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Title ANALYSIS OF CRITICAL BENCHMARK EXPERIMENTS FOR CONFIGURATIONS EXTERNAL TO WP

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PURPOSE AND SUMMARY OF RESULTS:

The purpose of this calculation is to select and review the critical benchmark experiments that are appropriate for the validation of the criticality calculational methodology that is to be used for assessing the criticality potential of the configurations external to the waste package. For the benchmark experiments associated with each group of external configurations, a lower bound tolerance limit is evaluated using the generic methodology described in Reference 1. The lower bound tolerance limit is derived from the bias and uncertainties associated with the employed criticality code and the modeling process of the critical experiments. All benchmark experiments used in this calculation are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5). For critical benchmark experiments that were not previously used in similar analysis, benchmark models and inputs for MCNP neutron transport code have been prepared and run. Five sets of criticality benchmark experiments have been constructed based on the fissile content of the external configurations (HEU, IEU, LEU, U+Pu and ^{233}U). They accommodate large variations in the range of parameters of the external configurations and also provide adequate statistics for the lower bound tolerance limit calculations. The range of applicability of the benchmark experiments is presented for each set of experiments.

The results of this calculation are consisting of values or expressions for the lower bound tolerance limit for each set of benchmark experiments. For the first two sets, the LUTB method (Ref. 10) for calculating the lower bound tolerance limit was identified as applicable and applied as implemented in CLREG code

1. HEU set (187 benchmark cases): $f(AENCF) = 0.970611$ for $0\ \text{MeV} < AENCF < 0.247\ \text{MeV}$
   $f(AENCF) = -1.7411e\text{-}02 * AENCF + 0.97491$ for $0.247\ \text{MeV} \leq AENCF < 0.902\ \text{MeV}$
2. IEU set (109 benchmark cases): $f(AENCF) = 0.97841$ for $0\ \text{MeV} < AENCF < 0.1518\ \text{MeV}$
   $f(AENCF) = -1.9322e\text{-}02 * AENCF + 0.981339$ for $0.1518\ \text{MeV} \leq AENCF < 0.482\ \text{MeV}$

For the last three sets of benchmark experiments, the DFTL method as described in Reference 6 was identified as appropriate to calculate the lower bound tolerance limit:

3. LEU set (96 benchmark cases): $f = 0.9842$
4. U+Pu set (120 benchmark cases): $f = 0.9644$
5. ^{233}U set (83 benchmark cases): $f = 0.9748$

This engineering calculation supports the disposal criticality methodology in Ref. 1 and is performed in accordance with the AREVA/FANP procedure for preparing and processing calculations (Ref. 3) and Quality Management Manual (Ref. 4).

THE FOLLOWING COMPUTER CODES HAVE BEEN USED IN THIS DOCUMENT:

CODE/VERSION/REV	CODE/VERSION/REV
MCNP4.B2	
CLREG1.0	

THE DOCUMENT CONTAINS ASSUMPTIONS THAT MUST BE VERIFIED PRIOR TO USE ON SAFETY-RELATED WORK

☐ YES ☒ NO

RECORD OF REVISIONS

Revision Number	Description	Date
00	Original issue	June 2004

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1. PURPOSE

The *Disposal Criticality Analysis Methodology Topical Report* (Reference 1) states that the accuracy of the criticality analysis methodology (MCNP Monte Carlo code and cross-section data) designated to assess the potential for criticality of various configurations in the Yucca Mountain proposed repository is established by evaluating appropriately selected benchmark critical experiments.

The purpose of this calculation is to select and review the critical benchmark experiments that are appropriate for the validation of the criticality calculational methodology that is to be used for assessing the criticality potential of the configurations external to the waste package. For the benchmark experiments associated with each group of external configurations, a lower bound tolerance limit is evaluated using the methodology described in Reference 1. The lower bound tolerance limit is derived from the bias and uncertainties associated with the employed criticality code and the modeling process of the critical experiments.

The results of this calculation will be used to validate the MCNP code's ability to accurately predict the effective neutron multiplication factor (k_{eff}) for a range of conditions spanned by various critical configurations representative of the configurations postulated to occur in locations external to the waste packages.

This report is an engineering calculation supporting the validation of the criticality methodology for disposal of commercial and DOE (Department of Energy) spent nuclear fuel in Yucca Mountain (Reference 1). The calculation was performed in accordance with the AREVA/FANP procedure in References 3 and the Framatome Quality Management Manual (Reference 4).

2. METHOD

An essential element of validating the methods and models used for calculating the effective neutron multiplication factor, k_{eff}, for configurations internal or external to a waste package is the determination of a critical limit for each class of configurations. The critical limit (CL) is the value of k_{eff} at which a configuration is considered potentially critical and accounts for the criticality method bias and uncertainty. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

This calculation presents a detailed description of the first three steps outlined above for specific groups of benchmark critical experiments selected for the postulated external configurations. The external configurations have been grouped based on the possible fissile material content, which is a criterion not explicitly presented in the external configuration classes description presented in Reference 1. More precisely, the configuration classes for external configurations described in Reference 1 (p. 3-16) are mainly grouped based on the possible mechanisms (scenarios) that can lead to the accumulation of fissile material in an external location. They have been regrouped for the purpose of the present calculation using the possible fissile content as the main criterion. The configurations considered include relatively homogeneous distributions of fissile material and moderator in various compact geometries. These types of configurations have been shown to have potential for criticality in a preliminary criticality analysis (Reference 2).

The criticality benchmark experiments for each group of external configurations have been selected using their fissile content as a first criterion, the presence of moderator as a second criterion, and geometry of the experiment as a third criterion. The benchmark experiments are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (Reference 2). The sets of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the external configurations and also to provide adequate statistics for the lower bound tolerance limit calculations.

The second step in the process is establishing a range of applicability for the selected experiments. This was done by identifying or calculating important physical and spectral parameters for each experiment and including them in comprehensive tables. This information can later be used in constructing a collective range of applicability to be compared with the range of parameters of the configurations. The parameters included in the tables constructed for this report characterize fissile materials, moderator, neutron absorbers and reflectors, geometry, and neutron energy (spectral parameters).

The third step in the process (establishing a lower bound tolerance limit for each group of benchmark experiments) was performed by following an approach similar to that developed for the internal configurations of the waste package (Reference 10). The approach is based on the methodology described in Reference 1 and is summarized in the next subsection. The individual sections of this document describe results for each group of benchmark experiments and include a detailed explanation of all steps involved in establishing the lower bound tolerance limit, specific to the conditions encountered during analysis of each group.

2.1 Lower Bound Tolerance Limit Calculation

The process for calculating the lower bound tolerance limit is presented in Figure 3-6 of Reference 1. The process starts by applying regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p. 8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value

(k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}. To normalize, the following formula applies:

$$k_{norm}=k_{calc}/k_{exp} \qquad (1)$$

Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (e.g., average energy of a neutron causing fission [AENCF], enrichment, ratio of hydrogen to fissile atoms [H/X]), using the build-in regression analysis tool from the Excel software. The AENCF is defined as the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. The H/X ratio is the ratio of mole of hydrogen to mole of fissile materials (U-235 and/or Pu-239). Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p.3-47). If trending is identified for one set, the LUTB method is used to calculate the lower bound tolerance limit (Reference 1, p. 3-49). The LUTB method is currently implemented in the personal computer code CLReg (Reference 11) that is used in this calculation.

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic (Reference 7, p. 390) can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the y values about their mean that can be attributed to a linear relation between y and x.

Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (b) (Reference 7, p. 382). The slope test requires calculating the test statistic "T" as shown in Equation 2 along with the statistical parameters in Equations 3 and 4 (Reference 7, p. 382 and p. 371).

$$T=b\sqrt{\frac{(n-2)S_{xx}}{SS_E}} \qquad (2)$$

where

b is the slope of the fitted linear regression equation

$$S = \sum_{i=1,n}(x_i - \bar{x})^2 \qquad (3)$$

and

$$SS_E = \sum_{i=1,n}(y_i - a - bx_i)^2 \qquad (4)$$

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and n-2 degrees of freedom (Reference 7, p. 659), where n is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied (Reference 7, p.377, p.401). The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals.

If the subset shows no trending, according to the methodology summarized in Reference 1 (Figure 3-6), the subset is tested for normality using an omnibus normality test. The omnibus Anderson-Darling test is used (Reference 8, p. 372) that tests the goodness-of-fit to a normal distribution constructed with the subset's sample average and standard deviation.

Given that the k_{eff} values produced by the criticality code for the benchmark experiments are shown to be normally distributed, the lower bound tolerance limit can be calculated using normal distribution tolerance limit method (NDTL) described in Reference 1 (p. 3-50) as:

$$CL = k_{ave} - k(\gamma, P, n) * S_P \qquad (5)$$

where: k_{ave} is the average of the k_{eff} values, unless k_{ave} is greater than unity (1.0), in which instance the appropriate value for k_{ave} should be 1.0 to disallow positive bias; k (γ, P, n) is a multiplier (Reference 9, pp. 1-14 and 1-15) in which γ is the confidence level, P is the proportion of the population covered, and n is the number of degrees of freedom. The S_P term is the square root of the sum of the inherent variance of the critical experiment data set plus the average of the criticality code variances for the critical experiment data set (Reference 1, p.3-51). Reference 6 (p.11) recommends that the lower tolerance limits, at a minimum, should be calculated with a 95% confidence that 95% of the data lies above the limit. This is quantified by using the multipliers provided in Table 1 (Reference 6, Table 2.1; Reference 9, pp.1-14 and 1-15).

Table 1. Multiplier Used in Calculating Lower Bound Tolerance Limit with NDTL

Number of Experiments (n)	Multiplier k (γ, P, n) for γ=95%; P=95%
10	2.911
11	2.815
12	2.736
13	2.670
14	2.614
15	2.566
16	2.523

Table 1. Multiplier Used in Calculating Lower Bound Tolerance Limit with NDTL (Continued)

Number of Experiments (n)	Multiplier k (γ, P, n) for γ=95%; P=95%
17	2.486
18	2.453
19	2.423
20	2.396
21	2.371
22	2.350
23	2.329
24	2.309
25	2.292
30	2.220
35	2.166
40	2.126
45	2.092
50	2.065

Source: Reference 6, Table 2.1

If the data does not have a normal statistical distribution, a non-parametric statistical treatment must be used as described in Reference 1 (p. 3-51) as the distribution-free tolerance limit (DFTL). A particularization of the method is presented in Reference 6 (p.14), resulting in the determination of the degree of confidence that a fraction of the true population of k_{eff} data lies above the smallest value observed. The more data are available in the sample, the higher the degree of confidence. Non-parametric techniques do not require reliance upon distributions, but are rather an analysis of ranks. Therefore, the k_{eff} values in a sample are ranked from the smallest to the largest.

For a desired population fraction of 95% and a rank order of 1 (the smallest k_{eff} value in data sample), the following equation determines the percent confidence that the specified fraction of the population is above the lowest observed value:

$$\beta = 1 - q^n = 1 - 0.95^n \tag{6}$$

For non-parametric data analysis, Reference 6 (p. 14) suggests that the lower bound tolerance limit be determined by:

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM) (7)

where:

Non-parametric margin (NPM) is added to account for small sample size (where appropriate).

Reference 6 (p.15) recommends a set of values for NPM based on the confidence level (β) calculated above. The values are presented in Table 2.

Table 2. Non-parametric Margins

Degree of Confidence (β) for 95% of Population	Non-parametric Margin
>90%	0.0
>80%	0.01
>70%	0.02
>60%	0.03
>50%	0.04
>40%	0.05
≤40%	Additional data needed.

Source: Reference 6, Table 2.2

If the smallest k_{eff} value is greater than 1, then the non-parametric lower bound tolerance limit becomes:

$$\textit{lower bound tolerance limit} = 1 - S_P - NPM \qquad (8)$$

where: S_P is the square root of the pooled variance.

All calculations described above have been applied, where appropriate, to each subset of k_{eff} data for the set of criticality benchmarks selected for each group of external configurations. The applicable theoretical steps presented are repeated for clarity in each section presenting the results for the benchmarks groups. The actual calculations are performed using simple Excel spreadsheets that are summarized in Attachments I to V.

3. ASSUMPTIONS

No specific assumptions are used in developing the current calculation.

4. USE OF COMPUTER SOFTWARE AND MODELS

4.1 CLREG

This calculation uses the CLReg (Reference 11) personal computer code to calculate the lower bound tolerance limit and critical limits for sets of k_{eff} data that show valid trending with spectral and/or physical parameters. The code was obtained and used in accordance with the requirements of procedure 0402-01(Reference 3, Section VII.C) which details the usage of computer programs written for personal computers. It requires that these programs be documented and verified. Reference 11 provides full documentation (including validation) of the code. Verification and confirmation for the purpose of the present calculation is carried out in Attachment VI. Section 7 presents a listing of the output files generated for the present calculation (including the reference test cases). The files were uploaded on the COLD server, such that an independent repetition of the calculations could be performed.

4.2 MCNP

The calculations in this document have been performed using the computer program MCNP (Reference 12) version 4B2. The program was used to calculate the neutron multiplication factor (k_{eff}) for various critical benchmark experiments. This version of the code is fully certified according the Framatome ANP procedure 0902-06 on various workstations, except "gr0" and "gr1". These workstations have been used to certify this version of the MCNP code according to DOE-OCWRM (U.S. Department of Energy, Office of Civilian Radioactive Waste Management) procedures and to perform work under specific contract requirements. The "gr0" and "gr1" workstations were used in the current calculation to assure consistency with previous MCNP 4B2 results obtained on these workstations, results that are referenced in YMP (Yucca Mountain Project) documents (Reference 10). A part of these legacy results are also utilized in the current calculation.

In order to fulfill the requirements of Framatome ANP's procedure 0402-01, *Preparing and Processing FANP Calculations* (Reference 3, Section VII.B), an additional verification of the code was performed in this document to independently demonstrate that the code results are correct. The full set of reference and verification test cases have been run and the results are presented in Attachment VII. All output files (including current k_{eff} calculations and test cases) were uploaded on the COLD server, such that an independent repetition of the calculations could be performed.

5. RESULTS AND DISCUSSION

5.1 CALCULATIONS FOR BENCHMARK CRITICALS APPLICABLE TO EXTERNAL CONFIGURATIONS CONTAINING HIGHLY ENRICHED URANIUM (HEU)

As mentioned in Section 2, an essential element of validating the methods and models used for calculating effective neutron multiplication factor, k_{eff}, for a waste package is determination of critical limit. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

In the following, the first three steps of the process of establishing a critical limit for the external configurations containing HEU mixtures are detailed.

5.1.1 Selection of the Criticality Benchmark Experiments

The criticality experiments selected for inclusion in the validation of the criticality model must be representative of the types of materials, conditions, and parameters to be modeled using the criticality calculational method (criticality model). A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a model, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results (Reference 6, p. 5).

For the present application (configurations with highly enriched uranium external to the waste package), the criticality benchmark experiments have been selected based on their fissile content, moderator content and geometry. The benchmark experiments are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (*External Criticality Calculation for DOE SNF Codisposal Waste Packages* [Reference 2]). The set of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the configurations and also to provide adequate statistics for the lower bound tolerance limit calculations.

The selected benchmark experiments containing a total of 187 individual cases are presented in Table 3 together with the results of the MCNP 4B2 code calculations. All cases have been run using the isotopic libraries described in Reference 10 (Table 2).

Table 3. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Highly Enriched Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
Experiment HEU-MET - MIXED-005 (5 cases)	hmm5_1	1.0007	0.0027	1.01308	0.00057	0.307
	hmm5_2	1.0003	0.0028	1.0217	0.00055	0.247
	hmm5_3	1.0012	0.0029	1.01904	0.00052	0.212
	hmm5_4	1.0016	0.003	1.0145	0.0006	0.3175
	hmm5_5	1.0005	0.004	1.00682	0.00052	0.377
Experiment HEU-MET-THERM-001 (1 case)	hmt001	1.0010	0.0060	1.0097	0.0010	0.0215
Experiment HEU-MET-THERM-014 (1 case)	hmt14	0.9939	0.0015	1.0125	0.0004	0.0233
Experiment HEU-COMP-MIXED-001 (26 cases)	hcm-1	1.0000	0.0059	1.0027	0.001	0.1045
	hcm-2	1.0012	0.0059	1.0059	0.0011	0.1053
	hcm-5	0.9985	0.0056	0.9963	0.001	0.7833
	hcm-6	0.9953	0.0056	0.9899	0.001	0.7962
	hcm-7	0.9997	0.0038	0.9949	0.001	0.8015
	hcm-8	0.9984	0.0052	0.9915	0.0011	0.6872
	hcm-9	0.9983	0.0052	0.9931	0.0011	0.6536
	hcm-10	0.9979	0.0052	0.9941	0.001	0.6494
	hcm-11	0.9983	0.0052	0.9934	0.0011	0.6385
	hcm-12	0.9972	0.0052	0.9960	0.0011	0.6358
	hcm-13	1.0032	0.0053	0.9977	0.0011	0.6309
	hcm-15	1.0083	0.005	0.9949	0.0011	0.4671
	hcm-16	1.0001	0.0046	0.9926	0.0011	0.4692
	hcm-17	0.9997	0.0046	1.0012	0.0011	0.4647
	hcm-18	1.0075	0.0046	1.0000	0.001	0.4625
	hcm-19	1.0039	0.0047	1.0000	0.0011	0.5191
	hcm-20	1.006	0.0065	1.0051	0.0015	0.5357
	hcm-21	1.0026	0.0064	1.0046	0.0016	0.5378
	hcm-22	1.0013	0.0064	0.9995	0.0016	0.5371
	hcm-23	0.9995	0.0053	1.0056	0.0015	0.535
	hcm-24	1.002	0.0053	1.0003	0.0016	0.5352
	hcm-25	0.9983	0.0053	0.9970	0.0014	0.5333
	hcm-26	0.9998	0.0053	1.0001	0.0015	0.5283
	hcm-27	0.9991	0.0053	0.9978	0.0016	0.5302
	hcm-28	1.0037	0.0053	1.0033	0.0015	0.541
	hcm-29	0.9992	0.0052	0.9998	0.0014	0.5401
Experiment HEU-COMP-MIXED-002 (23 cases)	hcm02_1	1.0000	0.0085	0.9866	0.0017	0.868
	hcm02_10	1.0000	0.0081	0.9856	0.0019	0.57
	hcm02_11	1.0000	0.0088	0.9829	0.0019	0.568
	hcm02_12	1.0000	0.0078	0.9900	0.0019	0.556
	hcm02_13	1.0000	0.0083	0.9874	0.0017	0.559
	hcm02_14	1.0000	0.0112	0.9880	0.0017	0.735
	hcm02_15	1.0000	0.0111	0.9850	0.0017	0.73
	hcm02_16	1.0000	0.0108	0.9861	0.0017	0.735
	hcm02_17	1.0000	0.0112	0.9861	0.0016	0.732

Table 3. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Highly Enriched Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	hcm02_18	1.0000	0.0111	0.9902	0.0017	0.727
	hcm02_19	1.0000	0.0107	0.9910	0.0017	0.712
	hcm02_2	1.0000	0.0088	0.9907	0.0017	0.865
	hcm02_20	1.0000	0.0108	0.9824	0.0018	0.735
	hcm02_21	1.0000	0.0092	0.9843	0.0016	0.902
	hcm02_22	1.0000	0.009	0.9879	0.0019	0.899
	hcm02_23	1.0000	0.0093	0.9866	0.0016	0.896
	hcm02_3	1.0000	0.0093	0.9914	0.0016	0.724
	hcm02_4	1.0000	0.0087	0.9923	0.0017	0.716
	hcm02_5	1.0000	0.0089	0.9933	0.0017	0.722
	hcm02_6	1.0000	0.0093	0.9852	0.0018	0.574
	hcm02_7	1.0000	0.0086	0.9813	0.0019	0.578
	hcm02_8	1.0000	0.0068	0.9943	0.0018	0.537
	hcm02_9	1.0000	0.0076	0.9913	0.0018	0.541
Experiment HEU-SOL-THERM-001 (10 cases)	hest1-1	1.0000	0.0025	1.00241	0.00131	0.01582
	hest1-2	1.0000	0.0025	0.99816	0.00209	0.03873
	hest1-3	1.0000	0.0025	1.00453	0.00199	0.01546
	hest1-4	1.0000	0.0025	1.0013	0.00203	0.0405
	hest1-5	1.0000	0.0025	1.00361	0.00166	0.00651
	hest1-6	1.0000	0.0025	1.01038	0.00187	0.00678
	hest1-7	1.0000	0.0025	1.0023	0.00201	0.01501
	hest1-8	1.0000	0.0025	1.00505	0.00213	0.0161
	hest1-9	1.0000	0.0025	0.99973	0.00212	0.04099
	hest110	1.0000	0.0025	0.99468	0.00178	0.00757
Experiment HEU-SOL-THERM-002 (14 cases)	hest2-1	1.0000	0.002	1.00548	0.00148	0.01558
	hest2-2	1.0000	0.002	1.00773	0.00235	0.01516
	hest2-3	1.0000	0.002	1.00219	0.0022	0.0374
	hest2-4	1.0000	0.002	1.00809	0.00242	0.03541
	hest2-5	1.0000	0.002	1.01049	0.0023	0.01622
	hest2-6	1.0000	0.002	1.00968	0.00215	0.01496
	hest2-7	1.0000	0.002	1.00691	0.00224	0.03747
	hest2-8	1.0000	0.002	1.01131	0.00206	0.03511
	hest2-9	1.0000	0.002	1.00348	0.00209	0.00654
	hest2-10	1.0000	0.002	1.00937	0.00202	0.00663
	hest2-11	1.0000	0.002	1.00875	0.00211	0.01595
	hest2-12	1.0000	0.002	1.0127	0.00209	0.01487
	hest2-13	1.0000	0.002	0.99869	0.00232	0.03676
	hest2-14	1.0000	0.002	1.01062	0.00238	0.03377
Experiment HEU-SOL-THERM-007 (17 cases)	CASE_1	1.0000	0.0035	1.0164	0.0019	0.0071
	CASE_2	1.0000	0.005	1.0178	0.0025	0.0361
	CASE_3	1.0000	0.0035	1.0084	0.0019	0.0071
	CASE_4	1.0000	0.0035	1.0144	0.0019	0.0357
	CASE_5	1.0000	0.0035	1.0112	0.0019	0.0835
	CASE_6	1.0000	0.0035	1.0045	0.0023	0.0376

Table 3. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Highly Enriched Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	CASE_7	1.0000	0.0035	1.0067	0.0019	0.0085
	CASE_8	1.0000	0.0035	1.0026	0.0025	0.0390
	CASE_9	1.0000	0.0035	1.0087	0.0021	0.0088
	CASE_10	1.0000	0.0035	1.0144	0.0018	0.0087
	CASE_11	1.0000	0.0035	1.0097	0.0020	0.0356
	CASE_12	1.0000	0.0035	1.0091	0.0019	0.0088
	CASE_13	1.0000	0.0035	1.0095	0.0023	0.0345
	CASE_14	1.0000	0.0035	1.0097	0.0021	0.0363
	CASE_15	1.0000	0.0035	1.0046	0.0021	0.0369
	CASE_16	1.0000	0.0035	1.0043	0.0022	0.0368
	CASE_17	1.0000	0.0035	1.0120	0.0023	0.0368
Experiment HEU-SOL-THERM-008 (5 cases evaluated)	heust81	1.0000	0.003	1.00316	0.00134	0.00661
	heust83	1.0000	0.003	0.9973	0.0019	0.00644
	heust86	1.0000	0.003	1.00969	0.0023	0.03669
	heust89	1.0000	0.003	1.00373	0.00116	0.0066
	hest813	1.0000	0.003	1.00331	0.002	0.03616
Experiment HEU-SOL-THERM-009 (4 cases)	heust9c1	1.0000	0.0057	1.0051	0.0006	0.058
	heust9c2	1.0000	0.0057	1.0045	0.0006	0.045
	heust9c3	1.0000	0.0057	1.0047	0.0007	0.029
	heust9c4	1.0000	0.0057	0.9994	0.0007	0.018
Experiment HEU-SOL-THERM-033 (26 cases)	hst33d_02a	1.0000	0.0111	1.00007	0.00128	0.036
	hst33d_02b	1.0000	0.0108	0.99792	0.00113	0.036
	hst33d_02c	1.0000	0.0065	0.99796	0.00119	0.036
	hst33d_03a	1.0000	0.0114	1.00634	0.00108	0.033
	hst33d_03b	1.0000	0.0111	1.00608	0.00115	0.034
	hst33d_03c	1.0000	0.007	1.01079	0.00118	0.032
	hst33d_04a	1.0000	0.0114	1.0057	0.00109	0.035
	hst33d_04b	1.0000	0.0111	1.0116	0.00117	0.035
	hst33d_05a	1.0000	0.0111	1.01126	0.00114	0.035
	hst33d_05b	1.0000	0.0108	1.00608	0.00128	0.035
	hst33d_06a	1.0000	0.0111	1.00936	0.00112	0.035
	hst33d_06b	1.0000	0.0108	1.00915	0.00114	0.034
	hst33d_07a	1.0000	0.0111	1.00453	0.00107	0.035
	hst33d_07b	1.0000	0.0108	1.00406	0.00109	0.035
	hst33d_08a	1.0000	0.0111	1.00558	0.00113	0.034
	hst33d_08b	1.0000	0.0108	1.00213	0.00111	0.035
	hst33d_09a	1.0000	0.0111	1.00228	0.00115	0.036
	hst33d_09b	1.0000	0.0108	0.99359	0.00113	0.035
	hst33d_09c	1.0000	0.0104	0.99619	0.00116	0.036
	hst33d_10a	1.0000	0.0114	1.00267	0.00113	0.034
	hst33d_10c	1.0000	0.007	1.00333	0.00103	0.032
	hst33d_10d	1.0000	0.0104	0.99286	0.00111	0.033
	hst33d_11a	1.0000	0.0111	1.00669	0.0011	0.035
	hst33d_11b	1.0000	0.0108	1.00176	0.00097	0.034

