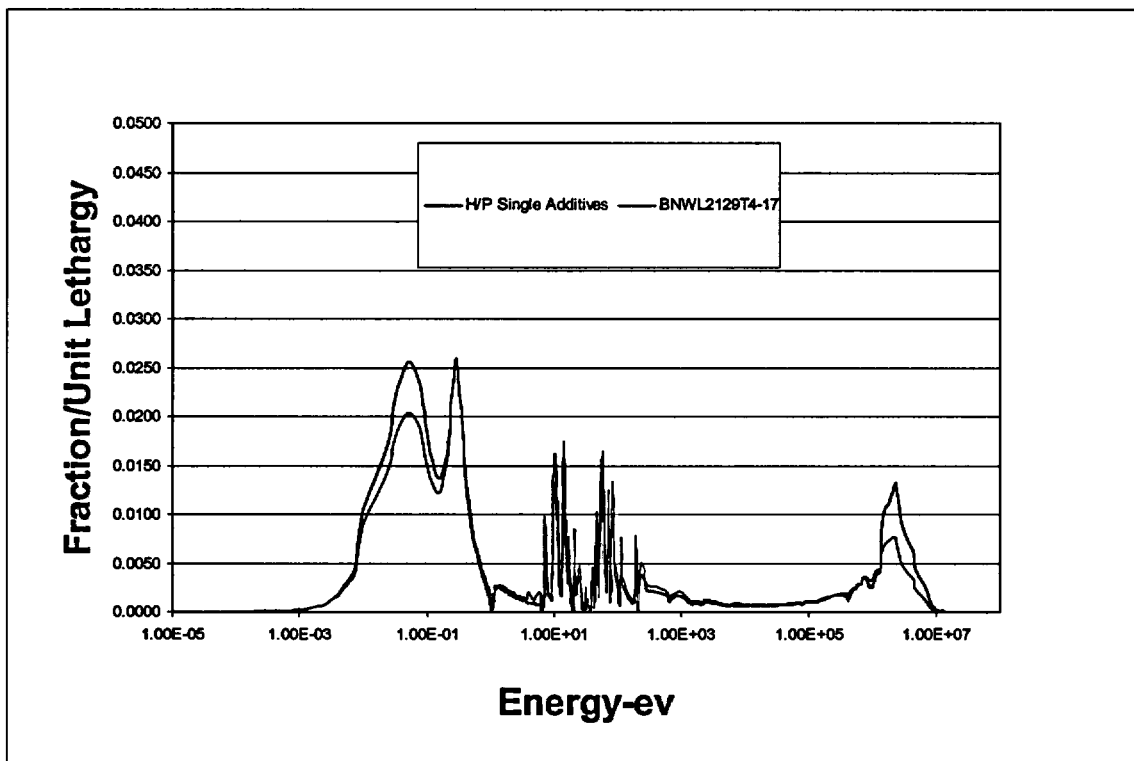


Figure 5-16 Neutron spectra comparison between BNWL2129T4-17 and MFFF typical design application

Thus the presence of various neutron absorbers do not significantly affect the neutron spectra causing fissions. Since other major characteristics of this set, such as the H/X, the fissile media content and moderator are in good agreement with the screening range, this experiment set is judged acceptable.

#### 5.2.5 Pu-8-1

Pu-8 is a set of four experiments that involve ~8% plutonium oxide and depleted uranium oxide that has been homogeneously blended with polystyrene, and then compacted into cubes. The plutonium consisted of ~11.5 wt.%  $^{240}\text{Pu}$  (~88.5 wt.%  $^{239}\text{Pu}$ ) and the  $^{235}\text{U}$  content of the depleted uranium was ~0.2 wt.%. For all four cases, the resulting H/(Pu + U) atomic ratio of the compacts was 7.33, a value slightly above the AOA(4) revised screening upper range of 3.84. The cubes in each experiment are stacked in array configurations with full reflection by Plexiglas.

This experiment set is within the revised screening range for AOA(4) except for the H/(Pu + U) values. In addition to the wt.%  $^{239}\text{Pu}$  and wt.%  $^{235}\text{U}$  values (and corresponding wt.%  $^{240}\text{Pu}$  and  $^{238}\text{U}$  values) mentioned in the above paragraph, the EALFs for the four cases are in the thermal range and vary between 0.632 – 0.643 eV.

These four cases have been included in the AOA(4) benchmark set because the 7.33 H/(Pu + U) ratio is not much above the 3.84 upper value for the revised screening range, which is considered



to be an insignificant deviation, and the inclusion of these experiments adds EALF values that are important in filling gaps within the desired EALF validation range. Additionally, the Pu content of this set, 8%, is very near to the maximum Pu content in MFFF final blend (6.3%). This inclusion of this set in the AOA(4) benchmarks is also justified by the neutron spectra causing fissions illustration shown in Figure 5-17, which shows a comparison of the neutron spectra causing fissions for a typical AOA(4) design application, involving final blend, (Homogenizer/Pelletizer with a bounding double amount of additives) and experiment Case 1.

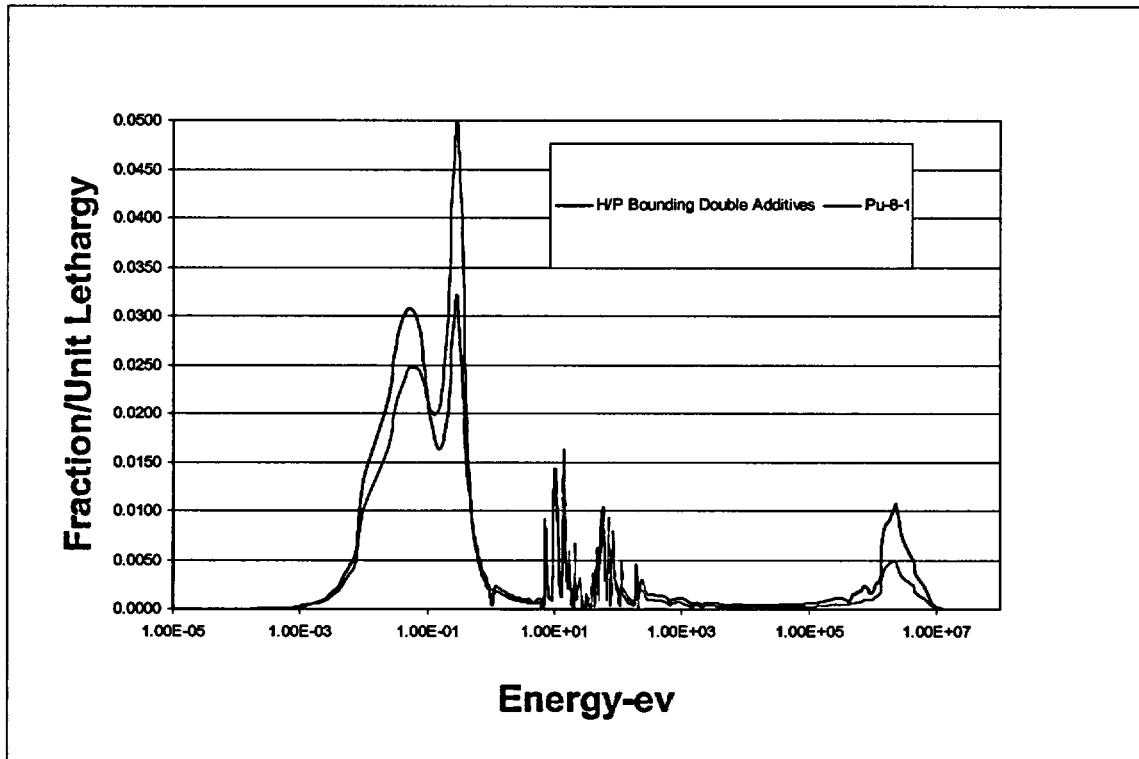


Figure 5-17 Neutron spectra comparison between Pu-8-1 and MFFF typical design application

As can be seen from Figure 5-17, in both cases the neutron spectra causing fissions are essentially identical in shape with similar fissions occurring throughout the low, intermediate and high energy ranges providing additional justification for the applicability of this experiment to AOA(4).