Table 3. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Highly Enriched Uranium Mixtures

Experiment	**Case Name**	**Benchmark Values**		**Calculated Values (MCNP)**		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	**AENCF**
	hst33d_12a	1.0000	0.0111	1.00386	0.00112	0.036
	hst33d_12b	1.0000	0.0108	1.00165	0.00107	0.035
Experiment HEU-SOL-THERM-038 (28 cases evaluated)	CASE_1	1.0000	0.0025	0.9995	0.0004	0.0437
	CASE_2	1.0000	0.0025	0.9989	0.0004	0.0405
	CASE_3	1.0000	0.0025	1.0022	0.0004	0.0421
	CASE_4	1.0000	0.0025	1.0007	0.0004	0.0438
	CASE_5	1.0000	0.0025	1.0011	0.0004	0.0434
	CASE_6	1.0000	0.0025	0.9985	0.0004	0.0405
	CASE_7	1.0000	0.0032	1.0013	0.0004	0.0420
	CASE_8	1.0000	0.0026	1.0016	0.0004	0.0416
	CASE_9	1.0000	0.0033	1.0009	0.0004	0.0412
	CASE_10	1.0000	0.0026	1.0007	0.0004	0.0425
	CASE_11	1.0000	0.0025	1.0017	0.0004	0.0434
	CASE_12	1.0000	0.0025	1.0006	0.0004	0.0434
	CASE_13	1.0000	0.0050	1.0066	0.0004	0.0440
	CASE_14	1.0000	0.0050	1.0060	0.0004	0.0443
	CASE_15	1.0000	0.0050	1.0065	0.0004	0.0442
	CASE_16	1.0000	0.0050	1.0065	0.0004	0.0442
	CASE_17	1.0000	0.0026	1.0013	0.0004	0.0432
	CASE_18	1.0000	0.0032	1.0017	0.0004	0.0431
	CASE_19	1.0000	0.0032	1.0011	0.0004	0.0430
	CASE_20	1.0000	0.0032	1.0021	0.0004	0.0430
	CASE_21	1.0000	0.0025	0.9994	0.0004	0.0412
	CASE_22	1.0000	0.0027	0.9998	0.0004	0.0407
	CASE_23	1.0000	0.0027	0.9997	0.0004	0.0408
	CASE_24	1.0000	0.0026	1.0027	0.0004	0.0438
	CASE_25	1.0000	0.0032	1.0025	0.0004	0.0429
	CASE_26	1.0000	0.0032	1.0018	0.0004	0.0429
	CASE_27	1.0000	0.0032	1.0012	0.0004	0.0483
	CASE_28	1.0000	0.0025	1.0013	0.0004	0.0425
Experiment HEU-SOL-THERM-042 (8 cases)	CASE_1	0.9957	0.0045	0.9982	0.0003	0.0024
	CASE_2	0.9965	0.0040	0.9983	0.0003	0.0024
	CASE_3	0.9994	0.0028	1.0011	0.0002	0.0022
	CASE_4	1.0000	0.0034	1.0025	0.0002	0.0021
	CASE_5	1.0000	0.0034	0.9997	0.0002	0.0020
	CASE_6	1.0000	0.0037	1.0005	0.0002	0.0021
	CASE_7	1.0000	0.0036	1.0011	0.0002	0.0021
	CASE_8	1.0000	0.0035	1.0013	0.0001	0.0021
Experiment HEU-SOL-THERM-043 (3 cases)	heust43c1	0.9986	0.0017	0.9995	0.0007	0.014
	heust43c2	0.9995	0.0041	1.0082	0.0004	0.003
	heust43c3	0.999	0.0044	1.0033	0.0004	0.003
Experiment HEU-SOL-THERM-044 (16 cases)	hst4410	0.9944	0.0077	0.9909	0.0018	0.039
	hst4411	0.9944	0.0078	0.9847	0.002	0.041
	hst4412	0.9944	0.0078	0.9872	0.0017	0.040

Table 3. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Highly Enriched Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	hst4413	0.9964	0.0067	1.0000	0.0018	0.042
	hst4416	0.9974	0.0062	1.0178	0.0018	0.043
	hst4417	0.9964	0.0057	0.9987	0.0017	0.044
	hst4419	0.9974	0.0063	1.0079	0.0018	0.045
	hst4444	0.9984	0.0057	1.0004	0.0017	0.045
	hst4449	0.9964	0.0047	1.0116	0.0017	0.034
	hst4450	0.9946	0.0047	0.9881	0.0018	0.038
	hst4451	0.9984	0.0057	1.0047	0.0017	0.046
	hst4453	0.9984	0.0064	1.0189	0.0018	0.047
	hst4454	0.9984	0.0065	1.0142	0.0015	0.046
	hst4455	0.9984	0.0065	1.0196	0.0017	0.046
	hst447	0.9944	0.0097	0.9948	0.0018	0.037
	hst448	0.9946	0.0083	0.9955	0.0021	0.042

Source: Critical benchmark experiments are evaluated in NEA 2003 and MCNP calculations are summarized in Reference 10 except cases from experiments HEU-MET-THERM-001, HEU-MET-THERM-014, HEU-SOL-THERM-007, HEU-SOL-THERM-038 and HEU-SOL-THERM-042 which have been run for the current calculation (output files are listed in Section 7 and uploaded on the COLD server)

The experiments listed in Table 3 are considered appropriate to represent degraded configurations containing mixtures highly enriched in ^{235}U external to the waste package (Reference 1, p. 3-15).

5.1.2 Range of Applicability of Selected Criticality Benchmark Experiments

This subsection summarizes in a set of tables (Tables 4 to 6) the range of applicability of the experiments listed in Table 3. The information is partly excerpted from Reference 10. The tables have been enhanced by adding information regarding the spectral characteristics of the experiments (available for the majority of the benchmarks from Reference 5). The purpose is to enable the construction of a collective area of applicability that can be used to directly compare the range of applicability of this set of benchmark experiments with the range of parameters of the postulated external configurations.

Table 4. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures Highly Enriched in ^{235}U (set 1)

Category/ Description	Parameter	Experiment HEU-MET-MIXED-005 (5 cases)	Experiment HEU-MET-THERM-001 (1 case)	Experiment HEU-MET THERM-014 (1case)	Experiment HEU-COMP-MIXED-001 (26 cases)	Experiment HEU-COMP-MIXED-002 (23 cases)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Uranium metal pellets	Uranium metal foils	Uranium metal foils	UO_2	UO_2
	Isotopic Composition	89.39 wt% ^{235}U	93.23 wt% ^{235}U	93.23 wt% ^{235}U	93.15 wt% ^{235}U	89.42 and 89.6 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 4.24e-02	^{235}U: 3.84e-02 to 4.28e-02	^{235}U: 3.84e-02 to 4.38e-02	^{235}U: 4.48e-03 to 1.39e-02	^{235}U: 1.26e-02 and 1.32e-02
	Temperature	Room Temp.	Room Temp.	293 K	Room Temp.	Room Temp.

Category/ Description	Parameter	Experiment HEU-MET-MIXED-005 (5 cases)	Experiment HEU-MET-THERM-001 (1 case)	Experiment HEU-MET THERM-014 (1case)	Experiment HEU-COMP-MIXED-001 (26 cases)	Experiment HEU-COMP-MIXED-002 (23 cases)
Materials/ Moderator	**Element**	Si as scatterer H in sand	H, C Si as scatterer	H, C Si as scatterer	H	H and Deuterium (D)
	Physical form	SiO_2 pellets interspersed with U pellets	Plates of polyethylene and silicon glass	Plates of polyethylene and silicon glass	Water, alcohol-water solution, Plexiglas	Mixture water with heavy water
	Atomic density (atoms/b-cm)	Si: 1.99e-02 H: 2.65e-05	H: 8.23e-02 to 8.28e-02 C: 4.11e-02 to 4.14e-02 Si: 2.17 to 2.24e-02	H: 8.19e-02 to 8.34e-02 C: 4.10e-02 to 4.17e-02 Si: 2.20 to 2.28e-02	Fuel Region: 2.16e-2 (7 cases) 5.68e-2 (Plexiglas) 6.24e-2 (alcohol-water)	H: 7.36e-03 to 6.67e-02 D: 0 to 5.91e-02
	Ratio to fissile material	Not available	Not available	H/X: Not available Si/^{235}U = 42	0 - 49	Not available
	Temperature	Room Temp.	Room Temp.	Room Temp.	Room Temp.	Room Temp.
Materials/ Reflector	**Material/Physical form**	Reflected by polyethylene, SiO_2 sand and concrete	Reflected by polyethylene	Reflected by polyethylene	Reflected by polyethylene	Reflected by water stainless steel and concrete walls
Materials/ Neutron Absorber	**Element**	Boron	None	None	None	None
	Physical form	Impurity in SiO_2	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	^{10}B: 4.40e-08	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Complex hexagonal geometry of pellets in Al tubes	Rectangular column of plates and foils	Rectangular column of plates and foils	Complex arrays of cans in rectangular geometry	Hexagonal array of tubes containing UO_2 in a cylindrical tank
	Shape	Cylinder	Parallelepiped	Parallelepiped	Cylinder	Cylinder
Neutron Energy	**AENCF**	0.212 to 0.377 MeV	0.0212 MeV	0.0234 MeV	0.1045-0.8015 MeV	0.537 – 0.899 MeV
	EALF	1.48 to 5150 eV	0.0865 eV	Not Available	0.438 to 2.14e-03	237 to 4.61e04 eV
	Neutron Energy Spectra[a]	T: 0.3 to 25.0 % I: 28.1 to 50.5 % F: 46.8 to 54.2 %	T: 22.7 % I: 27.7 % F: 49.7 %	Not Available	T: 4.3 to 26.1 % I: 14.2 to 25.9 % F: 48.3 to 81.4 %	T: 0.4 – 8.0 % I: 16.0 – 33.8 % F:65.1 – 82.9 %
	Fission Rate vs Neutron Energy[a]	T: 4.4 to 68.4 % I: 20.5 to 68.4 % F: 11.1 to 27.2 %	T: 91.2 % I: 7.7 % F: 1.2 %	Not Available	T: 25.4 to 78.0 % I: 16.4 to 43.1 % F: 5.6 to 49.3 %	T: 3.8 – 34.5 % I: 26.8 – 54.6 % F: 31.9 – 63.6 %

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 5. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures Highly Enriched in ^{235}U (set 2)

Category/ Description	Parameter	Experiment HEU-SOL-THERM-001 (10 cases)	Experiment HEU-SOL-THERM-002 (14 cases)	Experiment HEU-SOL-THERM-007 (17 cases)	Experiment HEU-SOL-THERM-008 (5 cases)	Experiment HEU-SOL-THERM-009 (4 cases)
Materials/ Fissionable Material	**Fissionable Element**	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranium oxyfluoride

Category/ Description	Parameter	Experiment HEU-SOL-THERM-001 (10 cases)	Experiment HEU-SOL-THERM-002 (14 cases)	Experiment HEU-SOL-THERM-007 (17 cases)	Experiment HEU-SOL-THERM-008 (5 cases)	Experiment HEU-SOL-THERM-009 (4 cases)
	Isotopic Composition	93.17 wt% ^{235}U	93.17 wt% ^{235}U	93.17 wt% ^{235}U	93.17 wt% ^{235}U	93.18 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 1.31e-04 to 8.54E-04 ^{238}U: 7.46e-06 to 4.86e-05	^{235}U: 1.42e-04 to 7.99e-04 ^{238}U: 8.11e-06 to 4.55e-05	^{235}U: 1.60e-04 to 8.69e-04 ^{238}U: 9.14e-6 to 1.03e-05	^{235}U: 1.44e-04 to 8.50e-04 ^{238}U: 8.20e-6 to 4.84e-05	^{235}U: 5.09e-04 to 1.66e-03 ^{238}U: 2.88e-5 to 9.41e-05
	Temperature	Room Temp.	Room Temp.	Room Temp.	Room Temp.	Room Temp.
Materials/ Moderator	**Element**	H	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	5.82e-02 to 6.54e-02	5.88e-02 to 6.53e-02	5.78e-02 to 6.48e-02	5.84e-02 to 6.53e-02	5.96e-02 to 6.44e-02
	Ratio to fissile material	86 to 499	74 to 460	65 to 405	69 to 454	35.8 to 126.5
	Temperature	Room Temp.	Room Temp.	Room Temp.	Room Temp.	Room Temp.
Materials/ Reflector	**Material/Physical form**	Unreflected (concrete walls)	Reflected by concrete walls	Concrete	Plexiglas	Water
Materials/ Neutron Absorber	**Element**	None	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a cylindrical tank	Arrays of cylindrical tanks placed in a rectangular geometry	Arrays of cylindrical tanks placed in a rectangular geometry	Homogeneous solution contained in a spherical vessel made of Al.
	Shape	Cylinder	Cylinder	Cylinder	Cylinder	Sphere
Neutron Energy	**AENCF**	0.0065 to 0.0410 MeV	0.0066 to 0.0375 MeV	0.0071 to 0.0369 MeV	0.0064 to 0.0367 MeV	0.0180 to 0.0450 MeV
	EALF	0.04 to 0.29 eV	0.04 to 0.25 eV	0.046 to 0.27 eV	0.04 to 0.25 eV	0.09 to 0.52 eV
	Neutron Energy Spectra[a]	T:8.1 to 31.1 % I: 29.1 to 36.5% F:39.8 to 55.6%	T:8.7 to 30.4 % I: 29.6 to 36.7% F:39.9-55.2%	T:8.3 to 28.7 % I: 30.5 to 37.0 % F:40.8 to 55.0 %	T:8.5 to 30.8 % I: 29.1 to 36.3% F:40.0 to 55.5%	T:5.8 to 15.4 % I: 34 to 35.7% F:50.6 to 58.5%
	Fission Rate vs Neutron Energy[a]	T: 77.5 to 95.5% I: 4.1 to 20.3% F: 0.4 to 2.2%	T: 79.2 to 90.3% I: 4.2 to 18.8% F: 0.4 to 2.0%	T: 78.2 to 95.0% I: 4.6 to 19.7% F: 0.4 to 2.1%	T: 78.9 to 95.5% I: 4.1 to 19.0% F: 0.4 to 2.1%	T: 71.8 to 89.1% I: 9.9 to 25.0 % F: 1.0 to 3.2%

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 6. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures Highly Enriched in ^{235}U (set 3)

Category/ Description	Parameter	Experiment HEU-SOL-THERM-033 (26 cases)	Experiment HEU-SOL-THERM-038 (28 cases)[b]	Experiment HEU-SOL-THERM-042 (8 cases)	Experiment HEU-SOL-THERM-043 (3 case)	Experiment HEU-SOL-THERM-044 (16 cases)
Materials/ Fissionable Material	**Fissionable Element**	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranium oxyfluoride	Aqueous solution of uranyl nitrate
	Isotopic Composition	93.2 wt% ^{235}U	93.1 wt% ^{235}U	92.78 to 93.22 wt% ^{235}U	93.2 wt% ^{235}U	93.17 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 8.54e-4 ^{238}U: 4.85e-5	^{235}U: 9.64e-04 ^{238}U: 5.90e-05	^{235}U: 3.24e-05 to 4.13e-05 ^{238}U: 1.89e-6 to 2.34e-06	^{235}U: 4.77e-05 to 3.20e-04 ^{238}U: 2.86e-06 to 1.79e-05	^{235}U: 8.65e-4 ^{238}U: 4.95e-5
	Temperature	Room Temp.	Room Temp.	Room Temp.	300 K	Room Temp
Materials/ Moderator	**Element**	H	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	5.81e-02	5.78e-02	6.62e-02 to 6.648e-02	6.53e-2 to 6.67e-2	5.81e-02
	Ratio to fissile material	68.1	60.0	1602 to 2050	204 to 1392	67.2
	Temperature	Room Temp.	Room Temp.	Room Temp.	300 K	Room Temp.
Materials/ Reflector	**Material/Physical form**	Concrete	Reflected by various plates (Pb, U, Be, Cd, Polyethylene, Stainless steel, Boraflex, etc) and concrete walls	Unreflected	Unreflected	Concrete
Materials/ Neutron Absorber	**Element**	B and Cd	B, Cd, Pb, U, Fe, etc	None	None	B, Cl, Cd and Gd
	Physical form	B and Cd in solution	Absorbers were inserted as plates	N/A	N/A	Absorbers are in various forms (pyrex glass, boraflex rubber,Cd sleeves etc.)
	Atomic density (atoms/b-cm)	B-10:1.74e-8 Cd: 1.49e-8	Not available	N/A	N/A	B-10:6.99e-03 to 9.57e-4 Cd: 5.19e-03 to 4.63e-02
Geometry	**Heterogeneity**	Homogeneous solution contained in a nested structure of cylindrical tanks made of stainless steel.	Homogeneous solution contained in two cylindrical tanks	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a spherical vessel made of Al.	Homogeneous solution contained in a nested structure of cylindrical tanks made of stainless steel.
	Shape	Cylinder	Cylinder	Cylinder	Sphere	Cylinder
Neutron Energy	**AENCF**	0.032 to 0.036 MeV	0.041 to 0.048 MeV	0.0020 to 0.0024 MeV	0.003 – 0.014 MeV	0.0340 – 0.0470 MeV
	EALF	0.269 to 0.316 eV	0.31 to 0.41 eV	0.031 to 0.032 eV	0.033- 0.075 eV	Not available

Category/ Description	Parameter	Experiment HEU-SOL-THERM-033 (26 cases)	Experiment HEU-SOL-THERM-038 (28 cases)[b]	Experiment HEU-SOL-THERM-042 (8 cases)	Experiment HEU-SOL-THERM-043 (3 case)	Experiment HEU-SOL-THERM-044 (16 cases)
	Neutron Energy Spectra[a]	T:8.1 to 8.8 % I: 38.2 to 39 % F:52.6 to 53.4 %	T:5.0 to 26.0 % I: 31.7 to 40.4 % F: 41.5 to 57.7%	T:52.1 to 56.4 % I: 19.6 to 21.3 % F: 24.0 to 26.6 %	T:18.0 to 49.8 % I: 22.2 to 33.7 % F:28.0 to 48.3 %	Not available
	Fission Rate vs Neutron Energy[a]	T: 76.2 to 78.0 % I: 20.1 to 21.7 % F: 1.9 to 2.1 %	T: 73.8 to 76.9 % I: 20.8 to 23.6 % F: 2.3 to 2.6 %	T: 98.1 to 98.4% I: 1.5 to 1.8% F: 0.1%	T: 90.8 to 97.9 % I: 1.9 to 8.4 % F: 0.1 to 0.8 %	Not available

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

[b] Spectral data include only selected cases for HEU-SOL-THERM-038 (cases 1 to 28)

5.1.3 Calculation of the Lower Bound Tolerance Limit

In the following paragraphs some of the information presented in Section 2 is repeated focusing on the steps that are actually applicable for the current group of benchmarks. The first step in calculating the lower bound tolerance limit is to apply regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p.8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}. Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (in this case, average energy of a neutron causing fission [AENCF]), using the build-in regression analysis tool from Excel software. The AENCF is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p.3-47).

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the *y* values about their mean that can be attributed to a linear relation between *y* and *x*. Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (*b*). The slope test requires calculating the test statistic "*T*" as described by Equations 2, 3 and 4 from Section 2.

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and *n*-2 degrees of freedom, where *n* is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied. The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals.

The results of the trending parameter analysis for the criticality benchmark subset representative for external configurations containing HEU are presented in Attachment I and summarized in Table 7. The trending parameters for AENCF (r^2, T, P-value) from Table 7, indicate a trend of k_{eff} with increasing AENCF. The normality test on the residuals failed marginally (Attachment I) and the residuals do not exhibit a visible pattern. This situation (strong trend parameters and residuals not following a normal distribution) is difficult to be categorized with respect to the validity of the linear trend. Since the residuals fail only marginally the normality test, the linear trend can be assumed to be valid based on the trending parameters.

Table 7. Trending Parameter Results for the Criticality Benchmark Subset Representative for Configurations Containing HEU External to the Waste Package

Trend Parameter	n	Intercept	Slope	r^2	T	$t_{0.025,n-2}$	P-value	Goodness-of-fit Tests	Valid Trend
AENCF	187	1.0055	-0.019	0.4264	-11.73	1.980[a]	4.2E-24	Passed (partially)	Yes

Source: Attachment I

Note: [a]Table A-4 from Reference 9 has a limited number of entries for n (t=1.98 for n=120 and t=1.96 for n close to infinity); using t=1.98 is conservative for the current application where n=187.

The lower bound tolerance limit is calculated for this situation using the CLReg code (Reference 11). Figure 1 presents the k_{eff} values and the calculated lower bound tolerance limit for this set of benchmark experiments. The following expression (Attachment I) describes the calculated lower bound tolerance limit:

$f(AENCF) = 0.970611$ for $0\ MeV < AENCF < 0.247\ MeV$

$f(AENCF) = -1.7411e{-}02*AENCF + 0.97491$ for $0.247\ MeV \leq AENCF < 0.902\ MeV$

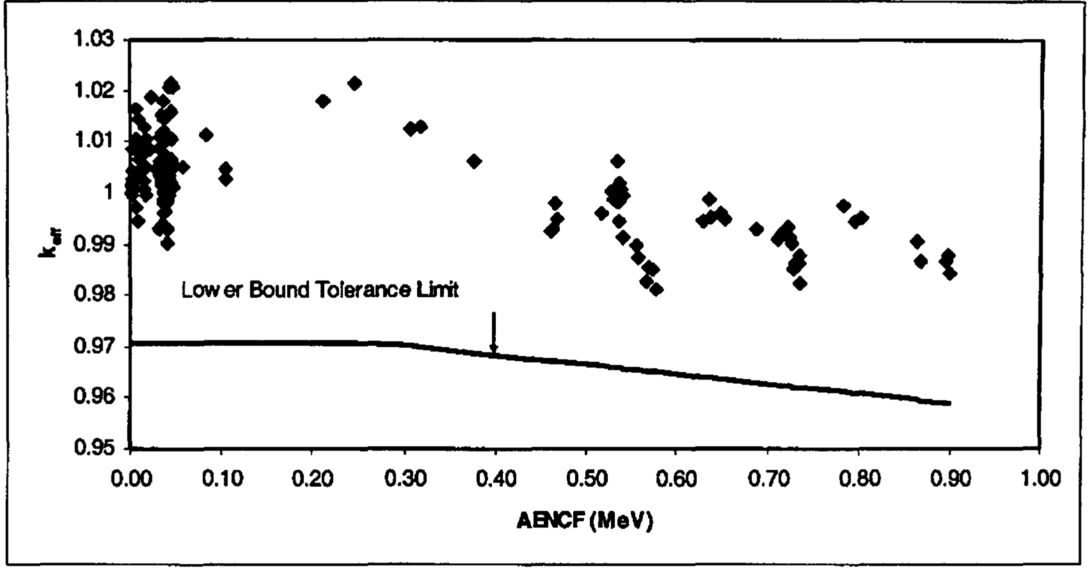

Figure 1. Lower Bound Tolerance Limit Applicable for Configurations Containing HEU External to the Waste Package

5.2 CALCULATIONS FOR BENCHMARK CRITICAL EXPERIMENTS SELECTED FOR EXTERNAL CONFIGURATIONS CONTAINING INTERMEDIATE ENRICHED URANIUM (IEU)

As mentioned in Section 2, an essential element of validating the methods and models used for calculating effective neutron multiplication factor, k_{eff}, for a waste package is determination of critical limit. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

In the following, the first three steps of the process of establishing a critical limit for the external configurations containing IEU mixtures are detailed.