As noted above, the fissile material in this set is plutonium oxide that very closely matches the fissile material in AOA(4). Hydrogen is contained in the polystyrene moderator for this set matching the hydrogen moderator in the AOA(4) MFFF materials.

The presence of a reflector in this set is consistent with the range of configurations analyzed for AOA(4) which includes reflected situations.

## 6. ANALYSIS OF VALIDATION RESULTS

As noted in previous sections, the selection process for applicable benchmarks is as follows:

- 1) Review areas of applications, identify key parameters, and identify key parameter ranges based upon both the established current design analyses and the potential needs of subsequent analyses.
- 2) Develop screening criteria.
- 3) Identify the applicable experiments in the database of benchmark experiments that meet the screening criteria.
- 4) Investigate and justify experiments which may be applicable based on similarity of key parameters.

Section 3.6 provides a description of the process. Section 4 implements the process. Section 5 discusses the various benchmark experiment sets. This section lists the experiments selected and analyzes the results to determine conservative limits to which calculations may be performed. This section also shows plots of the selected benchmarks as a function of key parameters.

### 6.1 DESIGN APPLICATION (3) – PuO<sub>2</sub> POWDER

The benchmark experiments identified in Section 5.1 are modeled with CSAS26/KENO VI using the 238 group library 238GROUPNDF5. The calculated  $k_{eff}$  values for selected benchmark experiments are presented in Table 6-1.

Figure 6-1 shows the distribution of calculated  $k_{eff}$  values for the experiments as calculated with SCALE 4.4a (KENO-VI Update 3) on the PC platform. The  $k_{eff}$  values are first analyzed statistically using the USLSTATS computer code. Although the data passes the test for normality employed in that analysis, a visual inspection of the histogram shown in Figure 6-1 suggests that the data is not normally distributed. Three subsequent statistical tests for normality (Anderson-Darling, Ryan-Joiner, and Kolmogorov-Smirnov) indicated that the data fails the test for normality with a likelihood greater than 0.99. Hence, the nonparametric technique described in Section 3.2.3 is employed.

With a total of 70 unique experiments for this AOA, the degree of confidence,  $\beta$ , obtained from Equation 3.3 is 97.2%. Hence, the required nonparametric margin obtained from Table 3-1 is 0.0. The minimum computed benchmark  $k_{eff}$  is  $0.9876 \pm 0.0006$  obtained for case PMF003-03 [5]. The experimental uncertainty determined for this case in the Handbook evaluation [5] is 0.0030. The resulting combined uncertainty associated with this benchmark calculation is

$$\sqrt{0.0030^2 + 0.0006^2} = 0.0031$$

The resulting USL for AOA(3) is then determined from Equation 3.1 as

USL = Smallest  $k_{eff}$  value – Uncertainty for smallest  $k_{eff}$  – Nonparametric margin –  $\Delta k_m$

$$\text{USL AOA(3)} = 0.9876 - 0.0031 - 0.0 - 0.05 = 0.9345$$

This USL is applicable for design applications falling within the validated range of key parameters shown in Table 5-2. For design applications outside the AOA, ANSI/ANS 8.1-1998 [2] permits extension of the AOA based on observed trends in the bias as a function of the extended parameter. In order to establish these trends, computed  $k_{eff}$  results are plotted as a function of trending parameter in Figure 6-2 through Figure 6-4. To facilitate trending analysis, the plotted data is fitted linearly. Data for EALF is fitted logarithmically due to the extended range of the parameter.

The USL for AOA(3) is 0.9345. This value includes a 0.05 administrative margin and consideration for calculational bias and allowance for uncertainties. Justification for an administrative margin of 0.05 is provided in Section 7.1.

## 6.2 DESIGN APPLICATION (4) – MOX POWDER

The benchmark experiments identified in Section 5.2 for AOA(4) are modeled with CSAS26/KENO VI using the 238 group library 238GROUPNDF5. The calculated  $k_{eff}$  values for selected benchmark experiments are presented in Table 6-2.

Figure 6-5 shows the distribution of calculated  $k_{eff}$  values for the experiments as calculated with SCALE 4.4a (KENO-VI Update 3) on the PC platform. The  $k_{eff}$  values are first analyzed statistically using the USLSTATS computer code. The data fails the test for normality employed in that analysis; hence, the nonparametric technique described in Section 3.2.3 is employed.

With a total of 59 unique experiments for this AOA, the degree of confidence,  $\beta$ , obtained from Equation 3.3 is 95.2%. Hence, the required nonparametric margin obtained from Table 3-1 is 0.0. The minimum computed benchmark  $k_{eff}$  is  $0.9924 \pm 0.0005$  obtained for case PU29-6 [23]. The benchmark experiment uncertainty for this experiment series is not included in the original paper describing the experiment. However, the experiment series is one of the Bierman series of criticality experiments performed at Battelle Pacific Northwest Laboratories, and uses substantially the same experimental configuration as that described in PU-COMP-MIXED-001 and PU-COMP-MIXED-002. Hence, the experimental error for PU29-6 is approximated by taking the maximum observed error reported for these benchmarks, 0.0075, which is reported for PCM-002 Cases 6-9. Combined with the observed calculational uncertainty for the minimum case, 0.0005, the resulting uncertainty is

$$\sqrt{0.0075^2 + 0.0005^2} = 0.0075$$

The resulting USL for AOA(4) is then determined from Equation 3.1 as

$$USL = \text{Smallest } k_{eff} \text{ value} - \text{Uncertainty for smallest } k_{eff} - \text{Nonparametric margin} - \Delta k_m$$

$$USL \text{ AOA(4)} = 0.9924 - 0.0075 - 0.0 - 0.05 = 0.9349$$

This USL is applicable for design applications falling within the range of key parameters shown in Table 5-4. For design applications outside the AOA, ANSI/ANS 8.1-1998 [2] permits extension of the AOA based on observed trends in the bias as a function of the extended parameter. In order to establish these trends, computed  $k_{eff}$  results are plotted as a function of trending parameter in Figure 6-6 through Figure 6-10. To facilitate trending analysis, the plotted

data is fitted linearly. Data for EALF is fitted logarithmically due to the extended range of the parameter.

The USL for AOA(4) is 0.9349. This value includes a 0.05 administrative margin and consideration for calculational bias and allowance for uncertainties. Justification for an administrative margin of 0.05 is provided in Section 7.1.

Table 6-1 Experiment Set and Benchmark Calculation Results for AOA(3)

Experiment	H/(Pu + U)	H/Pu	Wt % 240Pu	Wt % Pu	EALF (eV)	K6 keff	$\sigma$
BNWL2129T4-01	2.77	9.47	11.5%	29.3%	6.14E+00	1.0166	0.0005
NSE55T5-01	2.79	9.55	11.5%	29.3%	4.02E+01	1.0044	0.0005
NSE55T5-02	2.79	9.55	11.5%	29.3%	3.97E+01	1.0023	0.0005
NSE55T5-03	2.79	9.55	11.5%	29.3%	4.02E+01	1.0043	0.0006
NSE55T5-04	2.79	9.55	11.5%	29.3%	4.08E+01	1.0037	0.0005
NSE55T5-05	2.79	9.55	11.5%	29.3%	4.07E+01	1.0021	0.0005
NSE55T5-06	2.79	9.55	11.5%	29.3%	4.17E+01	1.0024	0.0005
NSE55T5-07	2.79	9.55	11.5%	29.3%	4.35E+01	1.0045	0.0005
NSE55T5-08	2.79	9.55	11.5%	29.3%	3.94E+01	1.0015	0.0005
NSE55T5-09	2.79	9.55	11.5%	29.3%	3.92E+01	1.0029	0.0005
NSE55T5-10	2.79	9.55	11.5%	29.3%	3.86E+01	1.0038	0.0005
PCM001-02	5.05	5.05	11.5%	100.0%	1.74E+03	1.0203	0.0007
PCM001-03	15.10	15.10	2.2%	100.0%	3.26E+01	1.0164	0.0006
PCM001-04	14.95	14.95	8.1%	100.0%	3.95E+01	0.9881	0.0006
PCM002-01	0.04	0.04	18.4%	100.0%	4.92E+03	1.0329	0.0006
PCM002-02	0.04	0.04	18.4%	100.0%	4.24E+03	1.0306	0.0006
PCM002-03	0.04	0.04	18.4%	100.0%	3.49E+03	1.0275	0.0005
PCM002-04	0.04	0.04	18.4%	100.0%	2.58E+03	1.0204	0.0006
PCM002-05	0.04	0.04	18.4%	100.0%	1.87E+03	1.0167	0.0005
PCM002-06	5.05	5.05	11.5%	100.0%	9.26E+01	1.0230	0.0005
PCM002-07	5.05	5.05	11.5%	100.0%	8.43E+01	1.0219	0.0006
PCM002-08	5.05	5.05	11.5%	100.0%	6.79E+01	1.0210	0.0006
PCM002-09	5.05	5.05	11.5%	100.0%	5.73E+01	1.0223	0.0006
PCM002-10	15.10	15.10	2.2%	100.0%	4.14E+00	1.0325	0.0006
PCM002-11	15.10	15.10	2.2%	100.0%	4.55E+00	1.0286	0.0005
PCM002-12	15.10	15.10	2.2%	100.0%	5.15E+00	1.0284	0.0006
PCM002-13	15.10	15.10	2.2%	100.0%	5.44E+00	1.0261	0.0006
PCM002-14	15.10	15.10	2.2%	100.0%	5.59E+00	1.0297	0.0006
PCM002-15	15.10	15.10	2.2%	100.0%	5.56E+00	1.0279	0.0006
PCM002-16	15.10	15.10	2.2%	100.0%	5.14E+00	1.0250	0.0006
PCM002-17	14.95	14.95	8.1%	100.0%	4.90E+00	1.0080	0.0006
PCM002-18	14.95	14.95	8.1%	100.0%	6.17E+00	1.0101	0.0005
PCM002-19	14.95	14.95	8.1%	100.0%	6.46E+00	1.0091	0.0005
PCM002-20	14.95	14.95	8.1%	100.0%	6.68E+00	1.0090	0.0005
PCM002-21	14.95	14.95	8.1%	100.0%	6.66E+00	1.0092	0.0005
PCM002-22	14.95	14.95	8.1%	100.0%	6.41E+00	1.0145	0.0006

Table 6-1 Experiment Set and Benchmark Calculation Results for AOA(3) – Continued

Experiment	H/(Pu + U)	H/Pu	Wt % 240Pu	Wt % Pu	EALF (eV)	K6 keff	$\sigma$
PMF001-01	0.00	0.00	4.5%	100.0%	1.24E+06	0.9957	0.0006
PMF003-01	0.00	0.00	6.0%	100.0%	1.24E+06	0.9946	0.0006
PMF003-02	0.00	0.00	6.0%	100.0%	6.94E+05	0.9930	0.0006
PMF003-03	0.00	0.00	6.0%	100.0%	1.24E+06	0.9876	0.0006
PMF003-04	0.00	0.00	6.0%	100.0%	6.28E+05	0.9922	0.0006
PMF003-05	0.00	0.00	6.0%	100.0%	1.25E+06	0.9914	0.0006
PMF016-01	0.00	0.00	6.0%	100.0%	1.17E+04	1.0128	0.0006
PMF016-02	0.00	0.00	6.0%	100.0%	8.56E+03	1.0008	0.0006
PMF016-03	0.00	0.00	6.0%	100.0%	8.23E+03	0.9994	0.0006
PMF016-04	0.00	0.00	6.0%	100.0%	8.08E+03	0.9983	0.0006
PMF016-05	0.00	0.00	6.0%	100.0%	7.96E+03	0.9986	0.0006
PMF016-06	0.00	0.00	6.0%	100.0%	7.80E+03	1.0003	0.0006
PMF017-01	0.00	0.00	6.0%	100.0%	7.83E+05	0.9896	0.0006
PMF017-02	0.00	0.00	6.0%	100.0%	4.07E+05	0.9912	0.0007
PMF017-03	0.00	0.00	6.0%	100.0%	2.31E+05	0.9951	0.0006
PMF017-04	0.00	0.00	6.0%	100.0%	4.57E+05	0.9903	0.0007
PMF017-05	0.00	0.00	6.0%	100.0%	9.38E+04	1.0004	0.0006
PMF033-01	0.00	0.00	5.9%	52.5%	4.00E+05	1.0072	0.0005
PMF037-01	0.00	0.00	6.0%	100.0%	1.46E+05	0.9977	0.0006
PMF037-05	0.00	0.00	6.0%	100.0%	5.12E+04	0.9969	0.0006
PMF037-07	0.00	0.00	6.0%	100.0%	3.32E+04	0.9978	0.0006
PMF037-10	0.00	0.00	6.0%	100.0%	2.58E+04	0.9985	0.0006
PMF037-12	0.00	0.00	6.0%	100.0%	2.36E+04	0.9996	0.0006
PMF037-15	0.00	0.00	6.0%	100.0%	1.83E+04	0.9992	0.0006
PMF037-16	0.00	0.00	6.0%	100.0%	2.84E+04	1.0007	0.0005
PU-29-1	2.77	9.47	11.5%	29.3%	4.16E+01	0.9934	0.0003
PU-29-2	2.77	9.47	11.5%	29.3%	4.07E+01	0.9931	0.0005
PU-29-3	2.77	9.47	11.5%	29.3%	4.10E+01	1.0029	0.0005
PU-29-4	2.77	9.47	11.5%	29.3%	3.80E+01	0.9928	0.0005
PU-29-5	2.77	9.47	11.5%	29.3%	3.78E+01	0.9935	0.0005
PU-29-6	2.77	9.47	11.5%	29.3%	3.67E+01	0.9924	0.0005
PU-29-7	2.77	9.47	11.5%	29.3%	3.52E+01	0.9938	0.0005
PU-29-8	2.77	9.47	11.5%	29.3%	3.45E+01	0.9926	0.0005
PU-29-9	2.77	9.47	11.5%	29.3%	3.46E+01	0.9968	0.0005