5.2.1 Selection of the Criticality Benchmark Experiments

The criticality experiments selected for inclusion in the validation of the criticality model must be representative of the types of materials, conditions, and parameters to be modeled using the calculational method (criticality model). A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a model, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results (Reference 6, p. 5).

For the present application (configurations with mixtures of IEU fissile material external to the waste package), the criticality benchmark experiments have been selected based on their fissile content, moderator content and geometry. The benchmark experiments are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (*External Criticality Calculation for DOE SNF Codisposal Waste Packages* [Reference 2]). The set of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the configurations and also to provide adequate statistics for the lower bound tolerance limit calculations. A set of critical experiments with enrichments close to 10 wt% have also been added to this group even if they are categorized as LEU in Reference 5.

The selected benchmark experiments containing a total of 109 individual cases are presented in Table 8 together with the results of the MCNP code calculations. All cases have been run using the isotopic libraries described in Reference 10 (Table 2).

Table 8. Critical Benchmark Experiments Selected for Validation of the Criticality Model for External Configurations Containing Intermediate Enrichment Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
Experiment IEU-COMP-THERM-001 (29 cases)	iect101	1.0000	0.004	0.9974	0.0009	0.21679
	iect102	1.0000	0.004	0.9960	0.0009	0.15817
	iect103	1.0000	0.004	0.9931	0.0010	0.10412
	iect104	1.0000	0.004	0.9974	0.0011	0.07405
	iect105	1.0000	0.004	1.0085	0.0009	0.04552
	iect106	1.0000	0.004	1.0003	0.0010	0.10793
	iect107	1.0000	0.004	0.9980	0.0010	0.11064
	iect108	1.0000	0.004	0.9960	0.0010	0.11867
	iect109	1.0000	0.004	1.0004	0.0008	0.1679
	iect110	1.0000	0.004	0.9967	0.0010	0.15756
	iect111	1.0000	0.004	0.9958	0.0010	0.15732
	iect112	1.0000	0.004	0.9964	0.0010	0.15568
	iect113	1.0000	0.004	0.9967	0.0010	0.0743
	iect114	1.0000	0.004	0.9979	0.0009	0.07375
	iect115	1.0000	0.004	0.9981	0.0010	0.074
	iect116	1.0000	0.004	1.0021	0.0009	0.05547
	iect117	1.0000	0.004	0.9965	0.0010	0.20814
	iect118	1.0000	0.004	0.9976	0.0011	0.13428
	iect119	1.0000	0.004	1.0045	0.0010	0.06114
	iect120	1.0000	0.004	1.0005	0.0009	0.15539
	iect121	1.0000	0.004	0.9988	0.0009	0.21334
	iect122	1.0000	0.004	0.9990	0.0011	0.19772
	iect123	1.0000	0.004	0.9952	0.0011	0.12826

Table 8. Critical Benchmark Experiments Selected for Validation of the Criticality Model for External Configurations Containing Intermediate Enrichment Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	iect124a	1.0000	0.004	1.0004	0.0011	0.13305
	iect125	1.0000	0.004	0.9987	0.0009	0.05992
	iect126	1.0000	0.004	1.0044	0.0010	0.05663
	iect127	1.0000	0.004	1.0032	0.0009	0.05633
	iect128	1.0000	0.004	1.0051	0.0009	0.15824
	iect129	1.0000	0.004	1.0012	0.0010	0.15184
Experiment IEU-COMP-THERM-005 (2 cases)	case2	0.980	0.003	0.9807	0.0004	0.48226
	case3	1.014	0.006	1.0158	0.0005	0.25976
Experiment LEU-SOL-THERM-003 (9 cases)	lst3-1	0.9997	0.0039	0.9993	0.0004	0.0186
	lst3-2	0.9993	0.0042	0.9971	0.00038	0.0166
	lst3-3	0.9995	0.0042	1.0015	0.00037	0.0164
	lst3-4	0.9995	0.0042	0.9954	0.00038	0.0162
	lst3-5	0.9997	0.0048	0.9990	0.00031	0.0133
	lst3-6	0.9999	0.0049	0.9992	0.0003	0.0129
	lst3-7	0.9994	0.0049	0.9972	0.0003	0.0127
	lst3-8	0.9993	0.0052	1.0008	0.00025	0.0114
	lst3-9	0.9996	0.0052	0.9973	0.00025	0.0114
Experiment LEU-SOL-THERM-004 (7 cases)	lst4_1	0.9994	0.0008	1.0029	0.0007	0.0188
	lst4_29	0.9999	0.0009	1.0034	0.0006	0.0179
	lst4_33	0.9999	0.0009	1.0013	0.0007	0.017
	lst4_34	0.9999	0.001	1.0037	0.0006	0.0157
	lst4_46	0.9999	0.001	1.0032	0.0006	0.0154
	lst4_51	0.9994	0.0011	1.0023	0.0005	0.0148
	lst4_54	0.9996	0.0011	1.0026	0.0005	0.0142
Experiment LEU-SOL-THERM-007 (5 cases)	leust7_1	0.9961	0.0009	0.9966	0.0002	0.02
	leust7_2	0.9973	0.0009	0.9995	0.0002	0.0187
	leust7_3	0.9985	0.001	0.9979	0.0002	0.0173
	leust7_4	0.9988	0.0011	1.0005	0.0002	0.0166
	leust7_5	0.9983	0.0011	0.9989	0.0002	0.0159
Experiment LEU-SOL-THERM-008 (4 cases)	lst8_72	0.9999	0.0014	1.0038	0.0002	0.0152
	lst8_74	1.0002	0.0015	1.0023	0.0002	0.0154
	lst8_76	0.9999	0.0014	1.0028	0.0002	0.0153
	lst8_78	0.9999	0.0014	1.0040	0.0002	0.0153
Experiment LEU-SOL-THERM-009 (3 cases)	lst9_92	0.9998	0.0014	1.0018	0.0005	0.0155
	lst9_93	0.9999	0.0014	1.0021	0.0002	0.0157
	lst9_94	0.9999	0.0014	1.0022	0.0002	0.0158
Experiment LEU-SOL-THERM-010 (4 cases)	lst10_83	0.9999	0.0153	1.0023	0.0003	0.0153
	lst10_85	0.9999	0.0154	1.0019	0.0003	0.0154
	lst10_86	1.0000	0.0153	1.0032	0.0003	0.0153
	lst10_88	1.0001	0.0154	1.0026	0.0003	0.0154
Experiment LEU-SOL-THERM-016 (7 cases)	lst16_05	0.9996	0.0013	1.0093	0.0007	0.0267
	lst16_13	0.9999	0.0013	1.0080	0.0006	0.0248
	lst16_25	0.9994	0.0014	1.0075	0.0006	0.0216
	lst16_29	0.9996	0.0014	1.0068	0.0006	0.0209

Table 8. Critical Benchmark Experiments Selected for Validation of the Criticality Model for External Configurations Containing Intermediate Enrichment Uranium Mixtures

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	lst16_31	0.9995	0.0014	1.0059	0.0005	0.0195
	lst16_40	0.9992	0.0015	1.0043	0.0005	0.0186
	lst16_96	0.9994	0.0015	1.0047	0.0005	0.018
Experiment LEU-SOL-THERM-017 (6 cases)	lst17_04	0.9981	0.0013	1.0051	0.0007	0.0275
	lst17_22	0.9986	0.0013	1.0049	0.0006	0.0258
	lst17_23	0.9989	0.0014	1.0052	0.0006	0.0224
	lst17_26	0.9992	0.0014	1.0043	0.0006	0.0212
	lst17_30	0.9987	0.0015	1.0043	0.0005	0.02
	lst17_47	0.9996	0.0015	1.0042	0.0006	0.0192
Experiment LEU-SOL-THERM-018 (6 cases)	RUN133	0.9992	0.001	1.0033	0.0002	0.0183
	RUN142	0.9996	0.001	1.0042	0.0003	0.0187
	RUN143	0.9996	0.001	1.0045	0.0003	0.0188
	RUN144	0.9997	0.001	1.0033	0.0003	0.0187
	RUN145	0.9992	0.001	1.0038	0.0003	0.0187
	RUN146	0.9996	0.001	1.0037	0.0003	0.0186
Experiment LEU-SOL-THERM-019 (6 cases)	RUN149	0.9997	0.0009	1.0043	0.0003	0.019
	RUN150	0.9995	0.0009	1.0043	0.0003	0.019
	RUN151	0.9999	0.0009	1.0049	0.0002	0.0191
	RUN152	0.9996	0.0009	1.0054	0.0003	0.0191
	RUN153	0.9998	0.0009	1.0050	0.0003	0.0191
	RUN183	0.9994	0.0009	1.0036	0.0003	0.0189
Experiment LEU-SOL-THERM-020 (4 cases)	LST20C1	0.9995	0.001	1.0014	0.0003	0.015
	LST20C2	0.9996	0.001	1.0000	0.0003	0.0143
	LST20C3	0.9997	0.0012	0.9993	0.0003	0.0131
	LST20C4	0.9998	0.0012	1.0004	0.0003	0.0125
Experiment LEU-SOL-THERM-021 (4 cases)	LST21C1	0.9983	0.0009	0.9991	0.0003	0.0154
	LST21C2	0.9985	0.001	0.9996	0.0003	0.0144
	LST21C3	0.9989	0.0011	0.9976	0.0003	0.0135
	LST21C4	0.9993	0.0012	0.9999	0.0003	0.0127
Experiment LEU-SOL-THERM-022 (4 cases)	case1	0.9999	0.0010	1.0049	0.0002	0.0185
	case2	0.9994	0.0010	1.0058	0.0002	0.0184
	case3	0.9993	0.0010	1.0055	0.0002	0.0185
	case4	0.9994	0.0010	1.0050	0.0002	0.0186
Experiment LEU-SOL-THERM-023 (9 cases)	261	0.9963	0.0009	1.0000	0.0005	0.0175
	274	0.9967	0.0009	0.9950	0.0005	0.0177
	273	0.9967	0.0009	1.0000	0.0005	0.0179
	262	0.9960	0.0009	0.9986	0.0005	0.0177
	263	0.9959	0.0009	0.9990	0.0005	0.0176
	264	0.9959	0.0009	0.9992	0.0005	0.0175
	267	0.9966	0.0009	0.9993	0.0005	0.0177
	268	0.9970	0.0009	0.9996	0.0005	0.0177
	269	0.9977	0.0009	0.9997	0.0005	0.0178

Source: Critical benchmark experiments are evaluated in Reference 5 and MCNP calculations are summarized in Reference 10 except cases from experiments IEU-COMP-THERM-005, LEU-SOL-THERM-022 and LEU-SOL-THERM-023 (output files are listed in Section 7 and uploaded on the COLD server)

The experiments listed in Table 8 are considered appropriate to represent degraded configurations containing mixtures of intermediate enriched uranium external to the waste package.

5.2.2 Range of Applicability of Selected Criticality Benchmark Experiments

This subsection summarizes in a set of tables (Tables 9 to 12) the range of applicability of the experiments listed in Table 8. The information is partly excerpted from Reference 10. The tables have been enhanced by adding information regarding the spectral characteristics of the experiments (available for the majority of the benchmarks from Reference 5) and also by including the benchmark experiments not presented in Reference 5. The purpose is to enable the construction of a collective area of applicability that can be used to directly compare the range of applicability of this set of benchmark experiments with the range of parameters of the postulated external configurations.

Table 9. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing IEU Mixtures (set 1)

Category/ Description	Parameter	Experiment IEU-COMP-THERM-001 (29 cases)	Experiment IEU-COMP-THERM-005 (2 cases)	Experiment LEU-SOL-THERM-003 (9 cases)	Experiment LEU-SOL-THERM-004 (7 cases)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium	Uranium
	Physical Form	UF_4 compound with polytetra-fluoroethylene	Mixture of UO_2 and Th metal	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate
	Isotopic Composition	29.83 wt% ^{235}U	90 wt% and 36 wt% ^{235}U	10 wt% ^{235}U	9.97 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 2.37e-03 ^{238}U: 5.50e-03	^{235}U: 5.39e-03 and 1.35E-02 ^{238}U: 1.47e-03 and 9.53e-03	^{235}U: 4.34e-05 to 7.64e-05 ^{238}U:3.82e-04 to 6.73e-04	^{235}U: 5.76e-05 to 7.92e-05 ^{238}U: 5.13e-04 to 7.06e-04
	Temperature	Room temp.	300 K	300 K	298 K
Materials/ Moderator	Element	H; C	H; C	H	H
	Physical form	Polyethylene	Polyethylene	Solution	Solution
	Atomic density (atoms/b-cm)	H:7.52e-02 C:3.92e-02	H: 7.2588-e02 C: 3.6294e-02	5.89e-02 to 6.23e-02	5.70e-02 to 5.86e-02
	Ratio to fissile material	$H/^{235}U$ = 4 to 222	$H/^{235}U$ = 0 to 10	770 to 1437	719 to 1018
	Temperature	Room temp.	300 K	300 K	298 K
Materials/ Reflector	Material/Physical form	Unreflected or reflected by paraffin	K_{inf} experimental set-up	Unreflected	Reflected by water
Materials/ Neutron Absorber	Element	B or Cd for some experiments	None	None	None
	Physical form	Metallic sheets	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	Cd: 4.64e-02 ^{10}B: 3.21e-03	N/A	N/A	N/A
Geometry	*Heterogeneity*	Heterogeneous small cubes of fissile compound interspersed with moderator cubes	Heterogeneous set of stainless steel tubes forming a hexagonal infinite lattice	Homogeneous solution in a spherical tank	Homogeneous solution in a cylindrical tank

Category/ Description	Parameter	Experiment IEU-COMP-THERM-001 (29 cases)	Experiment IEU-COMP-THERM-005 (2 cases)	Experiment LEU-SOL-THERM-003 (9 cases)	Experiment LEU-SOL-THERM-004 (7 cases)
	Shape	Cuboid	Cylinder	Sphere	Cylinder
Neutron Energy	**AENCF**	0.0455 to 0.2168 MeV	0.260 and 0.483 MeV	0.0114 to 0.0186 MeV	0.0142 to 0.0188 MeV
	EALF	0.11 to 9.09 eV	1e+02 and 2.97e+04 eV	3.46e-02 to 4.14e-02 eV	3.75e-02 to 4.21e-02 eV
	Neutron Energy Spectra[a]	T: 1.8 to 22.8% I: 24.9 to 40.2% F: 49.6 to 63%	T: 0 and 1.0% I: 35.0 and 43.0% F: 56.0 and 65.0%	T: 37.6 to 49.1 % I: 22.7 to 27.3% F: 28.2 to 35.1%	T: 36.8 to 43.1 % I: 25.3 to 27.8% F: 31.6 to 35.4%
	Fission Rate vs Neutron Energy[a]	T: 49.9 to 90.9% I: 7.1 to 42.8% F: 2.0 to 11.1%	T: 0.2 and 21.4% I: 56.5 and 63.6% F: 15 and 43.2%	T: 96.2 to 97.6% I: 2 to 3.1% F: 0.4 to 0.7%	T: 96.1 to 97.0% I: 2.5 to 3.2% F: 0.5 to 0.7%

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 10. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing IEU Mixtures (set 2)

Category/ Description	Parameter	Experiment LEU-SOL-THERM-007 (5 cases)	Experiment LEU-SOL-THERM-008 (4 cases)	Experiment LEU-SOL-THERM-009 (3 cases)	Experiment LEU-SOL-THERM-010 (4 cases)
Materials/ Fissionable Material	**Fissionable Element**	Uranium	Uranium	Uranium	Uranium
	Physical Form	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate
	Isotopic Composition	9.97 wt% ^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 6.18e-05 to 8.00e-05 ^{238}U:5.5e-04 to 7.12e-04	^{235}U: 6.14e-05 ^{238}U:5.47e-04	^{235}U: 6.26e-05 ^{238}U:5.57e-04	^{235}U: 6.18e-05 to 6.21e-05 ^{238}U: 5.51e-04 to 5.53e-04
	Temperature	298 K	298 K	298 K	298 K
Materials/ Moderator	**Element**	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	5.67e-02 to 5.82e-02	5.86e-02	5.85e-02	5.85e-02
	Ratio to fissile material	709 to 942	951 to 956	934 to 936	942 to 946
	Temperature	298 K	298 K	298 K	298 K
Materials/ Reflector	**Material/Physical form**	Unreflected	Reflected by concrete	Reflected by borated concrete	Reflected by polyethylene
Materials/ Neutron Absorber	**Element**	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a cylindrical tank
	Shape	Cylinder	Cylinder	Cylinder	Cylinder
Neutron Energy	**AENCF**	0.0159 to 0.0200 MeV	0.0152 to 0.0154 MeV	0.0155 to 0.0158 MeV	0.0153 to 0.0154 MeV
	EALF	3.87e-02 to 4.28e-02 eV	3.84e-02 eV	3.89e-02 eV	3.84e-02 V
	Neutron Energy Spectra[a]	T:35.9 to 41.1 % I: 26 to 28.1% F:32.9 to 36%	T: 41.5 to 41.7% I: 25.9 to 26% F: 32.4 to 35%	T: 40.8 to 41 % I: 26.2 to 26.3% F: 32.8 to 32.9%	T: 41.6 % I: 25.8 to 25.9% F: 32.5 to 32.6%
	Fission Rate vs Neutron Energy[a]	T: 95.9 to 96.7% I: 2.7 to 3.4% F: 0.6 to 0.7%	T: 96.8% I: 2.6% F: 0.6%	T: 96.7% I: 2.7% F: 0.6%	T: 96.8% I: 2.6% F: 0.6%

Source: Reference 5 and 10

Note: [a]Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 11. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing IEU Mixtures (set 3)

Category/ Description	**Parameter**	**Experiment LEU-SOL-THERM-016 (7 cases)**	**Experiment LEU-SOL-THERM-017 (6 cases)**	**Experiment LEU-SOL-THERM-018 (6 cases)**	**Experiment LEU-SOL-THERM-019 (6 cases)**
Materials/ Fissionable Material	**Fissionable Element**	Uranium	Uranium	Uranium	Uranium
	Physical Form	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate
	Isotopic Composition	9.97 wt% ^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 7.65e-5 to 1.19e-04 ^{238}U: 6.82e-04 to 1.06e-03	^{235}U: 8.05e-05 to 1.19e-04 ^{238}U:7.17e-04 to 1.06e-03	^{235}U: 7.87e-5 to 8.04e-05 ^{238}U:7.01e-04 to 7.16e-04	^{235}U: 8.07e-05 to 8.13e-05 ^{238}U:7.19e-04 to 7.24e-04
	Temperature	298 K	298 K	298 K	298 K
Materials/ Moderator	**Element**	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	5.56e-02 to 5.91e-02	5.56e-02 to 5.87e-02	5.87e-02 to 5.91e-02	5.87e-02
	Ratio to fissile material	469 to 772	469 to 729	731 to 751	721 to 728
	Temperature	293 K	298 K	298 K	298 K
Materials/ Reflector	**Material/Physical form**	Reflected by water	Unreflected	Reflected by concrete	Reflected by polyethylene
Materials/ Neutron Absorber	**Element**	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution in a rectangular slab tank	Homogeneous solution in a rectangular slab tank	Homogeneous solution in a rectangular slab tank	Homogeneous solution in a rectangular slab tank
	Shape	Rectangular slab	Rectangular slab	Rectangular slab	Rectangular slab
Neutron Energy	**AENCF**	0.0180 to 0.0267 MeV	0.0192 to 0.0275 MeV	0.0183 to 0.0188 MeV	0.0189 to 0.0191 MeV
	EALF	4.15e-02 to 5.22e-02 eV	4.24e-02 to 5.23e-02 eV	0.042 to 0.0425 eV	0.0425 to 0.0426 eV
	Neutron Energy Spectra[a]	T: 29.1 to 37.7 % I: 27.7 to 31.2% F: 34.7 to 39.7%	T: 28.9 to 36.5 % I: 28 to 31.1% F:35.5 to 40.0%	T: 36.5 to 37 % I: 28 to 28.3 % F: 34.9 to 35.2%	T: 36.4 to 36.5 % I: 28.1 to 28.2 % F: 35.4 %
	Fission Rate vs Neutron Energy[a]	T: 94.3 to 96.2% I: 3.2 to 4.6% F: 0.7 to 1.0%	T: 94.3 to 96.0% I: 3.3 to 4.6% F: 0.7 to 1.0%	T: 96 to 96.1% I: 3.3 % F: 0.7 %	T: 95.9 to 96.0% I: 3.3 % F: 0.7 %

Source: Reference 5 and 10

Note: [a]Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 12. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing IEU Mixtures (set 4)

Category/ Description	**Parameter**	**Experiment LEU-SOL-THERM-020 (4 cases)**	**Experiment LEU-SOL-THERM-021 (4 cases)**	**Experiment LEU-SOL-THERM-022 (4 cases)**	**Experiment LEU-SOL-THERM-023 (9 cases)**
Materials/	**Fissionable Element**	Uranium	Uranium	Uranium	Uranium

Category/ Description	**Parameter**	**Experiment LEU-SOL-THERM-020 (4 cases)**	**Experiment LEU-SOL-THERM-021 (4 cases)**	**Experiment LEU-SOL-THERM-022 (4 cases)**	**Experiment LEU-SOL-THERM-023 (9 cases)**
Fissionable Material	**Physical Form**	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate
	Isotopic Composition	9.97 wt% ^{235}U	9.97 wt%^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 4.95e-05 to 6.21e-05 ^{238}U: 4.41e-04 to 5.53e-04	^{235}U: 4.95e-5 to 6.21e-05 ^{238}U: 4.41e-04 to 5.53e-04	^{235}U: 7.88e-05 to 7.93e-05 ^{238}U:7.03e-04 to 7.07e-04	^{235}U: 7.42e-5 to 7.56e-05 ^{238}U:6.61e-04 to 6.73e-04
	Temperature	298 K	298 K	298 K	298 K
Materials/ Moderator	**Element**	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	6.03e-02 to 6.13e-02	6.03e-02 to 6.13e-02	5.90e-02 to 5.91e-02	5.93e-02 to 5.95e-02
	Ratio to fissile material	971 to 1239	971 to 1239	744 to 750	785 to 803
	Temperature	298 K	298 K	298 K	298 K
Materials/ Reflector	**Material/Physical form**	Reflected by water	Unreflected	Reflected by borated concrete	Unreflected
Materials/ Neutron Absorber	**Element**	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution in a cylindrical tank	Homogeneous solution in a cylindrical tank	Homogeneous solution in a rectangular slab tank	Homogeneous solution in a rectangular slab tank
	Shape	Cylinder	Cylinder	Rectangular slab	Rectangular slab
Neutron Energy	**AENCF**	0.0125 to 0.0150 MeV	0.0127 to 0.0154 MeV	0.0184 to 0.0186 MeV	0.0175 to 0.0179 MeV
	EALF	3.57e-02 to 3.81e-02	3.58e-02 to 3.83e-02	4.21e-02 to 4.22e-02	Not available
	Neutron Energy Spectra[a]	T: 42.2 to 46.6 % I: 23.8 to 25.6 % F: 29.6 to 32.2 %	T: 41.8 to 46.3 % I: 23.9 to 25.7 % F: 29.8 to 32.5 %	T:36.8 to 36.9 % I: 28.1% F:35.0 to 35.1 %	Not available
	Fission Rate vs Neutron Energy[a]	T: 96.8 to 97.3 % I: 2.2 to 2.6 % F: 0.5 to 0.6 %	T: 96.8 to 97.3 % I: 2.2 to 2.6 % F: 0.5 to 0.6 %	T: 96.0 to 96.1% I: 3.3% F: 0.7%	Not available

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

5.2.3 Calculation of the Lower Bound Tolerance Limit

In the following paragraphs some of the information presented in Section 2 is repeated focusing on the steps that are actually applicable for the current group of benchmarks. The first step in calculating the lower bound tolerance limit is to apply regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p.8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value

(k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}. Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (in this case, average energy of a neutron causing fission [AENCF],), using the build-in regression analysis tool from Excel software. The AENCF is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p.3-47).

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the *y* values about their mean that can be attributed to a linear relation between *y* and *x*.
Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (*b*). The slope test requires calculating the test statistic "*T*" as described in Equations 2, 3 and 4 from Section 2.

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and *n-2* degrees of freedom, where *n* is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied. The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals. The results of the trending parameter analysis for the criticality benchmark subset representative for external configurations containing IEU fissile material are detailed in (Attachment II) and summarized in Table 13.

Table 13. Trending Parameter Results for the Criticality Benchmark Experiments Representative for Configurations Containing IEU External to the Waste Package

Trend Parameter	n	Intercept	Slope	r^2	T	$t_{0.025,107}$	P-value	Goodness-of-fit Tests	Valid Trend
AENCF	109	1.0030	-0.0194	0.1708	-4.6939	1.984[a]	7.98e-06	Passed	Yes

Source: Attachment II.
Note: [a] Value interpolated from Table A-4 of Reference 9.

The trending parameters for AENCF (r^2, T, P-value) from Table 12 indicate a trend of k_{eff} with AENCF (Attachment II). The lower bound tolerance limit is calculated for this situation using the CLReg code (Reference 11). Figure 2 presents the k_{eff} values and the lower bound tolerance limit calculated with CLREG code. The following expression (Attachment II) describes the calculated lower bound tolerance limit:

f(AENCF) = 0.97841 for 0 MeV < AENCF < 0.1518 MeV

f(AENCF) = -1.9322e-02*AENCF +0.981339 for 0.1518 MeV ≤ AENCF < 0.482 MeV

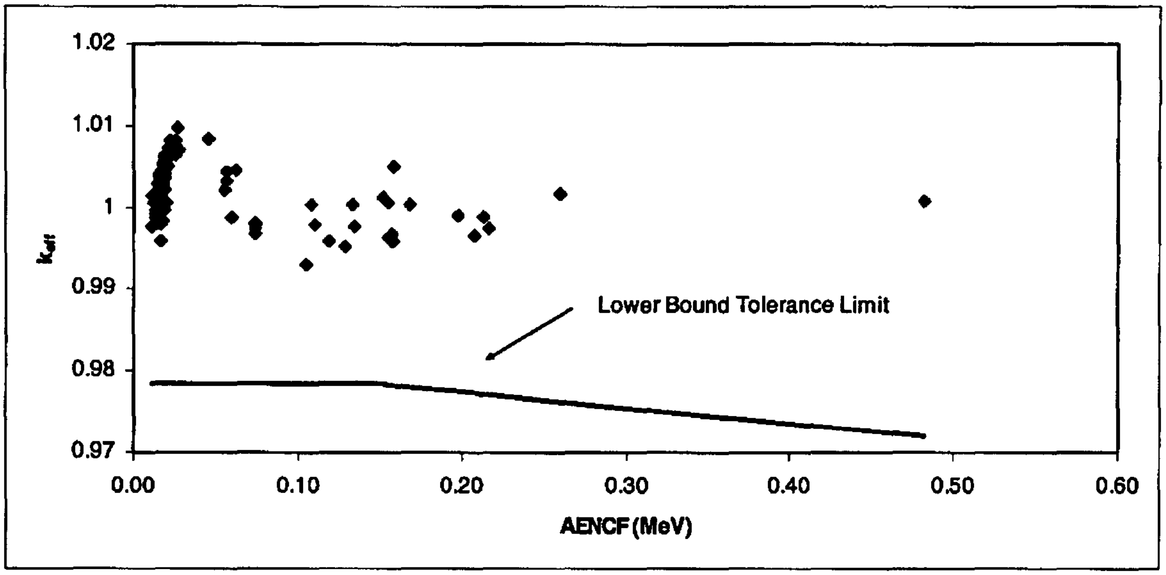

Figure 2. Lower Bound Tolerance Limit Applicable for Configurations Containing IEU Mixtures External to the Waste Package

5.3 CALCULATIONS FOR BENCHMARK CRITICAL EXPERIMENTS SELECTED FOR EXTERNAL CONFIGURATIONS CONTAINING LOW ENRICHED URANIUM (LEU)

As mentioned in Section 2, an essential element of validating the methods and models used for calculating effective neutron multiplication factor, k_{eff}, for a waste package is determination of critical limit. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

In the following, the first three steps of the process of establishing a critical limit for the external configurations containing LEU mixtures are detailed.

5.3.1 Selection of the Criticality Benchmark Experiments

The criticality experiments selected for inclusion in the validation of the criticality model must be representative of the types of materials, conditions, and parameters to be modeled using the calculational method (criticality model). A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a model, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results (Reference 6, p. 5).

For the present application (configurations with highly enriched uranium external to the waste package), the criticality benchmark experiments have been selected based on their fissile content, moderator and geometry. The benchmark experiments are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (*External Criticality Calculation for DOE SNF Codisposal Waste Packages* [Reference 2]). The set of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the configurations and also to provide adequate statistics for the lower bound tolerance limit calculations.

The selected benchmark experiments containing a total of 96 individual cases are presented in Table 14 together with the results of the MCNP 4B2 code calculations. All cases have been run using the isotopic libraries described in Reference 10 (Table 2).

Table 14. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures with Low Enriched Uranium

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
Experiment LEU-COMP-THERM-033 (52 cases)	case1	1.0000	0.0038	0.9945	0.0007	0.1791
	case2	1.0000	0.0038	0.9959	0.0006	0.1792
	case3	1.0000	0.0038	0.9965	0.0007	0.1789
	case4	1.0000	0.0038	0.9957	0.0006	0.1793
	case5	1.0000	0.0039	0.9993	0.0006	0.1379
	case6	1.0000	0.0039	1.0002	0.0007	0.1376
	case7	1.0000	0.0039	0.9983	0.0006	0.1371
	case8	1.0000	0.0040	0.9971	0.0006	0.1114
	case9	1.0000	0.0040	0.9957	0.0006	0.1119
	case10	1.0000	0.0039	0.9970	0.0007	0.0973
	case11	1.0000	0.0039	0.9963	0.0006	0.0972
	case12	1.0000	0.0039	0.9963	0.0006	0.0973
	case13	1.0000	0.0041	0.9973	0.0006	0.0840
	case14	1.0000	0.0051	0.9905	0.0005	0.0619
	case15	1.0000	0.0051	0.9915	0.0005	0.0623

Table 14. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures with Low Enriched Uranium

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	case16	1.0000	0.0051	0.9917	0.0005	0.0617
	case17	1.0000	0.0038	1.0048	0.0007	0.1657
	case18	1.0000	0.0038	1.0052	0.0007	0.1665
	case19	1.0000	0.0038	1.0058	0.0007	0.1657
	case20	1.0000	0.0038	1.0041	0.0007	0.1657
	case21	1.0000	0.0038	1.0061	0.0007	0.1650
	case22	1.0000	0.0039	1.0078	0.0007	0.1015
	case23	1.0000	0.0040	0.9946	0.0007	0.1952
	case24	1.0000	0.0040	0.9949	0.0007	0.1945
	case25	1.0000	0.0040	0.9950	0.0007	0.1953
	case26	1.0000	0.0039	0.9985	0.0007	0.1503
	case27	1.0000	0.0039	0.9992	0.0007	0.1503
	case28	1.0000	0.0039	0.9973	0.0007	0.1502
	case29	1.0000	0.0039	0.9993	0.0007	0.1503
	case30	1.0000	0.0039	0.9970	0.0007	0.1204
	case31	1.0000	0.0039	0.9981	0.0007	0.1199
	case32	1.0000	0.0039	0.9973	0.0006	0.1208
	case33	1.0000	0.0039	0.9955	0.0007	0.1209
	case34	1.0000	0.0039	0.9960	0.0007	0.1205
	case35	1.0000	0.0040	0.9965	0.0006	0.1047
	case36	1.0000	0.0040	0.9963	0.0006	0.1049
	case37	1.0000	0.0040	0.9950	0.0007	0.1047
	case38	1.0000	0.0040	0.9964	0.0006	0.1044
	case39	1.0000	0.0040	0.9964	0.0006	0.1047
	case40	1.0000	0.0040	0.9954	0.0006	0.1049
	case41	1.0000	0.0041	0.9965	0.0006	0.0901
	case42	1.0000	0.0041	0.9955	0.0006	0.0896
	case43	1.0000	0.0041	0.9946	0.0006	0.0890
	case44	1.0000	0.0050	0.9913	0.0005	0.0645
	case45	1.0000	0.0050	0.9908	0.0005	0.0637
	case46	1.0000	0.0050	0.9893	0.0005	0.0645
	case47	1.0000	0.0042	1.0110	0.0007	0.1880
	case48	1.0000	0.0042	1.0065	0.0007	0.1878
	case49	1.0000	0.0042	1.0063	0.0008	0.1889
	case50	1.0000	0.0041	1.0095	0.0007	0.1140
	case51	1.0000	0.0041	1.0127	0.0007	0.1146
	case52	1.0000	0.0041	1.0076	0.0007	0.1148
Experiment LEU-COMP-THERM-049 (18 cases)	lct49-01	1.0000	0.0034	0.9923	0.0006	0.294
	lct49-02	1.0000	0.0034	0.9937	0.0006	0.293
	lct49-03	1.0000	0.0034	0.9929	0.0006	0.297
	lct49-04	1.0000	0.0034	0.9931	0.0006	0.300
	lct49-05	1.0000	0.0042	0.9944	0.0007	0.255
	lct49-06	1.0000	0.0042	0.9946	0.0007	0.256
	lct49-07	1.0000	0.0042	0.9932	0.0007	0.253

Table 14. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures with Low Enriched Uranium

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	lct49-08	1.0000	0.0042	0.9921	0.0007	0.258
	lct49-09	1.0000	0.0037	0.9933	0.0006	0.227
	lct49-10	1.0000	0.0037	0.9946	0.0007	0.227
	lct49-11	1.0000	0.0037	0.9933	0.0006	0.227
	lct49-12	1.0000	0.0037	0.9924	0.0007	0.231
	lct49-13	1.0000	0.0036	0.9935	0.0006	0.271
	lct49-14	1.0000	0.0036	0.9941	0.0006	0.272
	lct49-15	1.0000	0.0036	0.9937	0.0006	0.271
	lct49-16	1.0000	0.0036	0.9938	0.0007	0.254
	lct49-17	1.0000	0.0036	0.9929	0.0007	0.258
	lct49-18	1.0000	0.003	0.997	0.0006	0.251
Experiment LEU-SOL-THERM-001 (1 case)	leust1	0.9991	0.0029	1.01182	0.00101	0.05186
Experiment LEU-SOL-THERM-002 (3 cases)	leust21	1.0038	0.004	0.99855	0.00058	0.02513
	leust22	1.0024	0.0037	0.99659	0.00064	0.0283
	leust23	1.0024	0.0044	1.0009	0.0006	0.02684
Experiment LEU-SOL-THERM-003 (9 cases)	lst3-1	0.9997	0.0039	0.9993	0.0004	0.0186
	lst3-2	0.9993	0.0042	0.9971	0.00038	0.0166
	lst3-3	0.9995	0.0042	1.0015	0.00037	0.0164
	lst3-4	0.9995	0.0042	0.9954	0.00038	0.0162
	lst3-5	0.9997	0.0048	0.9990	0.00031	0.0133
	lst3-6	0.9999	0.0049	0.9992	0.0003	0.0129
	lst3-7	0.9994	0.0049	0.9972	0.0003	0.0127
	lst3-8	0.9993	0.0052	1.0008	0.00025	0.0114
	lst3-9	0.9996	0.0052	0.9973	0.00025	0.0114
Experiment LEU-SOL-THERM-008 (4 cases)	lst8_72	0.9999	0.0014	1.0038	0.0002	0.0152
	lst8_74	1.0002	0.0015	1.0023	0.0002	0.0154
	lst8_76	0.9999	0.0014	1.0028	0.0002	0.0153
	lst8_78	0.9999	0.0014	1.0040	0.0002	0.0153
Experiment LEU-SOL-THERM-009 (3 cases	lst9_92	0.9998	0.0014	1.0018	0.0005	0.0155
	lst9_93	0.9999	0.0014	1.0021	0.0002	0.0157
	lst9_94	0.9999	0.0014	1.0022	0.0002	0.0158
Experiment LEU-SOL-THERM-018 (6 cases)	RUN133	0.9992	0.001	1.0033	0.0002	0.0183
	RUN142	0.9996	0.001	1.0042	0.0003	0.0187
	RUN143	0.9996	0.001	1.0045	0.0003	0.0188
	RUN144	0.9997	0.001	1.0033	0.0003	0.0187
	RUN145	0.9992	0.001	1.0038	0.0003	0.0187
	RUN146	0.9996	0.001	1.0037	0.0003	0.0186

Source: Critical benchmark experiments are evaluated in Reference 5 and MCNP calculations are summarized in Reference 10 except cases from experiments LEU-COMP-THERM-033, which have been run for the current calculation (output files are listed in Section 7 and uploaded on the COLD server)

The experiments listed in Table 14 are considered appropriate to represent degraded configurations containing mixtures with low enriched uranium external to the waste package.

5.3.2 Range of Applicability of Selected Criticality Benchmark Experiments

This subsection summarizes in a set of tables (Tables15 and 16) the range of applicability of the experiments listed in Table 14. The information is partly excerpted from Reference 10. The tables have been enhanced by adding information regarding the spectral characteristics of the experiments (available for the majority of the benchmarks from Reference 5). The purpose is to enable the construction of a collective area of applicability that can be used to directly compare the range of applicability of this set of benchmark experiments with the range of parameters of the postulated external configurations.

Table 15. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures with Low Enriched Uranium (set 1)

Category/ Description	Parameter	Experiment LEU-COMP-THERM-033 (52 cases)	Experiment LEU-COMP-THERM-049 (18 cases)	Experiment LEU-SOL-THERM-001 (1 case)	Experiment LEU-SOL-THERM-002 (3 cases)	Experiment LEU-SOL-THERM-003 (9 cases)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Uranium fluoride	UO_2	Aqueous solution of uranyl fluoride	Aqueous solution of uranium oxy-fluoride	Aqueous solution of uranyl nitrate
	Isotopic Composition	2 to 3 wt% ^{235}U	2.35 wt% ^{235}U	5 wt% ^{235}U	4.9 wt% ^{235}U	10 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 6.23e-05 to 2.35e-04	^{235}U: 3.69e-4 ^{238}U: 6.94e-03	^{235}U: 1.24e-4 ^{238}U: 2.35e-3	^{235}U: 5.67e-05 – 6.16e-05 ^{238}U:1.09e-03 – 1.18e-03	^{235}U: 4.34e-05 – 7.64e-05 ^{238}U:3.82e-04 – 6.73e-04
	Temperature	Room Temp.	295 K	298 K	298 K	300 K
Materials/ Moderator	Element	H, C	H	H	H	H
	Physical form	Paraffin	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	H: 3.09e-02 to 6.06e-02 C: 1.49e-02 to 2.91e-02	1.47e-02 – 2.20e-02	5.62e-02	6.17e-02 to 6.22e-02	5.89e-02 to 6.23e-02
	Ratio to fissile material	$H/^{235}U$ = 133.4 to 973	2-3	454	1001- 10098	770 - 1437
	Temperature	300 K	295 K	293 K	298 K	300 K
Materials/ Reflector	Material/Physical form	Reflected by paraffin, polyethylene or Plexiglas	Reflected by polyethylene	Unreflected	Unreflected or reflected by water	Unreflected
Materials/ Neutron Absorber	Element	None	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A	N/A
Geometry	Heterogeneity	Rectangular stacks of UF_2 or UF_4 – paraffin cubes	Array of boxes in rectangular geometry	Homogeneous solution in a cylindrical vessel	Homogeneous solution in a spherical vessel	Homogeneous solution in a spherical tank
	Shape	Parallelepiped	Parallelepiped	Cylinder	Sphere	Sphere
Neutron Energy	AENCF	0.0617 to 0.1953 MeV	0.2270-0.3000 MeV	0.0519 MeV	0.0251 – 0.0283 MeV	0.0114 – 0.0186 MeV
	EALF	0.0541 to 0.393 eV	0.899 to 27.8 eV	0.0629 eV	0.0395 to 0.0416 eV	3.46e-02 – 4.14e-02 eV
	Neutron Energy Spectra[a]	T: 13.4 to 42.4 % I: 26.2 to 41.3 % F: 31.5 to 45.3 %	T: 7.1 to 15.0 % I: 38.6 to 41.0 % F: 46.2 to 51.9 %	T: 28.6% I: 31.2% F: 40.2%	T: 43.9 to 45.5% I: 24.1 to 25.3% F: 30.4 to 32.1%	T: 37.6 – 49.1 % I: 22.7-27.3% F: 28.2-35.1%

Category/ Description	Parameter	Experiment LEU-COMP-THERM-033 (52 cases)	Experiment LEU-COMP-THERM-049 (18 cases)	Experiment LEU-SOL-THERM-001 (1 case)	Experiment LEU-SOL-THERM-002 (3 cases)	Experiment LEU-SOL-THERM-003 (9 cases)
	Fission Rate vs. Neutron Energy[a]	T: 80.6 to 95.4 % I: 2.6 to 12.9 % F: 2.0 to 6.6 %	T: 63.2 to 72.9 % I: 19.0 to 25.6 % F: 8.1 to 10.9 %	T: 93.6% I: 4.6% F: 1.8%	T: 96.6 to 96.9% I: 2.3 to 2.5% F: 0.8 to 1.1%	T: 96.2-97.6% I: 2-3.1% F: 0.4-0.7%

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 16. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures with Low Enriched Uranium (set 2)

Category/ Description	Parameter	Experiment LEU-SOL-THERM-008 (4 cases)	Experiment LEU-SOL-THERM-009 (3 cases)	Experiment LEU-SOL-THERM-018 (6 cases)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium
	Physical Form	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate	Aqueous solution of uranyl nitrate
	Isotopic Composition	9.97 wt% ^{235}U	9.97 wt% ^{235}U	9.97 wt% ^{235}U
	Atomic density (atoms/b-cm)	^{235}U: 6.14e-05 ^{238}U: 5.47e-04	^{235}U: 6.26e-05 ^{238}U: 5.57e-04	^{235}U: 7.87e-5 – 8.04e-05 ^{238}U: 7.01e-04 – 7.16e-04
	Temperature	298 K	298 K	298 K
Materials/ Moderator	Element	H	H	H
	Physical form	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	5.86e-02	5.85e-02	5.87e-02 – 5.91e-02
	Ratio to fissile material	951 - 956	934 - 936	731 – 751
	Temperature	298 K	298 K	298 K
Materials/ Reflector	Material/Physical form	Reflected by concrete	Reflected by borated concrete	Reflected by concrete
Materials/ Neutron Absorber	Element	None	None	None
	Physical form	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A
Geometry	Heterogeneity	Homogeneous solution contained in a cylindrical tank	Homogeneous solution contained in a cylindrical tank	Homogeneous solution in a rectangular slab tank
	Shape	Cylinder	Cylinder	Rectangular slab
Neutron Energy	AENCF	0.0152-0.0154 MeV	0.0155 – 0.0158 MeV	0.0183 - 0.0188 MeV
	EALF	3.84e-02 eV	3.89e-02 eV	0.042-0.0425 eV
	Neutron Energy Spectra[a]	T: 41.5-41.7% I: 25.9 - 26% F: 32.4 - 35%	T: 40.8 – 41 % I: 26.2-26.3% F: 32.8-32.9%	T: 36.5 – 37.0 % I: 28.0-28.3 % F: 34.9-35.2 %
	Fission Rate vs Neutron Energy[a]	T: 96.8% I: 2.6% F: 0.6%	T: 96.7% I: 2.7% F: 0.6%	T: 96.0% I: 3.3% F: 0.7

Source: Reference 5 and 10.

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

5.3.3 Calculation of the Lower Bound Tolerance Limit

In the following paragraphs some of the information presented in Section 2 is repeated focusing on the steps that are actually applicable for the current group of benchmarks. The first step in calculating the lower bound tolerance limit is to apply regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p. 8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}. Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (e.g., average energy of a neutron causing fission [AENCF]) using the build-in regression analysis tool from Excel software. The AENCF is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p.3-47). If trending is identified for one set, the LUTB method is used to calculate the lower bound tolerance limit (YMP 2003, p. 3-47).

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic (Reference 7, p. 390) can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the *y* values about their mean that can be attributed to a linear relation between *y* and *x*. Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (*b*). The slope test requires calculating the test statistic "*T*" as described by Equations 2, 3 and 4 from Section 2.

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and *n*-2 degrees of freedom (Reference 7, p. 659), where *n* is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied. The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals.

The results of the trending parameter analysis for the criticality benchmark subset representative for external configurations containing LEU mixtures are presented in Attachment III and summarized in Table 17. Some of the trending parameters for AENCF (r^2, T) from Table 17, indicate a slight trend of k_{eff} with increasing AENCF, but the analysis of the residuals do not finally confirm a valid trend of k_{eff} with AENCF (residuals are not normally distributed).

Table 17. Trending Parameter Results for the Criticality Benchmark Subset Representative for Configurations Containing LEU External to the Waste Package

Trend Parameter	n	Intercept	Slope	r^2	T	$t_{0.025,n-2}$	P-value	Goodness-of-fit Tests	Valid Trend
AENCF	96	1.0009	-0.0206	0.1175	-3.54	1.988[a]	0.0006	Failed	No

Source: Attachment III
Note: [a] Value interpolated from Table A-4 of Reference 9.

Because this set shows no valid trending, according to the methodology summarized in Figure 3-6 of Reference 1, the k_{eff} set is tested for normality using an omnibus normality test (Anderson-Darling). It tests the goodness-of-fit to a normal distribution constructed with the sample average and standard deviation of the k_{eff} set of values. The required steps to apply the test and specific test statistics are presented in Attachment III. The Anderson-Darling normality test performed for this set showed that the calculated k_{eff} values are not normally distributed.

If the set of k_{eff} values does not have a normal statistical distribution, a non-parametric statistical treatment must be used as described in Reference 1 (p. 3-51) as the distribution-free tolerance limit (DFTL). A more specific description of the method is presented in Reference 6 (p. 14), resulting in the determination of the degree of confidence that a fraction of the true population of data lies above the smallest value observed. The more data are available in the sample, the higher the degree of confidence. Non-parametric techniques do not require reliance upon distributions, but are rather an analysis of ranks. Therefore, the k_{eff} values in a sample are ranked from the smallest to the largest.

For a desired population fraction of 95% and a rank order of 1 (the smallest k_{eff} value in data sample), the confidence level calculated with Equation 5 from Section 2 for n = 96 points is 99.3%. For non-parametric data analysis, Reference 1 (p. 14) suggests that lower bound tolerance limit be determined by:

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM)

where: *Non-parametric margin (NPM)* is added to account for small sample size.

For the present value of the confidence level (99.3%), Table 2 (Section 2) indicates that the non parametric margin is 0.

The calculated lower bound tolerance limit value using DFTL method for the current set is f(x) = 0.9842 (Attachment III). Figure 3 presents the k_{eff} values and the calculated lower bound tolerance limit for this set of benchmark experiments.