Table 6-2 Experiment Set and Benchmark Calculation Results for AOA(4)

Experiment	H/(Pu + U)	H/Pu	Wt % 240Pu	Wt % Pu	EALF (eV)	K6 keff	$\sigma$
BNWL2129T4-01	2.77	9.47	11.5%	29.3%	6.14E+00	1.0166	0.0005
BNWL2129T4-02	2.77	9.47	11.5%	29.3%	4.50E+00	1.0181	0.0005
BNWL2129T4-03	2.77	9.47	11.5%	29.3%	3.38E+00	1.0190	0.0006
BNWL2129T4-04	2.77	9.47	11.5%	29.3%	5.00E+00	1.0180	0.0005
BNWL2129T4-05	2.77	9.47	11.5%	29.3%	3.21E+00	1.0186	0.0005
BNWL2129T4-06	2.77	9.47	11.5%	29.3%	2.21E+00	1.0193	0.0005
BNWL2129T4-07	2.77	9.47	11.5%	29.3%	4.90E+00	1.0165	0.0005
BNWL2129T4-08	2.77	9.47	11.5%	29.3%	2.38E+00	1.0177	0.0006
BNWL2129T4-09	2.77	9.47	11.5%	29.3%	5.76E+00	1.0178	0.0005
BNWL2129T4-10	2.77	9.47	11.5%	29.3%	5.23E+00	1.0165	0.0005
BNWL2129T4-11	2.77	9.47	11.5%	29.3%	3.50E+00	1.0171	0.0005
BNWL2129T4-12	2.77	9.47	11.5%	29.3%	3.71E+00	1.0210	0.0006
BNWL2129T4-13	2.77	9.47	11.5%	29.3%	2.52E+00	1.0220	0.0006
BNWL2129T4-14	2.77	9.47	11.5%	29.3%	1.49E+00	1.0194	0.0005
BNWL2129T4-15	2.77	9.47	11.5%	29.3%	5.00E+00	1.0155	0.0005
BNWL2129T4-16	2.77	9.47	11.5%	29.3%	5.21E+00	1.0168	0.0005
BNWL2129T4-17	2.77	9.47	11.5%	29.3%	4.24E+00	1.0188	0.0005
BNWL2129T4-18	2.77	9.47	11.5%	29.3%	3.56E+00	1.0180	0.0006
BNWL2129T4-19	2.77	9.47	11.5%	29.3%	4.03E+00	1.0186	0.0005
NSE55T5-01	2.79	9.55	11.5%	29.3%	4.02E+01	1.0044	0.0005
NSE55T5-02	2.79	9.55	11.5%	29.3%	3.97E+01	1.0023	0.0005
NSE55T5-03	2.79	9.55	11.5%	29.3%	4.02E+01	1.0043	0.0006
NSE55T5-04	2.79	9.55	11.5%	29.3%	4.08E+01	1.0037	0.0005
NSE55T5-05	2.79	9.55	11.5%	29.3%	4.07E+01	1.0021	0.0005
NSE55T5-06	2.79	9.55	11.5%	29.3%	4.17E+01	1.0024	0.0005
NSE55T5-07	2.79	9.55	11.5%	29.3%	4.35E+01	1.0045	0.0005
NSE55T5-08	2.79	9.55	11.5%	29.3%	3.94E+01	1.0015	0.0005
NSE55T5-09	2.79	9.55	11.5%	29.3%	3.92E+01	1.0029	0.0005
NSE55T5-10	2.79	9.55	11.5%	29.3%	3.86E+01	1.0038	0.0005

Table 6-2 Experiment Set and Benchmark Calculation Results for AOA(4) – Continued

Experiment	H/(Pu + U)	H/Pu	Wt % 240Pu	Wt % Pu	EALF (eV)	K6 keff	$\sigma$
PCM002-06	5.05	5.05	11.5%	100.0%	9.26E+01	1.0230	0.0005
PCM002-07	5.05	5.05	11.5%	100.0%	8.43E+01	1.0219	0.0006
PCM002-08	5.05	5.05	11.5%	100.0%	6.79E+01	1.0210	0.0006
PCM002-09	5.05	5.05	11.5%	100.0%	5.73E+01	1.0223	0.0006
PCM002-10	15.10	15.10	2.2%	100.0%	4.14E+00	1.0325	0.0006
PCM002-11	15.10	15.10	2.2%	100.0%	4.55E+00	1.0286	0.0005
PCM002-12	15.10	15.10	2.2%	100.0%	5.15E+00	1.0284	0.0006
PCM002-13	15.10	15.10	2.2%	100.0%	5.44E+00	1.0261	0.0006
PCM002-14	15.10	15.10	2.2%	100.0%	5.59E+00	1.0297	0.0006
PCM002-15	15.10	15.10	2.2%	100.0%	5.56E+00	1.0279	0.0006
PCM002-16	15.10	15.10	2.2%	100.0%	5.14E+00	1.0250	0.0006
PCM002-17	14.95	14.95	8.1%	100.0%	4.90E+00	1.0080	0.0006
PCM002-18	14.95	14.95	8.1%	100.0%	6.17E+00	1.0101	0.0005
PCM002-19	14.95	14.95	8.1%	100.0%	6.46E+00	1.0091	0.0005
PCM002-20	14.95	14.95	8.1%	100.0%	6.68E+00	1.0090	0.0005
PCM002-21	14.95	14.95	8.1%	100.0%	6.66E+00	1.0092	0.0005
PCM002-22	14.95	14.95	8.1%	100.0%	6.41E+00	1.0145	0.0006
PU-29-1	2.77	9.47	11.5%	29.3%	4.16E+01	0.9934	0.0003
PU-29-2	2.77	9.47	11.5%	29.3%	4.07E+01	0.9931	0.0005
PU-29-3	2.77	9.47	11.5%	29.3%	4.10E+01	1.0029	0.0005
PU-29-4	2.77	9.47	11.5%	29.3%	3.80E+01	0.9928	0.0005
PU-29-5	2.77	9.47	11.5%	29.3%	3.78E+01	0.9935	0.0005
PU-29-6	2.77	9.47	11.5%	29.3%	3.67E+01	0.9924	0.0005
PU-29-7	2.77	9.47	11.5%	29.3%	3.52E+01	0.9938	0.0005
PU-29-8	2.77	9.47	11.5%	29.3%	3.45E+01	0.9926	0.0005
PU-29-9	2.77	9.47	11.5%	29.3%	3.46E+01	0.9968	0.0005
PU-8-1	7.33	90.86	11.6%	8.1%	6.43E-01	1.0046	0.0006
PU-8-2	7.33	90.86	11.6%	8.1%	6.42E-01	1.0040	0.0005
PU-8-3	7.33	90.86	11.6%	8.1%	6.37E-01	1.0061	0.0005
PU-8-4	7.33	90.86	11.6%	8.1%	6.32E-01	1.0051	0.0005