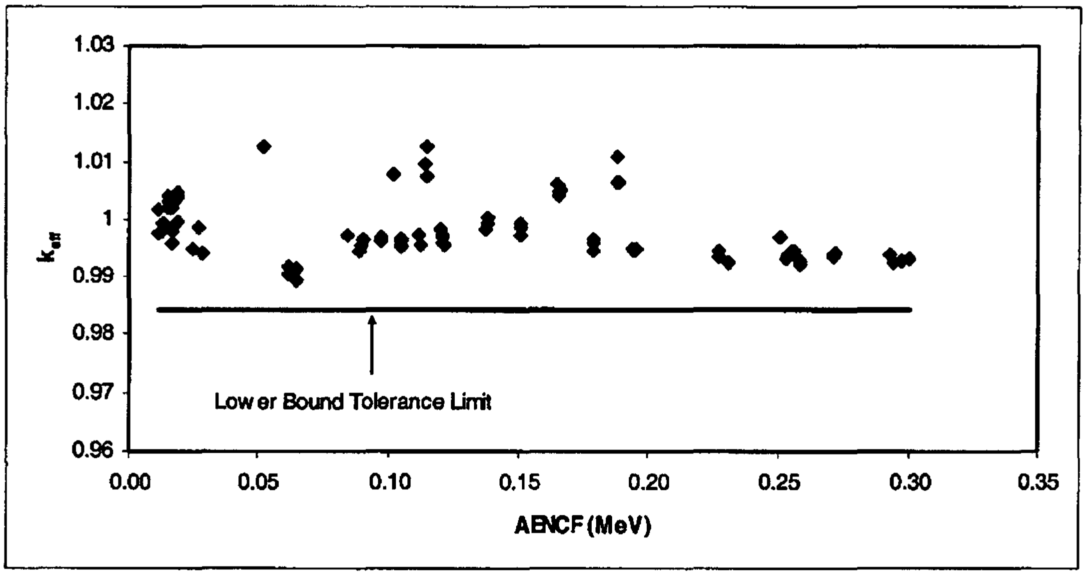

Figure 3. Lower Bound Tolerance Limit Applicable for Configurations Containing LEU External to the Waste Package

5.4 CALCULATIONS FOR BENCHMARK CRITICAL EXPERIMENTS SELECTED FOR EXTERNAL CONFIGURATIONS CONTAINING MIXTURES OF URANIUM AND PLUTONIUM FISSILE ISOTOPES

As mentioned in Section 2, an essential element of validating the methods and models used for calculating effective neutron multiplication factor, k_{eff}, for a waste package is determination of critical limit. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

In the following, the first three steps of the process of establishing a critical limit for the external configurations containing U+Pu mixtures are detailed.

5.4.1 Selection of the Criticality Benchmark Experiments

The criticality experiments selected for inclusion in the validation of the criticality model must be representative of the types of materials, conditions, and parameters to be modeled using the calculational method (criticality model). A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a model, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results (Reference 6, p. 5).

For the present application (configurations with mixtures of uranium and plutonium external to the waste package), the criticality benchmark experiments have been selected based on their fissile content, moderator content and geometry. The benchmark experiments are from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (*External Criticality Calculation for DOE SNF Codisposal Waste Packages* [Reference 2]). The set of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the configurations and also to provide adequate statistics for the lower bound tolerance limit calculations.

The selected benchmark experiments containing a total of 120 individual cases are presented in Table 18 together with the results of the MCNP 4B2 code calculations. All cases have been run using the isotopic libraries described in Reference 10 (Table 2).

Table 18. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures of Uranium and Plutonium Isotopes

Experiment	**Case Name**	**Benchmark Values**		**Calculated Values (MCNP)**		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	**AENCF**
Experiment MIX-SOL-THERM-001 (12 cases)	pnl3187	1.0000	0.0016	0.9976	0.0012	0.0417
	pnl3391	1.0000	0.0016	0.9943	0.0012	0.0411
	pnl3492	1.0000	0.0016	0.9975	0.0012	0.0431
	pnl3593	1.0000	0.0016	0.9973	0.0011	0.0459
	pnl3694	1.0000	0.0016	1.0026	0.0012	0.0445
	pnl3795	1.0000	0.0016	1.0017	0.0012	0.0400
	pnl3896	1.0000	0.0016	1.0024	0.0012	0.0232
	pnl3897	1.0000	0.0016	1.0045	0.0011	0.0142
	pnl3898	1.0000	0.0016	1.0029	0.0010	0.0299
	pnl3808	1.0000	0.0016	1.0020	0.0011	0.0213
	pnl3999	1.0000	0.0052	1.0092	0.0011	0.0296
	pnl5300	1.0000	0.0052	1.0080	0.0011	0.0288
Experiment MIX-SOL-THERM-002 (3 cases)	pnl1158	1.0000	0.0024	1.0069	0.0007	0.0038
	pnl1159	1.0000	0.0024	1.0074	0.0006	0.0037
	pnl1161	1.0000	0.0024	1.0079	0.0007	0.0061
Experiment MIX-SOL-THERM-003 (10 cases)	awre1	0.9985	0.0020	1.0147	0.0010	0.0315
	awre2	0.9960	0.0020	1.0157	0.0012	0.0315
	awre3	0.9935	0.0020	1.012	0.0012	0.0320
	awre4	0.9909	0.0020	1.0051	0.0012	0.0319
	awre5	0.9981	0.0022	1.0085	0.0010	0.0104
	awre6	0.9959	0.0022	1.0107	0.0010	0.0104
	awre7	0.9935	0.0022	1.0080	0.0010	0.0105
	awre8	0.9988	0.0025	1.0128	0.0008	0.0069
	awre9	0.9958	0.0025	1.0094	0.0009	0.0066
	awre10	0.9964	0.0025	1.0102	0.0008	0.0066
Experiment MIX-SOL-THERM-004 (9 cases)	pnl1577	1.0000	0.0033	0.9958	0.0012	0.0589
	pnl1678	1.0000	0.0033	0.9974	0.0012	0.0504
	pnl1783	1.0000	0.0078	0.9992	0.0012	0.0534
	pnl1868	1.0000	0.0078	1.0039	0.0013	0.0343
	pnl1969	1.0000	0.0033	1.0000	0.0012	0.0334
	pnl2070	1.0000	0.0033	0.9996	0.0014	0.0377
	pnl2565	1.0000	0.0033	1.0015	0.0012	0.0129
	pnl2666	1.0000	0.0033	1.0018	0.0011	0.0117
	pnl2767	1.0000	0.0078	1.0061	0.0011	0.0123
Experiment MIX-SOL-THERM-005 (7 cases)	msl5-63	1.0000	0.0037	0.9877	0.0008	0.013
	msl5-64	1.0000	0.0037	1.0045	0.0007	0.012
	msl5-71	1.0000	0.0037	1.0032	0.0008	0.033
	msl5-72	1.0000	0.0037	1.0001	0.0008	0.032
	msl5-74	1.0000	0.0037	0.9922	0.0009	0.037
	msl5-75	1.0000	0.0037	0.9898	0.0009	0.059
	msl5-76	1.0000	0.0037	0.9974	0.0007	0.049
Experiment MIX-SOL-THERM-006 (6 cases)	C1	1.0000	0.0011	0.9992	0.0006	0.0352
	C2	1.0000	0.0010	1.0018	0.0006	0.0375
	C3	1.0000	0.0012	1.0025	0.0005	0.0380

Table 18. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures of Uranium and Plutonium Isotopes

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	C4	1.0000	0.0016	1.0041	0.0005	0.0396
	C5	1.0000	0.0011	1.0039	0.0005	0.0405
	C6	1.0000	0.0014	1.0021	0.0005	0.0404
Experiment MIX-COMP-THERM-012 (33 cases)	c1_mc50	1.0042	0.0058	0.9764	0.0007	0.0709
	c2_mc50	1.0042	0.0058	0.9770	0.0007	0.0712
	c3_mc50	1.0042	0.0058	0.9743	0.0007	0.0708
	c4_mc50	1.0042	0.0058	0.9804	0.0007	0.0709
	c5_mc50	1.0042	0.0058	0.9756	0.0007	0.0710
	c6_mc50	1.0042	0.0058	0.9805	0.0007	0.0714
	c7_mc50	1.0023	0.0036	1.0353	0.0006	0.0268
	c8_mc50	1.0023	0.0036	1.0309	0.0006	0.0264
	c9_mc50	1.0023	0.0036	1.0281	0.0006	0.0267
	c10_mc50	1.0023	0.0036	1.0277	0.0006	0.0268
	c11_mc50	1.0023	0.0036	1.0264	0.0006	0.0265
	c12_mc50	1.0023	0.0036	1.0287	0.0007	0.0266
	c13_mc50	1.0023	0.0036	1.0372	0.0007	0.0266
	c14_mc50	1.0002	0.0027	1.0231	0.0007	0.0464
	c15_mc50	1.0002	0.0027	1.0234	0.0008	0.0464
	c16_mc50	1.0002	0.0027	1.0194	0.0007	0.0463
	c17_mc50	1.0002	0.0027	1.0188	0.0007	0.0457
	c18_mc50	1.0002	0.0027	1.0172	0.0007	0.0459
	c19_mc50	1.0002	0.0027	1.0167	0.0007	0.0456
	c20_mc50	1.0004	0.0037	1.0173	0.0008	0.0571
	c21_mc50	1.0004	0.0037	1.0160	0.0008	0.0581
	c22_mc50	1.0004	0.0037	1.0129	0.0008	0.0571
	c23_mc50	0.9997	0.0049	1.0108	0.0007	0.0388
	c24_mc50	0.9997	0.0049	1.0122	0.0008	0.0386
	c25_mc50	0.9997	0.0049	1.0112	0.0007	0.0384
	c26_mc50	0.9997	0.0049	1.0092	0.0007	0.0382
	c27_mc50	0.9997	0.0049	1.0089	0.0007	0.0380
	c28_mc50	0.9997	0.0049	1.0104	0.0007	0.0381
	c29_mc50	0.9997	0.0049	1.0113	0.0007	0.0376
	c30_mc50	0.9997	0.0049	1.0090	0.0007	0.0379
	c31_mc50	1.0007	0.0052	0.9963	0.0009	0.0493
	c32_mc50	1.0007	0.0052	0.9970	0.0008	0.0490
	c33_mc50	1.0007	0.0052	0.9935	0.0008	0.0498
Experiment PU-MET-MIXED-001 (6 cases)	81-1-B5	1.0002	0.0037	1.0003	0.0017	0.4567
	81-1AB5	1.0002	0.0032	0.9991	0.0019	0.4505
	81-2-B5	1.0005	0.0025	1.0040	0.0019	0.3800
	81-3-b5	1.0000	0.0025	1.0094	0.0019	0.3405
	81-4-b5	1.0001	0.0025	1.0165	0.0017	0.2178
	81-5-b5	1.0003	0.0025	1.0163	0.0017	0.2145
Experiment PU-COMP-MIXED-001 (5 cases)	case1	0.9986	0.0041	1.0286	0.0009	1.7019
	case2	1.0000	0.0068	1.0188	0.0013	0.6331

Table 18. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing Mixtures of Uranium and Plutonium Isotopes

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	case3	0.9990	0.0067	1.0150	0.0013	0.2753
	case4	1.0000	0.0066	0.9853	0.0014	0.2878
	case5	0.9989	0.0072	1.0084	0.0013	0.0999
Experiment PU-COMP-MIXED-002 (29 cases)	case1	0.9990	0.0046	1.0318	0.0009	1.0458
	case2	0.9990	0.0046	1.0309	0.0009	1.0303
	case3	0.9990	0.0046	1.0253	0.0008	1.0089
	case4	0.9990	0.0046	1.0199	0.0009	0.9807
	case5	0.9990	0.0046	1.0139	0.0008	0.9433
	case6	1.0000	0.0075	1.0168	0.0009	0.4377
	case7	1.0000	0.0075	1.0183	0.0008	0.4334
	case8	1.0000	0.0075	1.0177	0.0008	0.4234
	case9	1.0000	0.0075	1.0189	0.0009	0.4137
	case10	1.0000	0.0073	1.0282	0.0009	0.1836
	case11	1.0000	0.0073	1.0248	0.0009	0.1872
	case12	1.0000	0.0073	1.0250	0.0008	0.1919
	case13	1.0000	0.0073	1.0220	0.0010	0.1932
	case14	1.0000	0.0073	1.0268	0.0009	0.1933
	case15	1.0000	0.0073	1.0224	0.0009	0.1938
	case16	1.0000	0.0073	1.0188	0.0009	0.1917
	case17	0.9988	0.0055	1.0062	0.0009	0.1963
	case18	0.9988	0.0055	1.0071	0.0008	0.2040
	case19	0.9988	0.0055	1.0068	0.0009	0.2040
	case20	0.9988	0.0055	1.0078	0.0009	0.2060
	case21	0.9988	0.0055	1.0075	0.0009	0.2063
	case22	0.9988	0.0055	1.0118	0.0009	0.2038
	case23	1.0000	0.0068	1.0058	0.0009	0.0770
	case24	1.0000	0.0068	1.0090	0.0009	0.0770
	case25	1.0000	0.0068	1.0081	0.0009	0.0777
	case26	1.0000	0.0068	1.0103	0.0010	0.0774
	case27	1.0000	0.0068	1.0090	0.0009	0.0776
	case28	1.0000	0.0068	1.0095	0.0009	0.0777
	case29	1.0000	0.0068	1.0104	0.0009	0.0785

Source: Critical benchmark experiments are evaluated in Reference 5 and MCNP calculations are presented in Reference 10 except cases from experiments MIX-SOL-THERM-006, MIX-COMP-THERM-012, PU-MET-MIXED-001, PU-COMP-MIXED-001, PU-COMP-MIXED-002 that have been run for the current calculation (output files are listed in Section 7 and uploaded on the COLD server).

The experiments listed in Table 18 are considered appropriate to represent degraded configurations containing mixtures with plutonium and uranium external to the waste package.

5.4.2 Range of Applicability of Selected Criticality Benchmark Experiments

This subsection summarizes in a set of tables (Tables 19 to 21) the range of applicability of the experiments listed in Table 18. The information is partly excerpted from Reference 10. The tables have been enhanced by adding information regarding the spectral characteristics of the experiments (available for the majority of the benchmarks from Reference 5). The purpose is to enable the construction of a collective area of applicability that can be used to directly compare the range of applicability of this set of benchmark experiments with the range of parameters of the postulated external configurations.

Table 19. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures with Plutonium and Uranium (set 1)

Category/ Description	**Parameter**	**Experiment MIX-SOL-THERM-001 (12 cases)**	**Experiment MIX-SOL-THERM-002 (3 cases)**	**Experiment MIX-SOL-THERM-003 (10 cases)**	**Experiment MIX-SOL-THERM-004 (9 cases)**	**Experiment MIX-SOL-THERM-005 (7 cases)**
Materials/ Fissionable Material	**Fissionable Element**	Plutonium + Uranium	Plutonium + Uranium	Plutonium + Uranium	Plutonium + Uranium	Plutonium + Uranium
	Physical Form	Pu-U nitrate solution	Pu-U nitrate solution	Pu-U nitrate solution	Pu-U nitrate solution	Pu-U nitrate solution
	Isotopic Composition	91.1 to 91.57 wt% ^{239}Pu in Pu 0.44 to 0.71 wt % ^{235}U in U	91.1 wt% ^{239}Pu in Pu 0.7 to 2.29 wt % ^{235}U in U	94 wt% ^{239}Pu in Pu 0.72 wt % ^{235}U in U	91.1 wt% ^{239}Pu in Pu 0.56 wt % ^{235}U in U	91.1 wt% ^{239}Pu in Pu 0.56 wt % ^{235}U in U
	Atomic density (atoms/b-cm)	^{239}Pu: 1.08e-04 to 4.51e-04 ^{235}U: 1.35e-06 to 6.86e-06	^{239}Pu: 2.69e-05 to 2.80e-04 ^{235}U: 1.94e-06 to 4.6e-06	^{239}Pu: 7.47e-05 to 2.40e-04 ^{235}U: 7.6e-07 to 4.2e-06	^{239}Pu: 9.60e-05 to 3.98e-04 ^{235}U: 9.16e-07 to 3.8e-06	^{239}Pu: 9.42e-05 to 3.97e-04 ^{235}U: 9.09e-07 to 3.8e-06
	Temperature	Room Temp.	Room Temp.	Room Temp	Room Temp	Room Temp
Materials/ Moderator	**Element**	H	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	H: 5.45e-02 to 6.71e-02	H: 6.48e-02 to 6.55e-02	H: 5.73e-02 to 6.44e-02	H: 5.41e-02 to 6.35e-02	H: 5.40e-02 to 6.35e-02
	Ratio to fissile material	H/^{239}Pu = 125 to 569 (annular tank)	H/^{239}Pu = 2317 to 2434	H/^{239}Pu = 239 to 1556	H/^{239}Pu = 126 to 664	H/^{239}Pu = 136 to 674
	Temperature	Room Temp.	Room Temp.	Room Temp	Room Temp	Room Temp
Materials/ Reflector	**Material/Physical form**	Reflected by water	Reflected by water	Reflected by water and polyethylene	Reflected by water or concrete	Reflected by water or concrete
Materials/ Neutron Absorber	**Element**	B, Cd	None	None	None	None
	Physical form	B in concrete, Cd in inserts	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution in annular cylinder; Center contained solution and/or inserts	Homogeneous solution in a cylindrical vessel	Homogeneous solution in a cylindrical vessel	Homogeneous solution in a cylindrical vessel	Homogeneous solution in slab tank
	Shape	Cylinder	Cylinder	Cylinder	Cylinder	Parallelepiped
Neutron Energy	**AENCF**	0.0142 to 0.0459 MeV	0.0039 to 0.0061 MeV	0.0065 to 0.0320 MeV	0.0117 to 0.0589 MeV	0.012 to 0.059 MeV
	EALF	0.0541 to 0.393 eV	0.0423 to 0.0433 eV	0.0477 to 0.144 eV	0.06669 to 0.302 eV	0.0687 to 0.361 eV
	Neutron Energy Spectra[a]	T: 5.1 to 27.5 % I: 32.1 to 40.1 % F: 40.4 to 54.8 %	T: 47.4 to 48.5 % I: 22.6 to 23.1 % F: 28.7 to 29.5 %	T: 11.2 to 39.2 % I: 26.0 to 36.9 % F: 33.8 to 51.9 %	T: 6.1 to 24.6 % I: 31.8 to 39.0 % F: 43.6 to 55.7 %	T: 5.6 to 24.9 % I: 31.7 to 38.8 % F: 43.4 to 55.6 %
	Fission Rate vs. Neutron Energy[a]	T: 84.1 to 93.5 % I: 5.7 to 13.8 % F: 0.8 to 2.1 %	T: 98.3 to 98.5 % I: 1.3 to 1.4 % F: 0.1 to 0.3 %	T: 90.6 to 97.9% I: 1.8 to 7.9% F: 0.3 to 1.4%	T: 82.8 to 96.1% I: 3.4 to 14.5 % F: 0.5 to 2.7%	T: 82.7 to 96.1% I: 3.4 to 14.6 % F: 0.6 to 2.7%

Source: Reference 5 and 10

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – *20 MeV*]

Table 20. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing Mixtures with Plutonium and Uranium (set 2)

Category/ Description	Parameter	Experiment MIX-SOL-THERM-006 (6 cases)	Experiment MIX-COMP-THERM-012 (33 cases)	Experiment PU-MET-MIXED-001 (6 cases)	Experiment PU-COMP-MIXED-001 (5 cases)	Experiment PU-COMP-MIXED-002 (29 cases)
Materials/ Fissionable Material	**Fissionable Element**	Plutonium + Uranium	Plutonium + uranium	Plutonium	Plutonium	Plutonium
	Physical Form	Pu-U nitrate solution	Pu-U oxide (MOX)	Pu metal pellets	Pu oxide	Pu oxide
	Isotopic Composition	Pu: 75.4 wt % ^{239}Pu ; 20.4 wt % ^{240}Pu ; 2.9 wt % ^{241}Pu 0.56 wt % ^{235}U in U	Pu: 8 and 23 wt% ^{240}Pu in Pu 0.151 wt% ^{235}U in U	95.17 wt% ^{239}Pu	75.2 to 97.7 wt% ^{239}Pu in Pu	75.2 to 97.7 wt% ^{239}Pu in Pu
	Atomic density (atoms/b-cm)	^{239}Pu: 1.72e-04 to 1.73e-04 ^{235}U: 2.66e-06 to 2.7e-06	^{239}Pu: 6.51e-05 to 1.09e-04 ^{235}U: 1.01e-06 to 2.9e-06	^{239}Pu: 3.67e-02	^{239}Pu: 7.00e-04 to 1.09e-02	^{239}Pu: 7.00e-04 to 1.09e-02
	Temperature	Room Temp.	Room Temp	300 K	Room Temp	Room Temp
Materials/ Moderator	**Element**	H	H, C	H, C, Si as scatterer	H, C	H, C
	Physical form	Solution	Polystyrene	Polyethylene, sand	Polystyrene	Polystyrene
	Atomic density (atoms/b-cm)	H: 5.48e-02 to 5.52e-02	H: 4.15e-02 to 5.66e-02 C: 3.56e-02 to 4.54e-02	In Polythylene pellets: H: 7.83e-02 C: 3.91e-02 Silicone dioxide: Si:1.57e-02 and 1.98e-02	H: 5.51e-04 to 4.57e-02 C: 0 to 4.50e-02	H: 5.51e-04 to 4.57e-02 C: 0 to 4.50e-02
	Ratio to fissile material	H/X = 297 to 303	H/^{239}Pu = 174 to 724	Not available	H/^{239}Pu = 0.05 to 65.37	H/^{239}Pu = 0.05 to 65.37
	Temperature	Room Temp	Room Temp	300 K	Room Temp	Room Temp
Materials/ Reflector	**Material/Physical form**	Reflected by water	Unreflected or reflected by Plexiglas	Reflected by sand and depleted uranium	Unreflected	Reflected by Plexiglas
Materials/ Neutron Absorber	**Element**	Gd	None	B	None	None
	Physical form	Solution	N/A	B_4C	N/A	N/A
	Atomic density (atoms/b-cm)	Gd: 1.15e-07 to 2.67e-06	N/A	^{10}B: 1.10e-02 ^{11}B: 4.46e-02	N/A	N/A
Geometry	**Heterogeneity**	Homogeneous solution in cylindrical tank	Arrays of MOX/polystyrene compact blocks in rectangular configurations	Complex heterogeneous arrangements of Pu and silicon dioxide pellets placed in array of rods	Arrays of Pu-oxide/polystyrene compact blocks in rectangular configurations	Arrays of Pu-oxide/polystyrene compact blocks in rectangular configurations
	Shape	Cylinder	Slab, parallelepiped	Cylindrical array of rods	Rectangular slab	Rectangular slab
Neutron Energy	**AENCF**	0.035 to 0.040 MeV	0.026-0.071 MeV	0.214 –0.457 MeV	0.100 - 1.702 MeV	0.077 - 1.046 MeV
	EALF	Not available	0.070 to 0.264 eV	1.29 to 5540 eV	1.67 to 1.02e6 eV	0.749 to 6800 eV
	Neutron Energy Spectra[a]	Not available	T: 7.2 to 27.9% I: 31.2 to 38.8% F: 40.9 to 54.0%	T: 0.2 to 18.5% I: 31.9 to 52.3% F: 47.5 to 54.6%	T: 0 to 2.3 % I: 5.9 to 39.7 % F: 58. to 94.1 %	T: 0.1 to 3.2 % I: 13.9 to 39.2 % F: 57.6 to 86.0 %
	Fission Rate vs Neutron Energy[a]	Not available	T: 86.0 to 96% I: 3.0 to 11.8% F: 1.0 to 2.6%	T: 4.1 to 70.6% I: 18.1 to 63.7% F: 11.4 to 32.2%	T: 0.2 to 65.2% I: 5.3 to 57.7% F: 5.2 to 94.5 %	T: 23 to 72.4% I: 19.8 to 44.9% F: 4.0 to 57.2 %

Source: Reference 5 and 10

Note: [a] Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

5.4.3 Calculation of the Lower Bound Tolerance Limit

In the following paragraphs some of the information presented in Section 2 is repeated focusing on the steps that are actually used for the current group of benchmarks. The first step in calculating the lower bound tolerance limit is to apply regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p.8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}. Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (e.g., average energy of a neutron causing fission [AENCF]), using the build-in regression analysis tool from Excel software. The AENCF is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p. 3-47).

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the y values about their mean that can be attributed to a linear relation between y and x. Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (b). The slope test requires calculating the test statistic "T" as described by Equations 2, 3 and 4 from Section 2.

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and n-2 degrees of freedom, where n is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied. The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals.

The results of the trending parameter analysis for the criticality benchmark subset representative for external configurations containing U + Pu mixtures are presented in Attachment IV and summarized in Table 21. The results in Table 21 and the analysis of the residuals (Attachment IV) do not indicate a valid trend of k_{eff} with AENCF.

Table 21. Trending Parameter Results for the Criticality Benchmark Subset Representative for Configurations Containing U + Pu Mixtures External to the Waste Package

Trend Parameter	n	Intercept	Slope	r^2	T	$t_{0.025,n-2}$	P-value	Goodness-of-fit Tests	Valid Trend
AENCF	120	1.0062	-0.0168	0.1101	-3.82	1.980[a]	0.0002	Failed	No

Source: Attachment IV
Note: [a] Value taken from Table A-4 of Reference 9.