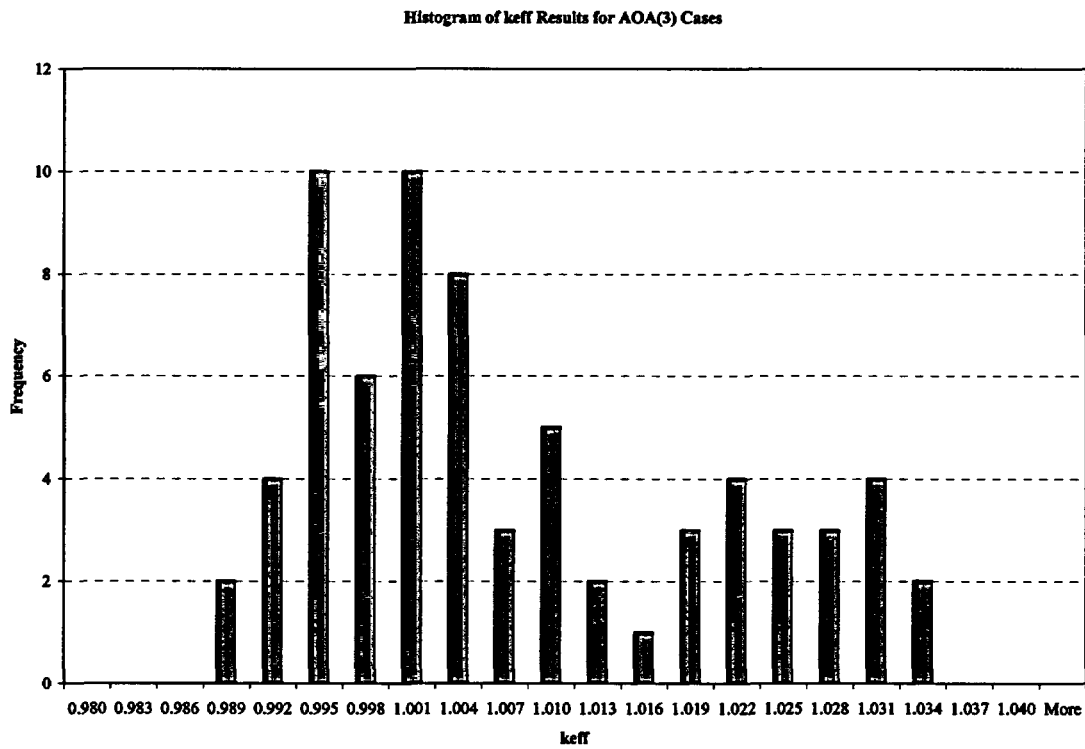


Figure 6-1 Histogram of  $k_{eff}$  occurrences for AOA(3)



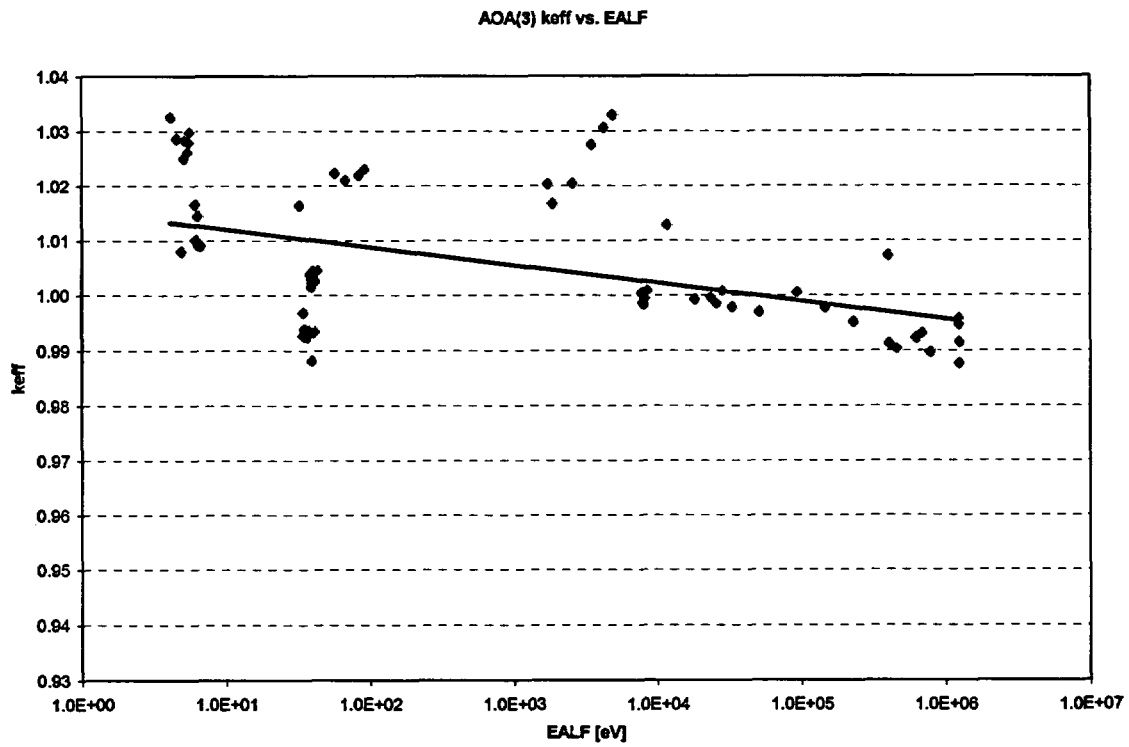


Figure 6-2 AOA(3)  $k_{eff}$  as a function of EALF

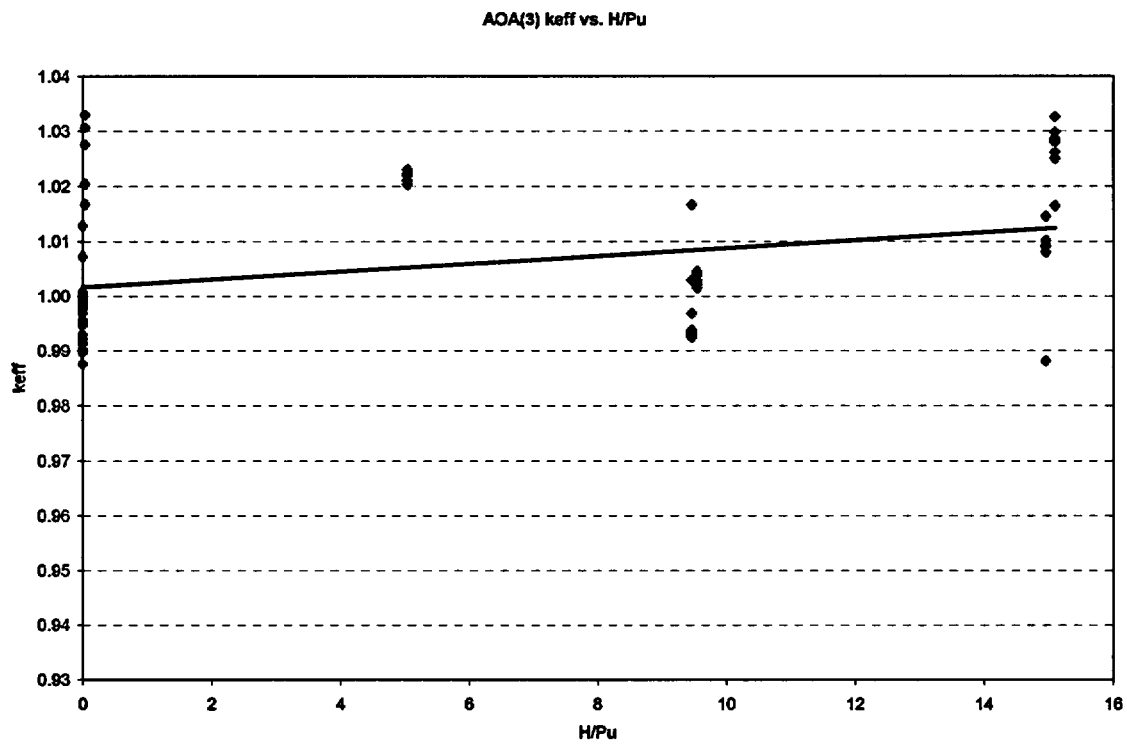


Figure 6-3 AOA(3)  $k_{eff}$  as a function of H/Pu

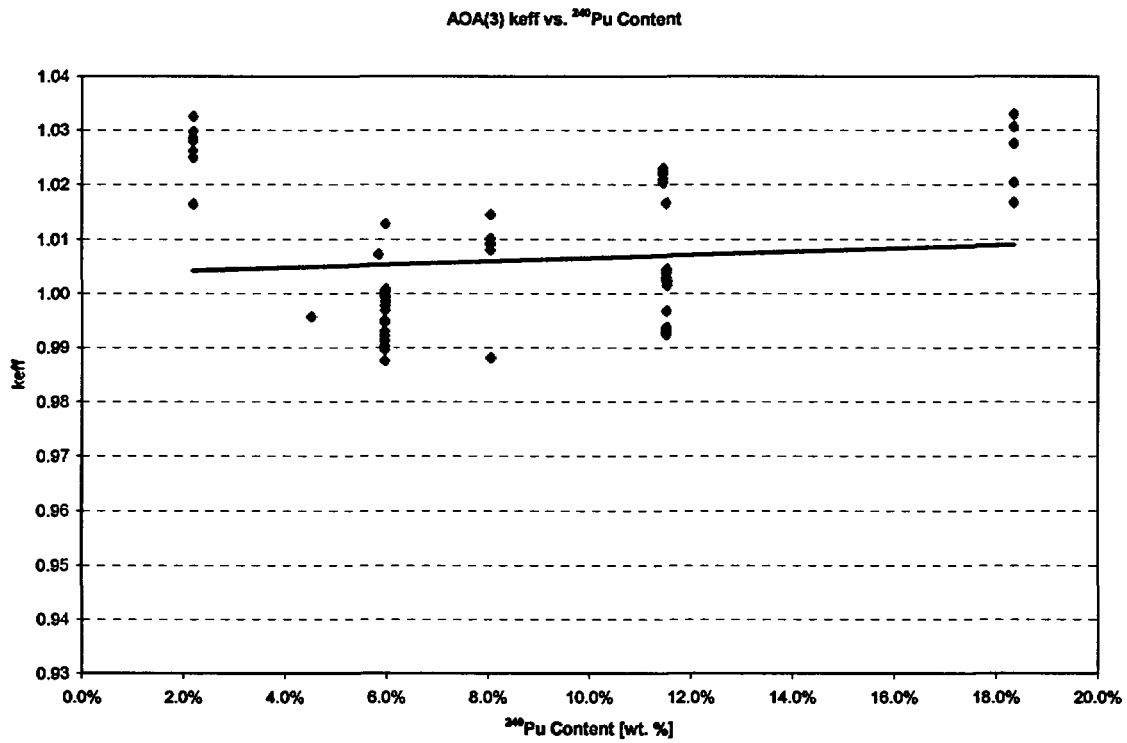


Figure 6-4 AOA(3)  $k_{eff}$  as a function of  $^{240}\text{Pu}$  content

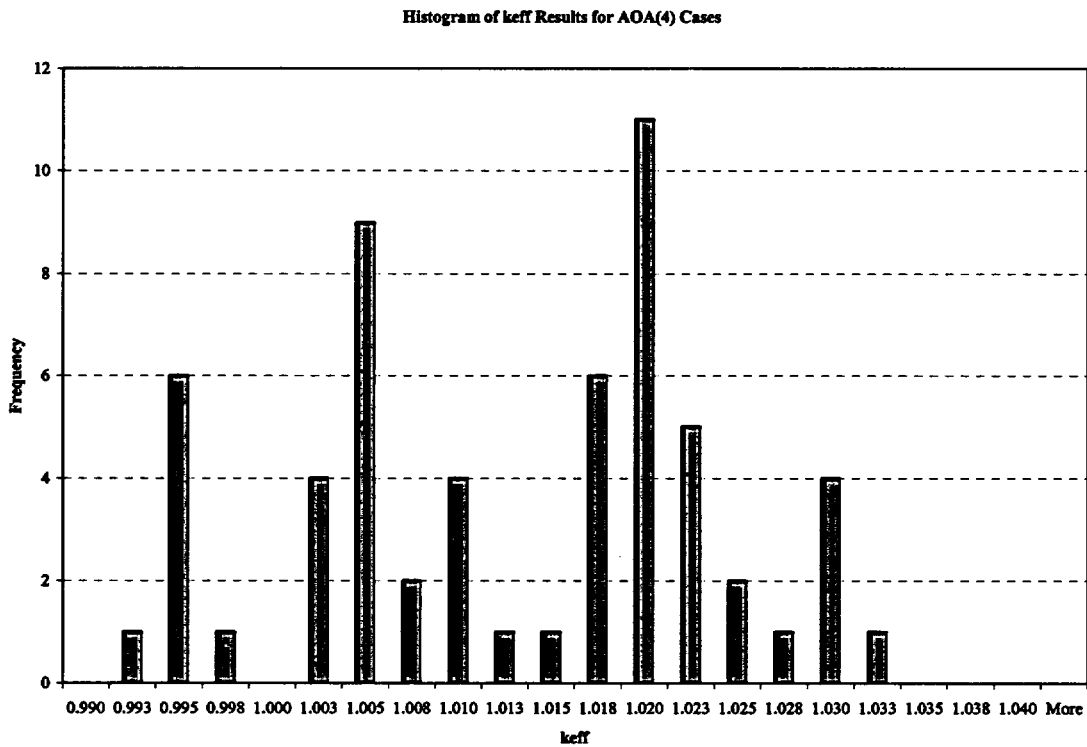


Figure 6-5 Histogram of  $k_{eff}$  occurrences for AOA(4)