Because this set shows no valid trending, according to the methodology summarized in Section 2, the set is tested for normality using an omnibus normality test (Anderson-Darling). It tests the goodness-of-fit to a normal distribution constructed with the sample average and standard deviation of the k_{eff} set of values. The required steps to apply the test and specific test statistics are presented in Attachment IV. The Anderson-Darling normality test performed for this set showed that the calculated k_{eff} values are not normally distributed.

If the set of values does not have a normal statistical distribution, a non-parametric statistical treatment must be used as described in Reference 1 (p. 3-51) as the distribution-free tolerance limit (DFTL). A more specific description of the method is presented in Reference 6 (p. 14), resulting in the determination of the degree of confidence that a fraction of the true population of data lies above the smallest value observed. The more data are available in the sample, the higher the degree of confidence. Non-parametric techniques do not require reliance upon distributions, but are rather an analysis of ranks. Therefore, the k_{eff} values in a sample are ranked from the smallest to the largest.

For a desired population fraction of 95% and a rank order of 1 (the smallest k_{eff} value in data sample), the confidence level calculated with Equation 5 from Section 2 for n = 96 points is 99.8%. For non-parametric data analysis, Reference 6 (p. 14) suggests that lower bound tolerance limit be determined by:

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM)

where: *Non-parametric margin (NPM)* is added to account for small sample size.

For the present case (n = 120) the non parametric margin was determined to be 0 based on a calculated confidence level (β) of 0.998 (Section 2 and Attachment IV) and the corresponding value of NPM from Table 2.

The final calculated lower bound tolerance limit value using DFTL method for this set of benchmark experiments is 0.9644 (Attachment IV). Figure 4 presents the k_{eff} values and the calculated lower bound tolerance limit.

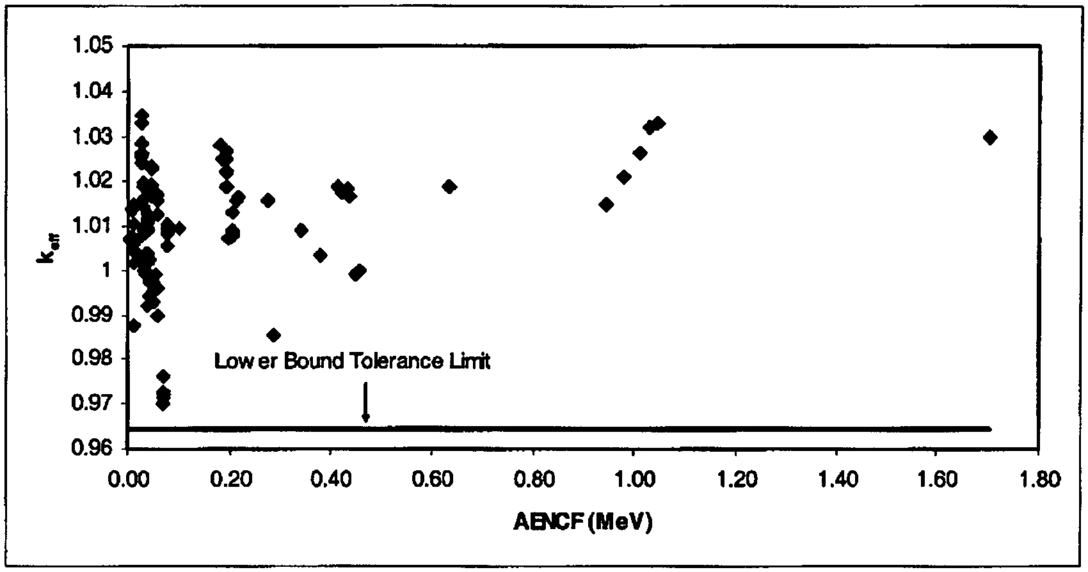

Figure 4. Lower Bound Tolerance Limit Applicable for Configurations Containing Mixtures of Plutonium and Uranium External to the Waste Package

5.5 CALCULATIONS FOR BENCHMARK CRITICAL EXPERIMENTS SELECTED FOR EXTERNAL CONFIGURATIONS CONTAINING MIXTURES WITH URANIUM-233

As mentioned in Section 2, an essential element of validating the methods and models used for calculating effective neutron multiplication factor, k_{eff}, for a waste package is determination of critical limit. The steps that need to be completed in establishing a critical limit are as follows (Reference 1, p.3-44): (1) selection of benchmark experiments; (2) establishment of the range of applicability of the benchmark experiments (identification of physical and spectral parameters that characterize the benchmark experiments); (3) establishment of a lower bound tolerance limit; and (4) establishment of additional uncertainties due to extrapolations or limitations in geometrical or material representations.

In the following, the first three steps of the process of establishing a critical limit for the external configurations containing mixtures with uranium-233 fissile isotope (^{233}U) are detailed.

5.5.1 Selection of the Criticality Benchmark Experiments

The criticality experiments selected for inclusion in the validation of the criticality model must be representative of the types of materials, conditions, and parameters to be modeled using the calculational method (criticality model). A sufficient number of experiments with varying experimental parameters should be selected for inclusion in the validation to ensure as wide an area of applicability as feasible and statistically significant results. While there is no absolute guideline for the minimum number of critical experiments necessary to validate a model, the use of only a few (i.e., less than 10) experiments should be accompanied by a suitable technical basis supporting the rationale for acceptability of the validation results (Reference 6, p. 5).

For the present application (configurations with U-233 fissile material external to the waste package), the criticality benchmark experiments have been selected based on their fissile content, moderator content and geometry. The benchmark experiments come from the *International Handbook of Evaluated Criticality Safety Benchmark Experiments* (Reference 5) unless otherwise noted. The selection process was based on a prior knowledge regarding the possible external configurations of the degraded fissile material carried outside the waste package (*External Criticality Calculation for DOE SNF Codisposal Waste Packages* [Reference 2]). The set of criticality benchmark experiments has been constructed to accommodate large variations in the range of parameters of the configurations and also to provide adequate statistics for the lower bound tolerance limit calculations.

The selected benchmark experiments containing a total of 83 individual cases are presented in Table 22 together with the results of the MCNP code calculations. All cases have been run using the isotopic libraries described in Reference 10 (Table 2).

Table 22. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing U-233

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
Experiment U233-SOL-THERM-001 (5 cases)	ust001-1	1	0.0031	1.0018	0.0005	0.0038
	ust001-2	1.0005	0.0033	1.0004	0.0006	0.0041
	ust001-3	1.0006	0.0033	0.9994	0.0006	0.0043
	ust001-4	0.9998	0.0033	0.9989	0.0006	0.0043
	ust001-5	0.9999	0.0033	0.9987	0.0006	0.0043
Experiment U233-SOL-THERM-002 (17 cases)	ust02-04	1.004	0.0087	1.0103	0.0011	0.026
	ust02-05	1.004	0.0087	0.9973	0.0011	0.0214
	ust02-08	1.004	0.0087	1.0113	0.001	0.0173
	ust02-10	1.004	0.0087	1.0096	0.0011	0.0138
	ust02-11	1.004	0.0087	1.0126	0.001	0.0115
	ust02-12	1.004	0.0087	1.0006	0.001	0.01
	ust02-14	1.004	0.0087	0.9875	0.0009	0.0098
	ust02-15	1.004	0.0087	1.0026	0.001	0.0083
	ust02-17	1.004	0.0087	0.9897	0.0009	0.0072
	ust02-18	1.004	0.0087	1.0029	0.0008	0.0066
	ust02-19	1.004	0.0087	1.0102	0.0008	0.0056
	ust02-22	1.004	0.0087	0.9967	0.0011	0.0356

Table 22. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing U-233

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	ust02-24	1.004	0.0087	0.9976	0.0012	0.049
	ust02-34	1.004	0.0087	1.0038	0.0011	0.0223
	ust02-35	1.004	0.0087	1.0103	0.0009	0.0155
	ust02-36	1.004	0.0087	1.0115	0.0009	0.0096
	ust02-38	1.004	0.0087	1.0097	0.0008	0.0075
Experiment U233-SOL-THERM-003 (10 cases)	ust03-40	0.9995	0.0087	1.008	0.001	0.0387
	ust03-41	0.9991	0.0151	1.026	0.0011	0.0397
	ust03-42	1.0007	0.0087	1.0044	0.0011	0.04
	ust03-45	1.0015	0.0126	1.014	0.0011	0.061
	ust03-55	1.0006	0.0122	1.0197	0.0011	0.0693
	ust03-57	1.0012	0.0087	1.0244	0.001	0.0209
	ust03-58	1.0016	0.0087	1.0167	0.001	0.0138
	ust03-61	1.0016	0.0087	1.0133	0.001	0.0108
	ust03-62	1.0018	0.0087	1.0107	0.001	0.0095
	ust03-65	1.0008	0.0087	1.0073	0.0008	0.0056
Experiment U233-SOL-THERM-004 (10 cases)	ust04-03	1.0039	0.0088	1.0086	0.0011	0.0257
	ust04-06	1.0034	0.0086	1.0113	0.001	0.0208
	ust04-20	1.0041	0.0089	1.0006	0.0011	0.0353
	ust04-25	1.0051	0.0089	0.9936	0.0011	0.0493
	ust04-27	1.002	0.0105	1.0119	0.0011	0.0479
	ust04-28	1.002	0.0104	1.0063	0.0011	0.0425
	ust04-30	1.0037	0.009	0.9988	0.0011	0.043
	ust04-33	1.002	0.0102	1.0087	0.0011	0.0215
Experiment U233-SOL-THERM-005 (2 cases)	ust05-01	1.000	0.004	1.0054	0.0009	0.0094
	ust05-02	1000	0.0049	1.0075	0.0009	0.0078
Experiment U233-SOL-THERM-008 (1 case)	ust008	1.0006	0.0029	0.9986	0.0004	0.003
Experiment U233-SOL-THERM-006 (12 cases)	m35	1.000	0.0035	1.023	0.0008	0.0576
	m36	1.000	0.0035	1.0113	0.0008	0.0583
	m37	1.000	0.0035	0.9996	0.0008	0.0588
	m38	1.000	0.0035	1.0011	0.0008	0.0584
	m45	1.000	0.0035	1.0186	0.0011	0.059
	m61	1.000	0.0035	1.0228	0.0008	0.0345
	m62	1.000	0.0035	1.0132	0.0008	0.0346
	m63	1.000	0.0035	0.9988	0.0008	0.0352
	m65	1.000	0.0035	0.9939	0.0008	0.0350
	m77	1.000	0.0035	0.9939	0.0011	0.0358
	m78	1.000	0.0035	0.9932	0.0011	0.0358
	m79	1.000	0.0035	0.9929	0.0011	0.0355
Experiment HEU-COMP-MIXED-001 (26 cases)	hcm-1	1.000	0.0059	1.0027	0.001	0.1045
	hcm-2	1.0012	0.0059	1.0059	0.0011	0.1053
	hcm-5	0.9985	0.0056	0.9963	0.001	0.7833
	hcm-6	0.9953	0.0056	0.9899	0.001	0.7962
	hcm-7	0.9997	0.0038	0.9949	0.001	0.8015

Table 22. Critical Benchmarks Selected for Validation of the Criticality Model for External Configurations Containing U-233

Experiment	Case Name	Benchmark Values		Calculated Values (MCNP)		
		k_{eff}	σ_{exp}	k_{eff}	σ_{calc}	AENCF
	hcm-8	0.9984	0.0052	0.9915	0.0011	0.6872
	hcm-9	0.9983	0.0052	0.9931	0.0011	0.6536
	hcm-10	0.9979	0.0052	0.9941	0.001	0.6494
	hcm-11	0.9983	0.0052	0.9934	0.0011	0.6385
	hcm-12	0.9972	0.0052	0.996	0.0011	0.6358
	hcm-13	1.0032	0.0053	0.9977	0.0011	0.6309
	hcm-15	1.0083	0.005	0.9949	0.0011	0.4671
	hcm-16	1.0001	0.0046	0.9926	0.0011	0.4692
	hcm-17	0.9997	0.0046	1.0012	0.0011	0.4647
	hcm-18	1.0075	0.0046	1	0.001	0.4625
	hcm-19	1.0039	0.0047	1	0.0011	0.5191
	hcm-20	1.006	0.0065	1.0051	0.0015	0.5357
	hcm-21	1.0026	0.0064	1.0046	0.0016	0.5378
	hcm-22	1.0013	0.0064	0.9995	0.0016	0.5371
	hcm-23	0.9995	0.0053	1.0056	0.0015	0.535
	hcm-24	1.002	0.0053	1.0003	0.0016	0.5352
	hcm-25	0.9983	0.0053	0.997	0.0014	0.5333
	hcm-26	0.9998	0.0053	1.0001	0.0015	0.5283
	hcm-27	0.9991	0.0053	0.9978	0.0016	0.5302
	hcm-28	1.0037	0.0053	1.0033	0.0015	0.541
	hcm-29	0.9992	0.0052	0.9998	0.0014	0.5401
Experiment HEU-MET-THERM-001 (1 case)	hmt001	1.0010	0.0060	1.0097	0.0010	0.0215
Experiment HEU-MET-THERM-014 (1 case)	hmt14	0.9939	0.0015	1.0125	0.0004	0.0233

Source: Critical benchmark experiments are evaluated in Reference 5 and MCNP calculations are summarized in Reference 10 except cases from experiments HEU-MET-THERM-001 and HEU-MET-THERM-014 which have been run for the current calculation (output files were uploaded on the COLD server and are listed in Section 7)

The experiments listed in Table 22 above are considered appropriate to represent degraded configurations containing U-233 alone or mixed with U-235 external to the waste package.

5.5.2 Range of Applicability of Selected Criticality Benchmark Experiments

This subsection summarizes in a set of tables (Tables 23 and 24) the range of applicability of the experiments listed in Table 22. The information is partly excerpted from Reference 10. The tables have been enhanced by adding information regarding the spectral characteristics of the experiments (available for the majority of the benchmarks from Reference 5). The purpose is to enable the construction of a collective area of applicability that can be used to directly compare the range of applicability of this set of benchmark experiments with the range of parameters of the postulated external configurations.

Table 23. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing U-233 (set 1)

Category/ Description	Parameter	Experiment U233-SOL-THERM-001 (5 cases)	Experiment U233-SOL-THERM-002 (17 cases)	Experiment U233-SOL-THERM-003 (10 cases)	Experiment U233-SOL-THERM-004 (8 cases)	Experiment U233-SOL-THERM-005 (2 cases)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Uranyl nitrate	Uranyl nitrate	Uranyl fluoride	Uranyl nitrate	Uranyl nitrate
	Isotopic Composition	97.7 wt% U-233	98.7 wt% U-233	98.7 wt% U-233	98.7 wt% U-233	98.7 wt% U-233
	Atomic density (atoms/b-cm)	U-233: 4.33e-05 to 5.00e-05	U-233: 8.71e-05 to 9.84e-04	U-233: 8.56e-05 to 1.55e-03	U-233: 4.15e-04 to 9.84e-04	U-233: 1.27e-04 and 1.60e-04
	Temperature	Room Temp.	Room Temp.	Room Temp.	Room Temp.	Room Temp.
Materials/ Moderator	Element	H	H	H	H	H
	Physical form	Solution	Solution	Solution	Solution	Solution
	Atomic density (atoms/b-cm)	6.63e-02 to 6.64e-02	5.62e-02 to 6.56e-02	6.05e-02 to 6.57e-02	5.62e-02 to 6.22e-02	6.50e-02 and 6.54e-02
	Ratio to fissile material	1324 to 1533	57.1 to 752.6	39.4 to 775	57.1 to 149.2	405 and 514
	Temperature	Room Temp.	Room Temp.	Room Temp.	Room Temp.	Room Temp.
Materials/ Reflector	Material/Physical form	Unreflected	Reflected by paraffin	Reflected by paraffin	Reflected by paraffin	Reflected by water
Materials/ Neutron Absorber	Element	B	None	None	None	None
	Physical form	Solution	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	B10:2.65e-07 to 1.01e-6	N/A	N/A	N/A	N/A
Geometry	Heterogeneity	Solution contained in an Al sphere	Solution contained in an Al sphere	Solution contained in single Al cylindrical vessel	Solution contained in single Al cylindrical vessel	Solution in spherical or cylindrical Al vessel
	Shape	Sphere	Sphere	Cylindrical	Cylindrical	Cylindrical/ Spherical
Neutron Energy	AENCF	0.0038-0.0043 MeV	0.0056-0.0490 MeV	0.0056-0.0693 MeV	0.0208-0.0493 MeV	0.0078-0.0094 MeV
	EALF	0.0392 to 0.0417 eV	0.0464 to 0.471 eV	0.046 to 1.03 eV	0.138 to 0.486 eV	0.055 to0.062 eV
	Neutron Energy Spectra[a]	T: 48.9 to 52.5 % I: 21.0 to 22.6% F: 26.5 to 28.5%	T: 7.7 to 42.2 % I: 24.8 to 33.9% F: 33.0 to 58.3%	T: 5.2 to 42.6 % I: 24.6 to 34.2 % F: 32.7 to 60.6 %	T: 7.8 to 17.2 % I: 32.4 to 34.0 % F: 50.4 to 58.3 %	T: 31.3 to 35.5 % I: 27.1 to 28.5 % F: 37.4 to 40.1 %
	Fission Rate vs Neutron Energy[a]	T: 94.0 to 94.8% I: 5.0 to 5.8% F: 0.2 %	T: 76.0 to 92.5% I: 7.1 to 33.5% F: 0.2 to 2.8 %	T: 54.5 to 92.7% I: 7.0 to 41.5 % F: 0.3 to 4.0 %	T: 63.8 to 79.5% I: 19.3 to 33.4 % F: 1.2 to 2.8 %	T: 88.9 to 90.5% I: 9.0 to 10.6 % F: 0.4 to 0.5 %

Source: Reference 5 and 10.

Note: [a]Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

Table 24. Range of Applicability of Critical Benchmark Experiments Selected for Comparison with External Configurations Containing U-233 (set 2)

Category/ Description	Parameter	Experiment U233-SOL-THERM-006 (6 cases)	Experiment U233-SOL-THERM-008 (1 case)	Experiment HEU-COMP-MIXED-001 (26 cases)	Experiment HEU-MET-THERM-001 (1 case)	Experiment HEU-MET THERM-014 (1case)
Materials/ Fissionable Material	Fissionable Element	Uranium	Uranium	Uranium	Uranium	Uranium
	Physical Form	Uranyl nitrate	Uranyl nitrate	UO_2	Uranium metal foils	Uranium metal foils
	Isotopic Composition	97.56 or 97.54 wt% U-233;	97.67 wt% U-233	93.15 wt% U-235	93.23 wt% U-235	93.23 wt% U-235

Category/ Description	Parameter	Experiment U233-SOL-THERM-006 (6 cases)	Experiment U233-SOL-THERM-008 (1 case)	Experiment HEU-COMP-MIXED-001 (26 cases)	Experiment HEU-MET-THERM-001 (1 case)	Experiment HEU-MET THERM-014 (1case)
	Atomic density (atoms/b-cm)	U-233:5.14e-04 to 8.64e-04	U-233: 3.34e-05	U-235: 4.48e-03 to 1.39e-02	U-235: 3.84e-02 to 4.28e-02	U-235: 3.84e-02 to 4.38e-02
	Temperature	293 K	293 K	293 K	Room Temp.	293 K
Materials/ Moderator	Element	H	H	H	H, C Si as scatterer	H, C Si as scatterer
	Physical form	Water in aqueous solution of uranyl nitrate	Solution	Water, Alcohol-water solution, Plexiglas	Plates of polyethylene and silicon glass	Plates of polyethylene and silicon glass
	Atomic density (atoms/b-cm)	5.89e-02 to 6.15e-02	6.64e-02	Fuel Region: 2.16e-2 (few cases) 5.68e-2 (plexiglas) 6.24e-2 (alcohol-water)	H: 8.23e-02 to 8.28e-02 C: 4.11e-02 to 4.14e-02 Si: 2.17 to 2.24e-02	H: 8.19e-02 to 8.34e-02 C: 4.10e-02 to 4.17e-02 Si: 2.20 to 2.28e-02
	Ratio to fissile material	H/X = 69 to 121	H/X = 1324 to 1533	H/X = 0 to 49	Not available	H/X: Not available Si/U235 = 42
	Temperature	293 K	293 K	293 K	Room Temp.	Room Temp.
Materials/ Reflector	Material/ Physical form	Unreflected	Unreflected	Reflected by polyethylene	Reflected by polyethylene	Reflected by polyethylene
Materials/ Neutron Absorber	Element	None	None	None	None	None
	Physical form	N/A	N/A	N/A	N/A	N/A
	Atomic density (atoms/b-cm)	N/A	N/A	N/A	N/A	N/A
Geometry	Heterogeneity	Arrays of cans containing uranyl nitrate solution in rectangular geometry	Solution contained in an Al sphere	Complex arrays of cans in rectangular geometry	Rectangular column of plates and foils	Rectangular column of plates and foils
	Shape	Parallelepiped	Sphere	Cylinder	Parallelepiped	Parallelepiped
Neutron Energy	AENCF	0.0344-0.0599 MeV	0.0030 MeV	0.1045-0.8015 MeV	0.0212 MeV	0.0234 MeV
	EALF	0.303 to 0.896 eV	0.0037 eV	0.438 to 2070 eV	0.0865 eV	Not Available
	Neutron Energy Spectra[a]	T: 6.1 to 10.7 % I: 34.8 to 35.4 % F: 54.4 to 58.4 %	T: 57.0 % I: 19.3 % F: 23.7 %	T: 4.3 to 25.3 % I: 14.2 to 25.9 % F: 56.0 to 81.4 %	T: 22.7 % I: 27.7 % F: 49.7 %	Not Available
	Fission Rate vs Neutron Energy[a]	T: 55.0 to 68.4 % I: 29.7 to 41.7 % F: 2.0 to 3.3 %	T: 95.5 % I: 4.3 % F: 0.2 %	T: 25.4 to 78.0 % I: 16.4 to 43.1 % F: 5.6 to 49.9 %	T: 91.2 % I: 7.7 % F: 1.2 %	Not Available

Source: Reference 5 and 10.

Note: [a]Spectral range defined as follows: thermal (T) [0-1 eV], intermediate (I) [1eV -100 keV], fast (F) [100 keV – 20 MeV]

5.5.3 Calculation of the Lower Bound Tolerance Limit

In the following paragraphs some of the information presented in Section 2 is repeated focusing on the steps that are actually applicable for the current group of benchmarks. The first step in calculating the lower bound tolerance limit is to apply regression–based methods to identify any trending of the calculated values of k_{eff} with spectral and/or physical parameters. The trends show the results of systematic errors or bias inherent in the calculational method used to estimate criticality.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done as suggested in Reference 6 (p.8). This adjustment is done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). This normalization does not affect the inherent bias in the calculation due to very small differences in k_{eff}.

Each subset of normalized k_{eff} values is first tested for trending against available spectral and/or physical parameters (e.g., average energy of a neutron causing fission [AENCF], ratio of hydrogen to fissile atoms [H/X]), using the build-in regression analysis tool from Excel software. The AENCF is the energy per source particle lost to fission divided by the weight per source neutron lost to fission from the "problem summary section" of the MCNP output. Trending in this context is linear regression of k_{eff} on the predictor variable(s) (Reference 1, p. 3-47).

The linear regression fitted equation is in the form $y(x) = a + bx + \varepsilon$, where ε is the random error component (residuals). The trending is checked using well-established indicators or goodness-of-fit tests concerning the regression parameters. As a first indicator, the coefficient of determination (r^2) that is available as a result of using linear regression statistic can be used to evaluate the linear trending. It represents the proportion of the sum of squares of deviations of the y values about their mean that can be attributed to a linear relation between y and x. Another assessment of the adequacy of the linear model can be done by checking the goodness-of-fit against a null hypothesis on the slope (b). The slope test requires calculating the test statistic "T" as described by Equations 2, 3 and 4 from Section 2.