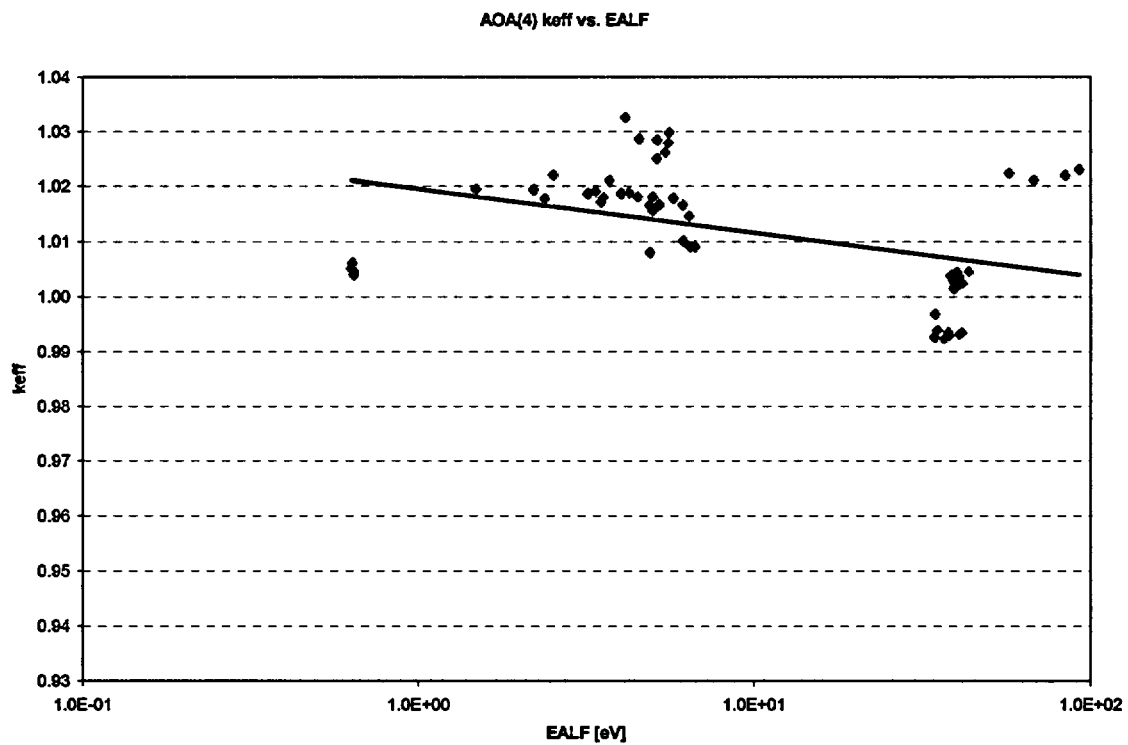


Figure 6-6 AOA(4)  $k_{eff}$  as a function of EALF

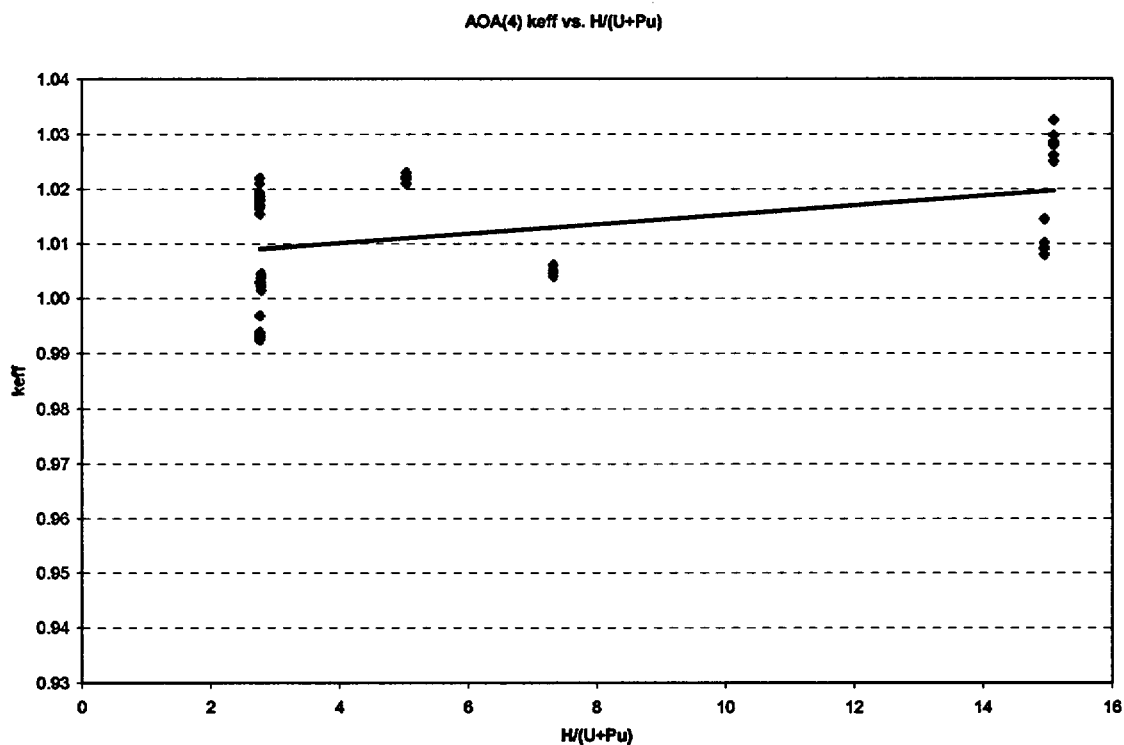


Figure 6-7 AOA(4)  $k_{eff}$  as a function of  $H/(U+Pu)$

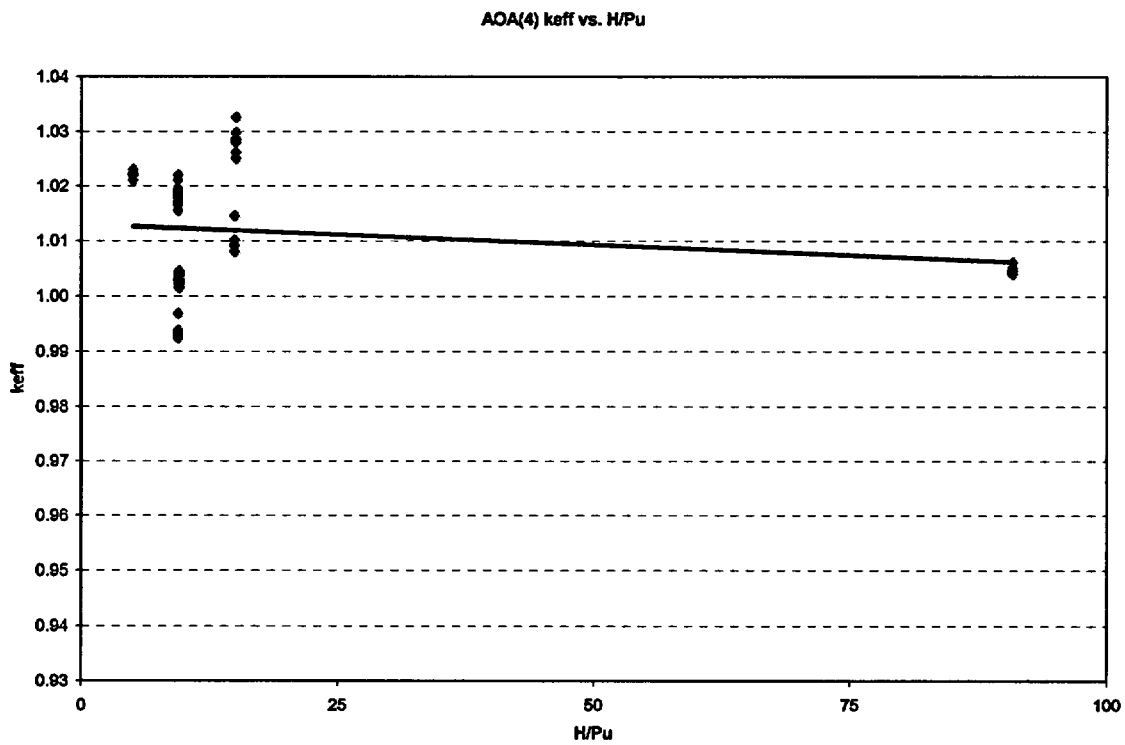


Figure 6-8 AOA(4)  $k_{eff}$  as a function of H/Pu

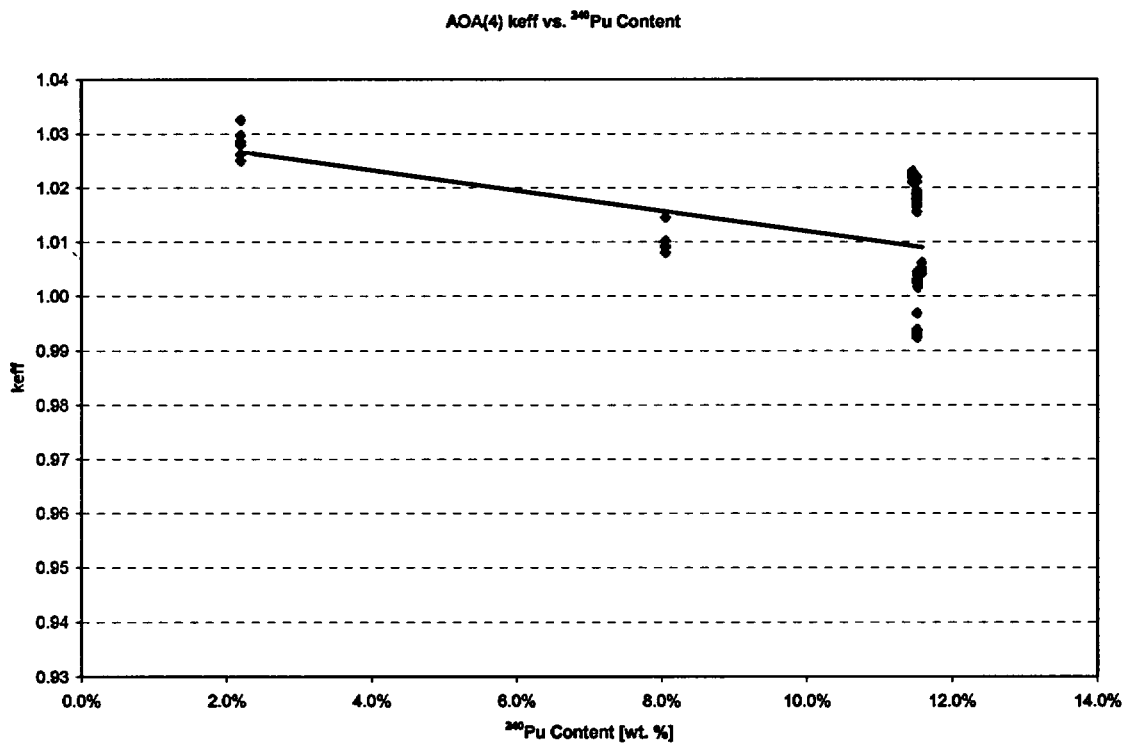


Figure 6-9 AOA(4)  $k_{eff}$  as a function of  $^{240}\text{Pu}$  content



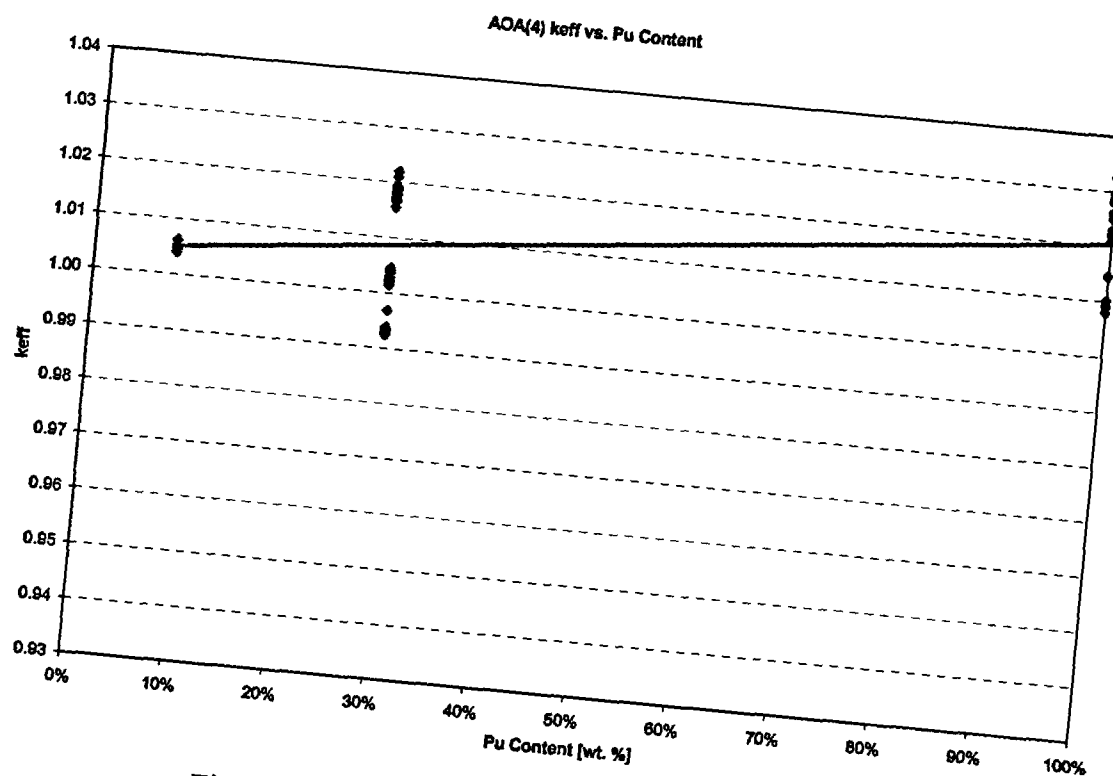


Figure 6-10 AOA(4)  $k_{eff}$  as a function of Pu content

## 7. CONCLUSIONS

The SCALE 4.4a code package using the CSAS26 (KENOVI) sequence and the 238 energy group cross-section library 238GROUPDF5 has been validated to perform criticality calculations for the MFFF on the PC platform. It has been validated for two of the design applications: AOA(3) PuO<sub>2</sub> powder and AOA(4) MOX powder.

The USL for the two design application areas is as follows:

- Design application (3) PuO<sub>2</sub> powder      USL AOA(3) = 0.9345
- Design application (4) MOX powder      USL AOA(4) = 0.9349

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.

Where extrapolation outside the range of applicability for AOA(3) or AOA(4) is necessary, ANSI/ANS-8.1 [2] allows extrapolating the trends established for the bias and USL. Results presented here provide the required trending regressions for determining adjusted USL values. If extrapolation is necessary, 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 nuclear criticality safety evaluation (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 for accident analysis conditions range from 0.02 to 0.05 as shown in Table 7-1. These values apply to applications within the validated AOA; 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 [20], 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 [20] 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) [19], 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 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 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, is justified and is sufficiently conservative to provide for an adequate margin of subcriticality.

**Table 7-1 Fuel Cycle and Industry Practice**

<b>Facility</b>	<b>Process/Application</b>	<b>Material</b>	<b>Administrative Margin</b>
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) <sup>239</sup> Pu c) <sup>239</sup> Pu d) <sup>239</sup> 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 <sup>1</sup>
Idaho National Engineering and Environmental Lab	Solutions/spent fuel/powders/pieces	Low to High Enriched U, including <sup>233</sup> U; some Pu	0.02 – 0.05 0.05 typical
Hanford Site	Waste tanks Packaging and transportation	Various	0.05

<sup>1</sup> Pending final approval of validation document.

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