The test statistic is compared to the Student's t-distribution ($t_{\alpha/2,n-2}$) with 95% confidence and n-2 degrees of freedom, where n is the initial number of points in the subset. Given a null hypothesis of "no statistically significant trend exists (slope is zero)", the hypothesis would be accepted if $|T| < t_{\alpha/2,n-2}$, and rejected otherwise. Unless the data is exceptional, the linear regression results will have a non-zero slope. By only accepting linear trends that the data supports with 95% confidence, trends due to the randomness of the data are eliminated. A good indicator of this statistical process is evaluation of the P-value probability (calculated by the regression tool in Excel) that gives a direct estimation of the probability of having a linear trending due only to chance.

The last step employed as part of the regression analysis is determining whether or not the final requirements of the simple linear regression model are satisfied. The error component (residuals) need to be normally distributed with mean zero, and also the residuals need to show a random scatter about the line y=0 (no pattern). These requirements were verified for the present calculation using the built-in statistical functions in Excel and by applying an omnibus normality test (Anderson-Darling [Reference 8, p.372]) on the residuals.

The results of the trending parameter analysis for the criticality benchmark subset representative for external configurations containing ^{233}U mixtures are presented in Attachment V and summarized in Table 25. The results in Table 25 and the analysis of the residuals (Attachment V) do not indicate a valid trend of k_{eff} with AENCF or H/X.

Table 25. Trending Parameter Results for the Criticality Benchmark Subset Representative for Configurations Containing ^{233}U External to the Waste Package

Trend Parameter	n	Intercept	Slope	r^2	T	$t_{0.025,n-2}$	P-value	Goodness-of-fit Tests	Valid Trend
AENCF	83	1.0045	-0.0121	0.1277	-3.4482	1.993^a	0.0009	Marginally failed	No
H/X	78	1.0024	-1.02E-06	2.304E-03	-0.4189	1.995^a	0.6765	Failed	No

Source: Attachment V
Note: [a]Values interpolated from Table A-4 of Reference 9.

The Anderson-Darling normality test performed for this subset (Attachment V) showed that the calculated k_{eff} values are not normally distributed. As indicated in Section 2, the lower bound tolerance limit value can be calculated in this situation with the DFTL method. The calculated lower bound tolerance limit value is 0.9748 (Attachment VI). Figure 5 presents the k_{eff} values and the calculated lower bound tolerance limit.

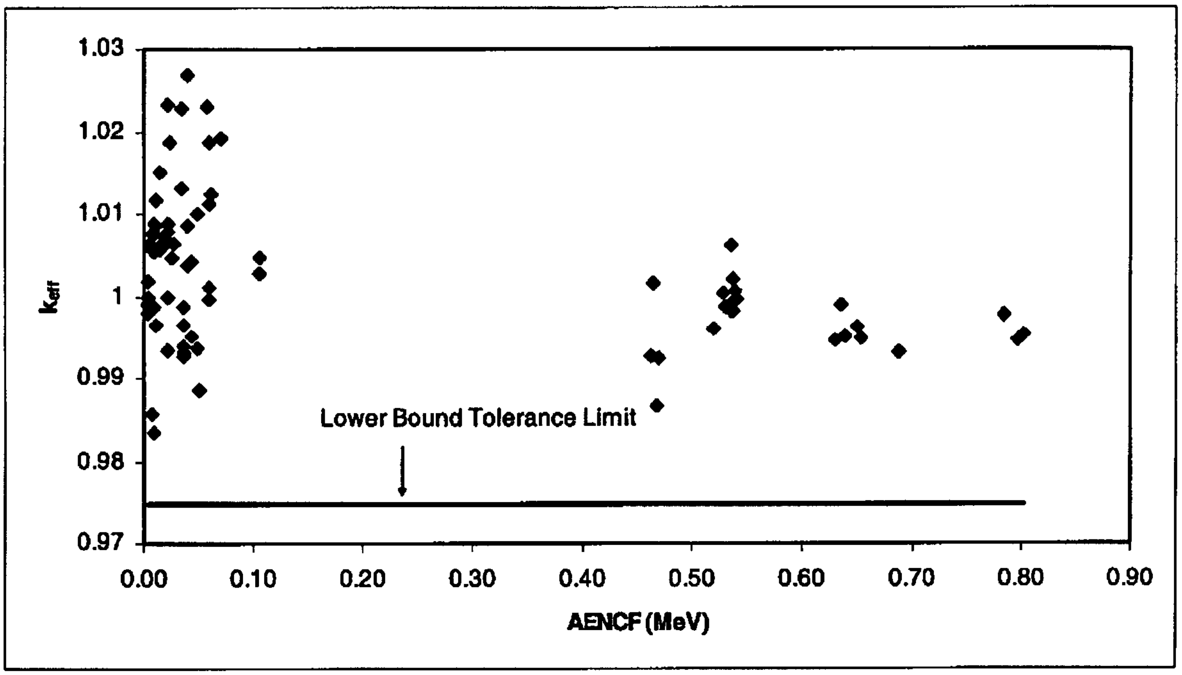

Figure 5. Lower Bound Tolerance Limit Applicable for Configurations Containing ^{233}U External to the Waste Package

6. REFERENCES

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7. COMPUTER OUTPUT

In the following the COLD server listing describing the MCNP output files associated with this engineering calculation is presented:

7.1 MCNP Output Files for Critical Benchmarks Experiments

Note: When transferred to COLD server, the output files for MCNP cases having identical names (e.g. CASE1, CASE2, etc) have been modified by affixing the benchmark experiment abbreviation (e.g. HST for HEU-SOL-THERM, etc). The content of the files have not been affected by this modification.

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7.2 CLREG Output Files from Calculation

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Analysis of Critical
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heuout.csv 32-5045840-00 06/26/2004 15:57:51
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Analysis of Critical
Benchmark Experiments for Configurations External to WP

ieu.utl 32-5045840-00 06/26/2004 15:57:51
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Analysis of Critical
Benchmark Experiments for Configurations External to WP

ieuout.csv 32-5045840-00 06/26/2004 15:57:51
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Analysis of Critical
Benchmark Experiments for Configurations External to WP

7.3. MCNP Verification Files

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Configurations External to WP

inp01o 32-5045840-00 06/09/2004 09:33:40
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Analysis of Critical Benchmark Experiments for Configurations External to WP

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Analysis of Critical Benchmark Experiments for Configurations External to WP

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Analysis of Critical Benchmark Experiments for Configurations External to WP

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Analysis of Critical Benchmark Experiments for Configurations External to WP

inp10o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp11o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp12o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp13o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp14o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp15o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp16o       32-5045840-00     06/09/2004 09:33:41
MOSCALU D        212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp17o       32-5045840-00     06/09/2004 09:33:41
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MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp18o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp19o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp20o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp21o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp22o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp23o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp24o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp25o 32-5045840-00 06/09/2004 09:33:41
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp26o 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp27o 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp28o 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

inp29o 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

leuct12_1.gr0 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for Configurations External to WP

leuct12_1.gr1 32-5045840-00 06/09/2004 09:33:42
MOSCALU D 212020
Analysis of Critical Benchmark Experiments for
Configurations External to WP

7.4 CLREG Verification Files

t1test.utl 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 01

t1testout.csv 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 01

t2test.utl 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 02

t2testout.csv 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 02

t3test.utl 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 03

t3testout.csv 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 03

t4test.utl 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 04

t4testout.csv 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 04

t5test.utl 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 05

t5testout.csv 32-5045840-00 06/15/2004
Mehmet Saglam 212020
CLReg Test Case 05

8. ATTACHMENTS

ATTACHMENT I: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing HEU

ATTACHMENT II: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing IEU

ATTACHMENT III: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing LEU

ATTACHMENT IV: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing Uranium and Plutonium Fissile Isotopes

ATTACHMENT V: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing ^{233}U

ATTACHMENT VI: CLREG V1.0 Software Validation and Verification

ATTACHMENT VII: MCNP 4B2 Software Independent Validation and Verification on HP Systems “gr0” and “gr1”.

ATTACHMENT I: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing HEU

This attachment presents additional information about the steps performed (Section 5.1) in the calculation of the lower bound tolerance limit including trending analysis and normality tests. The purpose is to provide to the individual reviewer all information necessary to replicate the current results by developing spreadsheets (in Excel or similar commercial software) independent of the originator. The k_{eff} data set used in this calculation contains the k_{eff} values calculated with MCNP for the critical benchmark experiments selected for external configurations containing HEU (Table 3, Section 5.1). The data set for the benchmark cases relevant to external configurations containing HEU has a size of n=187 cases.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} values calculated with MCNP (k_{calc}) was done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations. These values are included in Table A.I-1 together with the data from Table 3.

Table A.I-1. Summary of k_{eff} Data on Criticality Benchmark Experiments for External Configurations Containing HEU

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
hmm5_1	1.01308	0.00057	1.0007	0.0027	1.012371	0.307
hmm5_2	1.0217	0.00055	1.0003	0.0028	1.021394	0.247
hmm5_3	1.01904	0.00052	1.0012	0.0029	1.017819	0.212
hmm5_4	1.0145	0.0006	1.0016	0.003	1.012879	0.3175
hmm5_5	1.00682	0.00052	1.0005	0.004	1.006317	0.377
hmt001	1.0097	0.0010	1.001	0.006	1.008691	0.0215
hmt14	1.0125	0.0004	0.9939	0.0015	1.018744	0.0233
hcm-1	1.0027	0.001	1.0000	0.0059	1.0027	0.1045
hcm-2	1.0059	0.0011	1.0012	0.0059	1.004694	0.1053
hcm-5	0.9963	0.001	0.9985	0.0056	0.997797	0.7833
hcm-6	0.9899	0.001	0.9953	0.0056	0.994575	0.7962
hcm-7	0.9949	0.001	0.9997	0.0038	0.995199	0.8015
hcm-8	0.9915	0.0011	0.9984	0.0052	0.993089	0.6872
hcm-9	0.9931	0.0011	0.9983	0.0052	0.994791	0.6536
hcm-10	0.9941	0.001	0.9979	0.0052	0.996192	0.6494
hcm-11	0.9934	0.0011	0.9983	0.0052	0.995092	0.6385
hcm-12	0.996	0.0011	0.9972	0.0052	0.998797	0.6358
hcm-13	0.9977	0.0011	1.0032	0.0053	0.994518	0.6309
hcm-15	1.0063	0.0011	1.0083	0.005	0.998016	0.4671
hcm-16	0.9949	0.0011	1.0001	0.0046	0.994801	0.4692
hcm-17	0.9926	0.001	0.9997	0.0046	0.992898	0.4647
hcm-18	1.0000	0.001	1.0075	0.0046	0.992556	0.4625
hcm-19	1.0000	0.0011	1.0039	0.0047	0.996115	0.5191
hcm-20	1.0051	0.0015	1.006	0.0065	0.999105	0.5357

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
hcm-21	1.0046	0.0016	1.0026	0.0064	1.001995	0.5378
hcm-22	0.9995	0.0016	1.0013	0.0064	0.998202	0.5371
hcm-23	1.0056	0.0015	0.9995	0.0053	1.006103	0.535
hcm-24	1.0003	0.0016	1.002	0.0053	0.998303	0.5352
hcm-25	0.997	0.0014	0.9983	0.0053	0.998698	0.5333
hcm-26	1.0001	0.0015	0.9998	0.0053	1.0003	0.5283
hcm-27	0.9978	0.0016	0.9991	0.0053	0.998699	0.5302
hcm-28	1.0033	0.0015	1.0037	0.0053	0.999601	0.541
hcm-29	0.9998	0.0014	0.9992	0.0052	1.0006	0.5401
hcm02_1	0.9866	0.0017	1.0000	0.0085	0.9866	0.868
hcm02_10	0.9856	0.0019	1.0000	0.0081	0.9856	0.57
hcm02_11	0.9829	0.0019	1.0000	0.0088	0.9829	0.568
hcm02_12	0.99	0.0019	1.0000	0.0078	0.99	0.556
hcm02_13	0.9874	0.0017	1.0000	0.0083	0.9874	0.559
hcm02_14	0.988	0.0017	1.0000	0.0112	0.988	0.735
hcm02_15	0.985	0.0017	1.0000	0.0111	0.985	0.73
hcm02_16	0.9861	0.0017	1.0000	0.0108	0.9861	0.735
hcm02_17	0.9861	0.0016	1.0000	0.0112	0.9861	0.732
hcm02_18	0.9902	0.0017	1.0000	0.0111	0.9902	0.727
hcm02_19	0.991	0.0017	1.0000	0.0107	0.991	0.712
hcm02_2	0.9907	0.0017	1.0000	0.0088	0.9907	0.865
hcm02_20	0.9824	0.0018	1.0000	0.0108	0.9824	0.735
hcm02_21	0.9843	0.0016	1.0000	0.0092	0.9843	0.902
hcm02_22	0.9879	0.0019	1.0000	0.009	0.9879	0.899
hcm02_23	0.9866	0.0016	1.0000	0.0093	0.9866	0.896
hcm02_3	0.9914	0.0016	1.0000	0.0093	0.9914	0.724
hcm02_4	0.9923	0.0017	1.0000	0.0087	0.9923	0.716
hcm02_5	0.9933	0.0017	1.0000	0.0089	0.9933	0.722
hcm02_6	0.9852	0.0018	1.0000	0.0093	0.9852	0.574
hcm02_7	0.9813	0.0019	1.0000	0.0086	0.9813	0.578
hcm02_8	0.9943	0.0018	1.0000	0.0068	0.9943	0.537
hcm02_9	0.9913	0.0018	1.0000	0.0076	0.9913	0.541
hest1-1	1.00241	0.00131	1.0000	0.0025	1.00241	0.01582
hest1-2	0.99816	0.00209	1.0000	0.0025	0.99816	0.03873
hest1-3	1.00453	0.00199	1.0000	0.0025	1.00453	0.01546
hest1-4	1.0013	0.00203	1.0000	0.0025	1.0013	0.0405
hest1-5	1.00361	0.00166	1.0000	0.0025	1.00361	0.00651
hest1-6	1.01038	0.00187	1.0000	0.0025	1.01038	0.00678
hest1-7	1.0023	0.00201	1.0000	0.0025	1.0023	0.01501
hest1-8	1.00505	0.00213	1.0000	0.0025	1.00505	0.0161
hest1-9	0.99973	0.00212	1.0000	0.0025	0.99973	0.04099
hest110	0.99468	0.00178	1.0000	0.0025	0.99468	0.00757
hest2-1	1.00548	0.00148	1.0000	0.002	1.00548	0.01558
hest2-2	1.00773	0.00235	1.0000	0.002	1.00773	0.01516
hest2-3	1.00219	0.0022	1.0000	0.002	1.00219	0.0374
hest2-4	1.00809	0.00242	1.0000	0.002	1.00809	0.03541

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
hest2-5	1.01049	0.0023	1.0000	0.002	1.01049	0.01622
hest2-6	1.00968	0.00215	1.0000	0.002	1.00968	0.015
hest2-7	1.00691	0.00224	1.0000	0.002	1.00691	0.03747
hest2-8	1.01131	0.00206	1.0000	0.002	1.01131	0.03511
hest2-9	1.00348	0.00209	1.0000	0.002	1.00348	0.00654
hest2-10	1.00937	0.00202	1.0000	0.002	1.00937	0.00663
hest2-11	1.00875	0.00211	1.0000	0.002	1.00875	0.01595
hest2-12	1.0127	0.00209	1.0000	0.002	1.0127	0.01487
hest2-13	0.99869	0.00232	1.0000	0.002	0.99869	0.03676
hest2-14	1.01062	0.00238	1.0000	0.002	1.01062	0.03377
CASE_1	1.0164	0.0019	1.0000	0.0035	1.0164	0.0071
CASE_2	1.0178	0.0025	1.0000	0.005	1.0178	0.0361
CASE_3	1.0084	0.0019	1.0000	0.0035	1.0084	0.0071
CASE_4	1.0144	0.0019	1.0000	0.0035	1.0144	0.0357
CASE_5	1.0112	0.0019	1.0000	0.0035	1.0112	0.0835
CASE_6	1.0045	0.0023	1.0000	0.0035	1.0045	0.0376
CASE_7	1.0067	0.0019	1.0000	0.0035	1.0067	0.0085
CASE_8	1.0026	0.0025	1.0000	0.0035	1.0026	0.039
CASE_9	1.0087	0.0021	1.0000	0.0035	1.0087	0.0088
CASE_10	1.0144	0.0018	1.0000	0.0035	1.0144	0.0087
CASE_11	1.0097	0.002	1.0000	0.0035	1.0097	0.0356
CASE_12	1.0091	0.0019	1.0000	0.0035	1.0091	0.0088
CASE_13	1.0095	0.0023	1.0000	0.0035	1.0095	0.0345
CASE_14	1.0097	0.0021	1.0000	0.0035	1.0097	0.0363
CASE_15	1.0046	0.0021	1.0000	0.0035	1.0046	0.0369
CASE_16	1.0043	0.0022	1.0000	0.0035	1.0043	0.0368
CASE_17	1.012	0.0023	1.0000	0.0035	1.012	0.0368
heust81	1.00316	0.00134	1.0000	0.003	1.00316	0.00661
heust83	0.9973	0.0019	1.0000	0.003	0.9973	0.00644
heust86	1.00969	0.0023	1.0000	0.003	1.00969	0.03669
heust89	1.00373	0.00116	1.0000	0.003	1.00373	0.0066
hest813	1.00331	0.002	1.0000	0.003	1.00331	0.03616
heust9c1	1.0051	0.0006	1.0000	0.0057	1.0051	0.058
heust9c2	1.0045	0.0006	1.0000	0.0057	1.0045	0.045
heust9c3	1.0047	0.0007	1.0000	0.0057	1.0047	0.029
heust9c4	0.9994	0.0007	1.0000	0.0057	0.9994	0.018
hst33d_02a	1.00007	0.00128	1.0000	0.0111	1.00007	0.036
hst33d_02b	0.99792	0.00113	1.0000	0.0108	0.99792	0.036
hst33d_02c	0.99796	0.00119	1.0000	0.0065	0.99796	0.036
hst33d_03a	1.00634	0.00108	1.0000	0.0114	1.00634	0.033
hst33d_03b	1.00608	0.00115	1.0000	0.0111	1.00608	0.034
hst33d_03c	1.01079	0.00118	1.0000	0.007	1.01079	0.032
hst33d_04a	1.0057	0.00109	1.0000	0.0114	1.0057	0.035
hst33d_04b	1.0116	0.00117	1.0000	0.0111	1.0116	0.035
hst33d_05a	1.01126	0.00114	1.0000	0.0111	1.01126	0.035
hst33d_05b	1.00608	0.00128	1.0000	0.0108	1.00608	0.035

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
hst33d_06a	1.00936	0.00112	1.0000	0.0111	1.00936	0.035
hst33d_06b	1.00915	0.00114	1.0000	0.0108	1.00915	0.034
hst33d_07a	1.00453	0.00107	1.0000	0.0111	1.00453	0.035
hst33d_07b	1.00406	0.00109	1.0000	0.0108	1.00406	0.035
hst33d_08a	1.00558	0.00113	1.0000	0.0111	1.00558	0.034
hst33d_08b	1.00213	0.00111	1.0000	0.0108	1.00213	0.035
hst33d_09a	1.00228	0.00115	1.0000	0.0111	1.00228	0.036
hst33d_09b	0.99359	0.00113	1.0000	0.0108	0.99359	0.035
hst33d_09c	0.99619	0.00116	1.0000	0.0104	0.99619	0.036
hst33d_10a	1.00267	0.00113	1.0000	0.0114	1.00267	0.034
hst33d_10c	1.00333	0.00103	1.0000	0.007	1.00333	0.032
hst33d_10d	0.99286	0.00111	1.0000	0.0104	0.99286	0.033
hst33d_11a	1.00669	0.0011	1.0000	0.0111	1.00669	0.035
hst33d_11b	1.00176	0.00097	1.0000	0.0108	1.00176	0.034
hst33d_12a	1.00386	0.00112	1.0000	0.0111	1.00386	0.036
hst33d_12b	1.00165	0.00107	1.0000	0.0108	1.00165	0.035
CASE_1	0.9995	0.0004	1.0000	0.0025	0.9995	0.0437
CASE_2	0.9989	0.0004	1.0000	0.0025	0.9989	0.0405
CASE_3	1.0022	0.0004	1.0000	0.0025	1.0022	0.0421
CASE_4	1.0007	0.0004	1.0000	0.0025	1.0007	0.0438
CASE_5	1.0011	0.0004	1.0000	0.0025	1.0011	0.0434
CASE_6	0.9985	0.0004	1.0000	0.0025	0.9985	0.0405
CASE_7	1.0013	0.0004	1.0000	0.0032	1.00134	0.0420
CASE_8	1.0016	0.0004	1.0000	0.0026	1.00159	0.0416
CASE_9	1.0009	0.0004	1.0000	0.0033	1.00093	0.0412
CASE_10	1.0007	0.0004	1.0000	0.0026	1.00073	0.0425
CASE_11	1.0017	0.0004	1.0000	0.0025	1.00174	0.0434
CASE_12	1.0006	0.0004	1.0000	0.0025	1.00064	0.0434
CASE_13	1.0066	0.0004	1.0000	0.005	1.00658	0.0440
CASE_14	1.0060	0.0004	1.0000	0.005	1.00599	0.0443
CASE_15	1.0065	0.0004	1.0000	0.005	1.00647	0.0442
CASE_16	1.0065	0.0004	1.0000	0.005	1.00647	0.0442
CASE_17	1.0013	0.0004	1.0000	0.0026	1.00127	0.0432
CASE_18	1.0017	0.0004	1.0000	0.0032	1.00165	0.0431
CASE_19	1.0011	0.0004	1.0000	0.0032	1.00112	0.0430
CASE_20	1.0021	0.0004	1.0000	0.0032	1.00211	0.0430
CASE_21	0.9994	0.0004	1.0000	0.0025	0.9994	0.0412
CASE_22	0.9998	0.0004	1.0000	0.0027	0.9998	0.0407
CASE_23	0.9997	0.0004	1.0000	0.0027	0.9997	0.0408
CASE_24	1.0027	0.0004	1.0000	0.0026	1.00269	0.0438
CASE_25	1.0025	0.0004	1.0000	0.0032	1.00246	0.0429
CASE_26	1.0018	0.0004	1.0000	0.0032	1.00184	0.0429
CASE_27	1.0012	0.0004	1.0000	0.0032	1.00117	0.0483
CASE_28	1.0013	0.0004	1.0000	0.0025	1.0013	0.0425
CASE_1	0.9982	0.0003	0.9957	0.0045	1.002511	0.0024
CASE_2	0.9983	0.0003	0.9965	0.004	1.001806	0.0024

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
CASE_3	1.0011	0.0002	0.9994	0.0028	1.001701	0.0022
CASE_4	1.0025	0.0002	1.0000	0.0034	1.0025	0.0021
CASE_5	0.9997	0.0002	1.0000	0.0034	0.9997	0.002
CASE_6	1.0005	0.0002	1.0000	0.0037	1.0005	0.0021
CASE_7	1.0011	0.0002	1.0000	0.0036	1.0011	0.0021
CASE_8	1.0013	0.0001	1.0000	0.0035	1.0013	0.0021
heust43c1	0.9995	0.0007	0.9986	0.0017	1.000901	0.014
heust43c2	1.0082	0.0004	0.9995	0.0041	1.008704	0.003
heust43c3	1.0033	0.0004	0.999	0.0044	1.004304	0.003
hst4410	0.9909	0.0018	0.9944	0.0077	0.99648	0.039
hst4411	0.9847	0.002	0.9944	0.0078	0.990245	0.041
hst4412	0.9872	0.0017	0.9944	0.0078	0.992759	0.04
hst4413	1.0000	0.0018	0.9964	0.0067	1.003613	0.042
hst4416	1.0178	0.0018	0.9974	0.0062	1.020453	0.043
hst4417	0.9987	0.0017	0.9964	0.0057	1.002308	0.044
hst4419	1.0079	0.0018	0.9974	0.0063	1.010527	0.045
hst4444	1.0004	0.0017	0.9984	0.0057	1.002003	0.045
hst4449	1.0116	0.0017	0.9964	0.0047	1.015255	0.034
hst4450	0.9881	0.0018	0.9946	0.0047	0.993465	0.038
hst4451	1.0047	0.0017	0.9984	0.0057	1.00631	0.046
hst4453	1.0189	0.0018	0.9984	0.0064	1.020533	0.047
hst4454	1.0142	0.0015	0.9984	0.0065	1.015825	0.046
hst4455	1.0196	0.0017	0.9984	0.0065	1.021234	0.046
hst447	0.9948	0.0018	0.9944	0.0097	1.000402	0.037
hst448	0.9955	0.0021	0.9946	0.0083	1.000905	0.042

The set of normalized k_{eff} values is first tested for trending against the spectral parameter AENCF (e.g., average energy of a neutron causing fission) using the build-in regression analysis tool from the Excel software.

The linear regression is performed using the regression tool from Excel's menu by selecting the normalized k_{eff} (k_{norm}) as the y variable and the AENCF values as x variable. The full output of the regression tool contains statistics regarding validity of a trend, such as the coefficient of determination (r^2), standard error, t stat, etc., and is given below:

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.652958252
R Square	0.426354479
Adjusted R Square	0.423253692
Standard Error	0.00605197
Observations	187

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	5.0361E-03	0.005036078	137.4988	4.2106E-24
Residual	185	6.7759E-03	3.66263E-05		
Total	186	1.1812E-02			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.005503561	5.4207E-04	1854.937192	0	1.00443413	1.006573
X Variable 1	-0.0190719	1.6265E-03	-11.72598881	4.21E-24	-0.0222807	-0.01586

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 7 (Section 5.1). Since the absolute value of t-stat (renamed T in Table 7) is greater than $t_{0.025,185}$ and P-value is very low, the linear trend seems to be valid (Section 2).

In a second step, the assumptions used in deriving the linear model are verified. For a valid trend, the residuals (see Section 2) need to be normally distributed and with a mean of 0. The residuals are calculated by the regression tool in Excel (corresponding option need to be activated at the beginning of the process). Normality test of residuals is performed by applying the Anderson-Darling A^2 test (Reference 8, p. 372). The Anderson-Darling A^2 normality test consists of the following six steps:

1. The residuals, $X_{(i)}$, are arranged in ascending order,
   $X_{(1)} \leq \cdots \leq X_{(n)}$
2. The standardized values are calculated by using,
   $$y_{(i)} = \frac{X_{(i)} - X_{(avg)}}{S}$$
   where $X_{(avg)}$ is the average of the residual values and S is the standard deviation for the values.
3. P_i for i=1,......,n is calculated by the following formula,
   $$P_i = \Phi(Y_{(i)}) = \int_{-\infty}^{Y_{(i)}} \frac{e^{-t_2^2}}{\sqrt{2\pi}}\, dt$$
   here $\Phi(y)$ represents the cumulative distribution function (cdf) of the standard normal distribution and P_i is the cumulative probability corresponding to the standard value $Y_{(i)}$. The value of P_i can be found from standard normal tables or can be calculated using built in functions of spreadsheet programs such as Excel (i.e., NORMDIST).
4. The Anderson-Darling A^2 statistic is computed using,
   $$A^2 = \sum_{i=1}^{n} \left[(2i-1)\{\log P_i + \log(1-P_{n+1-i})\}/n\right] - n$$
   where log is log base e.
5. The modified statistics is calculated using,
   $A^* = A^2(1.0 + 0.75/n + 2.25/n^2)$

6. The null hypothesis of normality is rejected if A^* exceeds 0.752 at the 0.05 significance level.

The standardized residuals calculated in step 2 above as a function of AENCF are shown in Figure A.I-1.

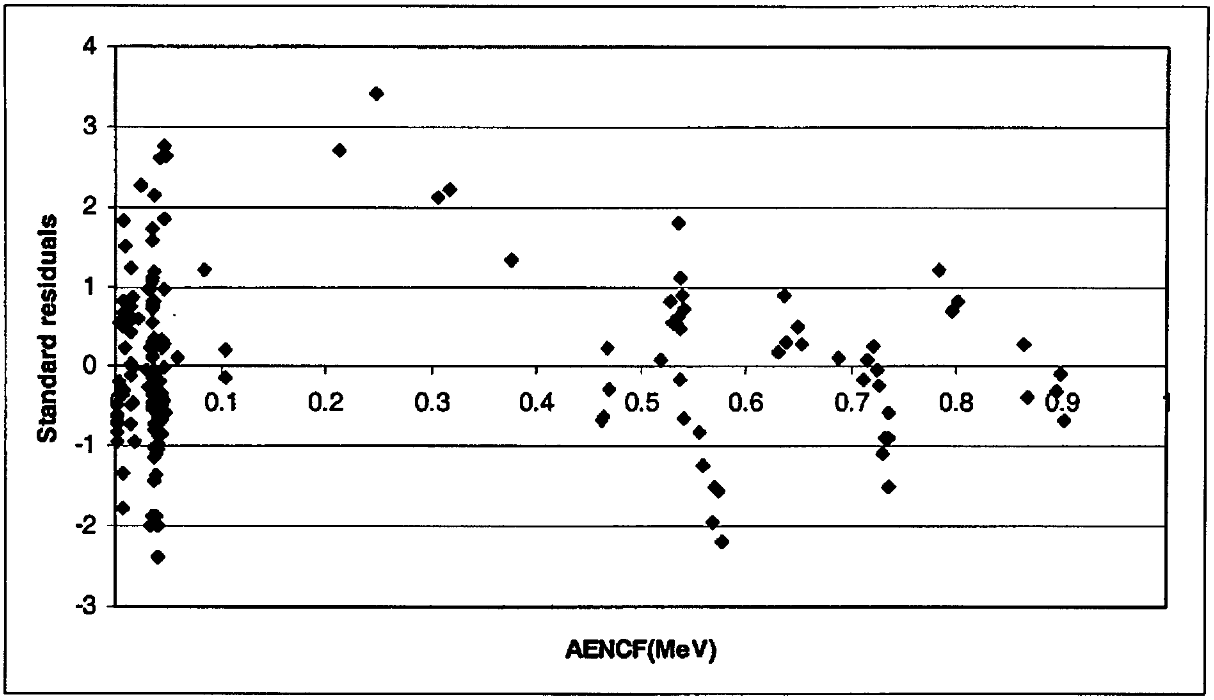

Figure A.I-1. Plot of Standardized Residuals for HEU Cases.

The Anderson-Darling A^2 test for the residuals results in $A^2 = 1.570$ and $A^* = 1.576$. Since $A^* > 0.752$, the residuals are not normally distributed. Inspection of Figure A.I-1 shows that the residuals do not exhibit a visible pattern. This situation (strong trend parameters and residuals not following a normal distribution) is difficult to be categorized with respect to the validity of the trend. Since the residuals fail only marginally the normality test, the linear trend can be assumed to be valid based on the trending parameters.

As mentioned in the criticality methodology (Section 2), for situations in which a valid trend is identified, the CLReg code (Reference 11) is used to calculate the lower bound tolerance limit. The input to the code consists of the results of the trending analysis (see above) and the initial points (k_{norm} and corresponding AENCF values). The CLReg output was attached to the COLD server ("heuout.csv"). The lower bound tolerance limit calculated by the code is presented in Figure 1 (Section 5.1) and the expression derived using the code calculation is:

f(AENCF) = 0.970611 for 0 MeV<AENCF < 0.247 MeV

f(AENCF) = -1.7411e-02*AENCF +0.97491 for 0.247 MeV ≤AENCF < 0.902 MeV

ATTACHMENT II: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing IEU

This attachment presents additional information about the steps performed (Section 5.2) in the calculation of the lower bound tolerance limit including trending analysis and normality tests. The purpose is to provide to the individual reviewer all information necessary to replicate the current results by developing spreadsheets (in Excel or similar commercial software) independent of the originator. The k_{eff} data set used in this calculation contains the k_{eff} values calculated with MCNP for the critical benchmark experiments selected for external configurations containing IEU (Table 8, Section 5.2). The data set for the benchmark cases relevant to external configurations containing IEU has a size of n=109 cases.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} value calculated with MCNP (k_{calc}) was done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations. These values are included in Table A.II-1 together with the data from Table 8.

Table A.II-1. Summary of k_{eff} Data on Criticality Benchmark Experiments for External Configurations Containing IEU

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
iect101	0.9974	0.0009	1.0000	0.0040	0.9974	0.2168
iect102	0.996	0.0009	1.0000	0.0040	0.996	0.1582
iect103	0.9931	0.001	1.0000	0.0040	0.9931	0.1041
iect104	0.9974	0.0011	1.0000	0.0040	0.9974	0.0741
iect105	1.0085	0.0009	1.0000	0.0040	1.0085	0.0455
iect106	1.0003	0.001	1.0000	0.0040	1.0003	0.1079
iect107	0.998	0.001	1.0000	0.0040	0.998	0.1106
iect108	0.996	0.001	1.0000	0.0040	0.996	0.1187
iect109	1.0004	0.0008	1.0000	0.0040	1.0004	0.1679
iect110	0.9967	0.001	1.0000	0.0040	0.9967	0.1576
iect111	0.9958	0.001	1.0000	0.0040	0.9958	0.1573
iect112	0.9964	0.001	1.0000	0.0040	0.9964	0.1557
iect113	0.9967	0.001	1.0000	0.0040	0.9967	0.0743
iect114	0.9979	0.0009	1.0000	0.0040	0.9979	0.0738
iect115	0.9981	0.001	1.0000	0.0040	0.9981	0.0740
iect116	1.0021	0.0009	1.0000	0.0040	1.0021	0.0555
iect117	0.9965	0.001	1.0000	0.0040	0.9965	0.2081
iect118	0.9976	0.0011	1.0000	0.0040	0.9976	0.1343
iect119	1.0045	0.001	1.0000	0.0040	1.0045	0.0611
iect120	1.0005	0.0009	1.0000	0.0040	1.0005	0.1554
iect121	0.9988	0.0009	1.0000	0.0040	0.9988	0.2133
iect122	0.999	0.0011	1.0000	0.0040	0.999	0.1977
iect123	0.9952	0.0011	1.0000	0.0040	0.9952	0.1283

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
iect124a	1.0004	0.0011	1.0000	0.0040	1.0004	0.1331
iect125	0.9987	0.0009	1.0000	0.0040	0.9987	0.0599
iect126	1.0044	0.001	1.0000	0.0040	1.0044	0.0566
iect127	1.0032	0.0009	1.0000	0.0040	1.0032	0.0563
iect128	1.0051	0.0009	1.0000	0.0040	1.0051	0.1582
iect129	1.0012	0.001	1.0000	0.0040	1.0012	0.1518
case2	0.9807	0.0004	0.9800	0.0030	1.000714	0.4823
case3	1.0158	0.0005	1.0140	0.0060	1.001775	0.2598
lst3-1	0.9993	0.0004	0.9997	0.0039	0.9996	0.0186
lst3-2	0.9971	0.00038	0.9993	0.0042	0.997798	0.0166
lst3-3	1.0015	0.00037	0.9995	0.0042	1.002001	0.0164
lst3-4	0.9954	0.00038	0.9995	0.0042	0.995898	0.0162
lst3-5	0.999	0.00031	0.9997	0.0048	0.9993	0.0133
lst3-6	0.9992	0.0003	0.9999	0.0049	0.9993	0.0129
lst3-7	0.9972	0.0003	0.9994	0.0049	0.997799	0.0127
lst3-8	1.0008	0.00025	0.9993	0.0052	1.001501	0.0114
lst3-9	0.9973	0.00025	0.9996	0.0052	0.997699	0.0114
lst4_1	1.0029	0.0007	0.9994	0.0008	1.003502	0.0188
lst4_29	1.0034	0.0006	0.9999	0.0009	1.0035	0.0179
lst4_33	1.0013	0.0007	0.9999	0.0009	1.0014	0.0170
lst4_34	1.0037	0.0006	0.9999	0.0010	1.0038	0.0157
lst4_46	1.0032	0.0006	0.9999	0.0010	1.0033	0.0154
lst4_51	1.0023	0.0005	0.9994	0.0011	1.002902	0.0148
lst4_54	1.0026	0.0005	0.9996	0.0011	1.003001	0.0142
leust7_1	0.9966	0.0002	0.9961	0.0009	1.000502	0.0200
leust7_2	0.9995	0.0002	0.9973	0.0009	1.002206	0.0187
leust7_3	0.9979	0.0002	0.9985	0.0010	0.999399	0.0173
leust7_4	1.0005	0.0002	0.9988	0.0011	1.001702	0.0166
leust7_5	0.9989	0.0002	0.9983	0.0011	1.000601	0.0159
lst8_72	1.0038	0.0002	0.9999	0.0014	1.0039	0.0152
lst8_74	1.0023	0.0002	1.0002	0.0015	1.0021	0.0154
lst8_76	1.0028	0.0002	0.9999	0.0014	1.0029	0.0153
lst8_78	1.004	0.0002	0.9999	0.0014	1.0041	0.0153
lst9_92	1.0018	0.0005	0.9998	0.0014	1.002	0.0155
lst9_93	1.0021	0.0002	0.9999	0.0014	1.0022	0.0157
lst9_94	1.0022	0.0002	0.9999	0.0014	1.0023	0.0158
lst10_83	1.0023	0.0003	0.9999	0.0153	1.0024	0.0153
lst10_85	1.0019	0.0003	0.9999	0.0154	1.002	0.0154
lst10_86	1.0032	0.0003	1.0000	0.0153	1.0032	0.0153
lst10_88	1.0026	0.0003	1.0001	0.0154	1.0025	0.0154
lst16_05	1.0093	0.0007	0.9996	0.0013	1.009704	0.0267
lst16_13	1.008	0.0006	0.9999	0.0013	1.008101	0.0248
lst16_25	1.0075	0.0006	0.9994	0.0014	1.008105	0.0216
lst16_29	1.0068	0.0006	0.9996	0.0014	1.007203	0.0209
lst16_31	1.0059	0.0005	0.9995	0.0014	1.006403	0.0195
lst16_40	1.0043	0.0005	0.9992	0.0015	1.005104	0.0186

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
lst16_96	1.0047	0.0005	0.9994	0.0015	1.005303	0.0180
lst17_04	1.0051	0.0007	0.9981	0.0013	1.007013	0.0275
lst17_22	1.0049	0.0006	0.9986	0.0013	1.006309	0.0258
lst17_23	1.0052	0.0006	0.9989	0.0014	1.006307	0.0224
lst17_26	1.0043	0.0006	0.9992	0.0014	1.005104	0.0212
lst17_30	1.0043	0.0005	0.9987	0.0015	1.005607	0.0200
lst17_47	1.0042	0.0006	0.9996	0.0015	1.004602	0.0192
RUN133	1.0033	0.0002	0.9992	0.0010	1.004103	0.0183
RUN142	1.0042	0.0003	0.9996	0.0010	1.004602	0.0187
RUN143	1.0045	0.0003	0.9996	0.0010	1.004902	0.0188
RUN144	1.0033	0.0003	0.9997	0.0010	1.003601	0.0187
RUN145	1.0038	0.0003	0.9992	0.0010	1.004604	0.0187
RUN146	1.0037	0.0003	0.9996	0.0010	1.004102	0.0186
RUN149	1.0043	0.0003	0.9997	0.0009	1.004601	0.0190
RUN150	1.0043	0.0003	0.9995	0.0009	1.004802	0.0190
RUN151	1.0049	0.0002	0.9999	0.0009	1.005001	0.0191
RUN152	1.0054	0.0003	0.9996	0.0009	1.005802	0.0191
RUN153	1.005	0.0003	0.9998	0.0009	1.005201	0.0191
RUN183	1.0036	0.0003	0.9994	0.0009	1.004203	0.0189
LST20C1	1.0014	0.0003	0.9995	0.0010	1.001901	0.0150
LST20C2	1	0.0003	0.9996	0.0010	1.0004	0.0143
LST20C3	0.9993	0.0003	0.9997	0.0012	0.9996	0.0131
LST20C4	1.0004	0.0003	0.9998	0.0012	1.0006	0.0125
LST21C1	0.9991	0.0003	0.9983	0.0009	1.000801	0.0154
LST21C2	0.9996	0.0003	0.9985	0.0010	1.001102	0.0144
LST21C3	0.9976	0.0003	0.9989	0.0011	0.998699	0.0135
LST21C4	0.9999	0.0003	0.9993	0.0012	1.0006	0.0127
case1	1.0049	0.0002	0.9999	0.0010	1.005001	0.0185
case2	1.0058	0.0002	0.9994	0.0010	1.006404	0.0184
case3	1.0055	0.0002	0.9993	0.0010	1.006204	0.0185
case4	1.005	0.0002	0.9994	0.0010	1.005603	0.0186
261	1.0000	0.0005	0.9963	0.0009	1.003714	0.0175
274	0.9986	0.0005	0.9967	0.0009	1.001906	0.0177
273	0.999	0.0005	0.9967	0.0009	1.002308	0.0176
262	0.9992	0.0005	0.9960	0.0009	1.003213	0.0175
263	0.9993	0.0005	0.9959	0.0009	1.003414	0.0177
264	0.9996	0.0005	0.9959	0.0009	1.003715	0.0177
267	0.9997	0.0005	0.9966	0.0009	1.003111	0.0178
268	1.0000	0.0005	0.9970	0.0009	1.003009	0.0179
269	0.995	0.0005	0.9977	0.0009	0.997294	0.0177

The set of normalized k_{eff} values is first tested for trending against the spectral parameter AENCF (e.g., average energy of a neutron causing fission) using the build-in regression analysis tool from the Excel software.

The linear regression is performed using the regression tool from Excel's menu by selecting the normalized k_{eff} (k_{norm}) as the "y" variable and the AENCF values as "x" variable. The full output of the regression tool contains statistics regarding validity of a trend, such as R^2, Standard Error, t stat, etc. , and is given below.

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.413220205
R Square	0.170750938
Adjusted R Square	0.163000946
Standard Error	0.003052808
Observations	109

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.000205	0.000205334	22.032404	7.98E-06
Residual	107	0.000997	9.31964E-06		
Total	108	0.001203			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.002968524	0.000363	2764.473515	1.605E-261	1.002249	1.003688
X Variable 1	-0.019394427	0.004132	-4.693868764	7.982E-06	-0.02759	-0.0112

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 13 (Section 5.2). Since the absolute value of t-stat (renamed T in Table 13) is greater than $t_{0.025,107}$ and P-value is very low, the linear trend seems to be valid (Section 2). In a second step, the assumptions used in deriving the linear model are verified. For a valid trend the residuals (see Section 2) need to be normally distributed and with a mean of 0. The residuals are calculated by the regression tool in Excel (corresponding option need to be activated at the beginning of the process). Normality test of residuals is performed by applying the Anderson-Darling A^2 test (Reference 8, p. 372). The Anderson-Darling A^2 normality test consists of the following six steps:

1. The residuals, $X_{(i)}$, are arranged in ascending order,
   $X_{(1)} \le \cdots \le X_{(n)}$
2. The standardized values are calculated by using,
   $$y_{(i)} = \frac{X_{(i)} - X_{(avg)}}{S}$$
   where $X_{(avg)}$ is the average of the residual values and S is the standard deviation for the values.

3. P_i for i=1,......,n is calculated by the following formula,

   $$P_i = \Phi(Y_{(i)}) = \int_{-\infty}^{Y_{(i)}} \frac{e^{-\frac{t^2}{2}}}{\sqrt{2\pi}}\, dt$$

   here $\Phi(y)$ represents the cumulative distribution function (cdf) of the standard normal distribution and P_i is the cumulative probability corresponding to the standard value $Y_{(i)}$. The value of P_i can be found from standard normal tables or can be calculated using built in functions of spreadsheet programs such as Excel (i.e., NORMDIST).
4. The Anderson-Darling A^2 statistic is computed using,

   $$A^2 = \sum_{i=1}^{n} \left[(2i-1)\{\log P_i + \log(1-P_{n+1-i})\}/n\right] - n$$

   where log is log base e.
5. The modified statistics is calculated using,

   $$A^* = A^2(1.0 + 0.75/n + 2.25/n^2)$$
6. The null hypothesis of normality is rejected if A^* exceeds 0.752 at the 0.05 significance level.

The standardized residuals calculated in step 2 above as a function of AENCF are shown in Figure A.II-1.

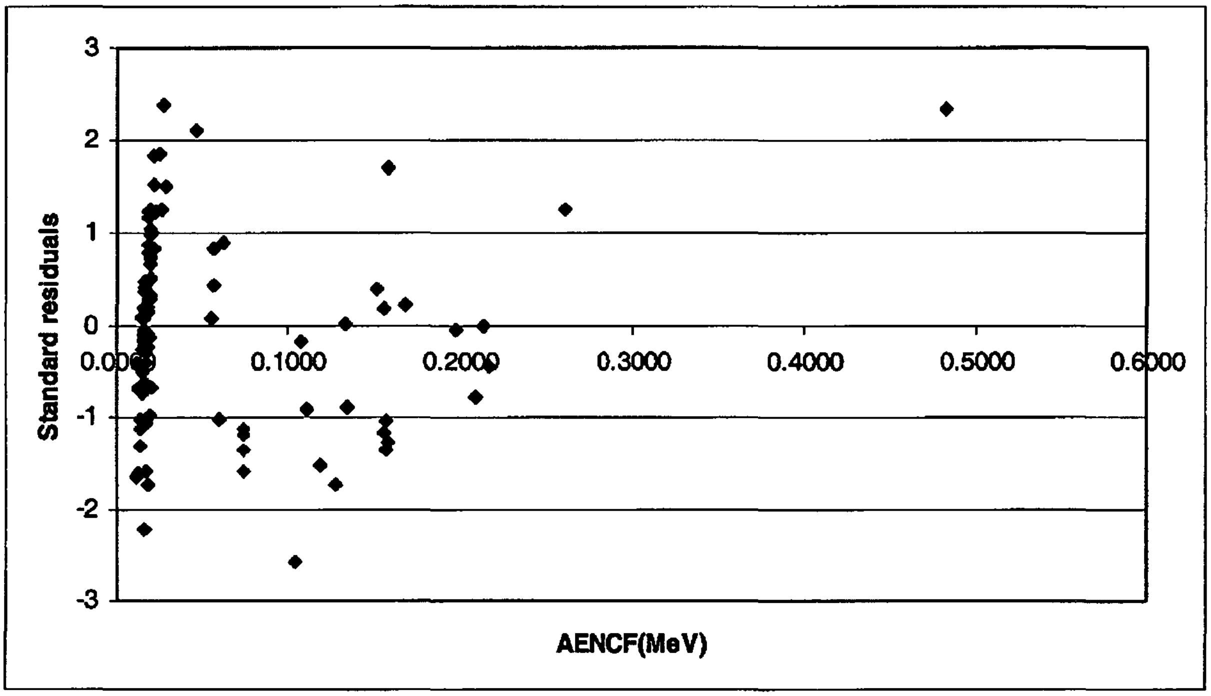

Figure A.II-1. Plot of Standardized Residuals for IEU Cases.

The Anderson-Darling A^2 test for the residuals results in $A^2 = 0.292579$ and A^* is 0.294648. *Since* $A^* < 0.752$, the residuals are considered to be normally distributed. Inspection of Figure A.II-1 shows that the residuals do not exhibit a visible pattern. This confirms the validity of the linear trend. As mentioned in the criticality methodology (Section 2), for situations in which a valid trend is identified, the CLReg code (Reference 11) is used to calculate the lower bound tolerance limit. The input to the code consists of the results of the trending analysis (see above) and the initial points (k_{norm} and corresponding AENCF values). The CLReg output was attached to the COLD server ("ieuout.csv"). The lower bound tolerance limit calculated by the code is presented in Figure 2 (Section 5) and the expression derived using the code calculation is:

f(AENCF) = 0.97841 for 0 MeV < AENCF < 0.1518 MeV

f(AENCF) = -1.9322e-02*AENCF +0.981339 for 0.1518 MeV ≤ AENCF < 0.482 MeV

ATTACHMENT III: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing LEU

This attachment presents additional information about the steps performed (Section 5.3) in the calculation of the lower bound tolerance limit including trending analysis and normality tests. The purpose is to provide to the individual reviewer all information necessary to replicate the current results by developing spreadsheets (in Excel or similar commercial software) independent of the originator. The k_{eff} data set used in this calculation contains the k_{eff} values calculated with MCNP for the critical benchmark experiments selected for external configurations containing LEU (Table 14, Section 5.3). The data set for the benchmark cases relevant to external configurations containing LEU has a size of n=96 cases.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} values calculated with MCNP (k_{calc}) was done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations. These values are included in Table A.III-1 together with the data from Table 14.

Table A.III-1. Summary of k_{eff} Data on Criticality Benchmark Experiments for External Configurations Containing LEU

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
case1	0.99453	0.00068	1.0000	0.0038	0.99453	0.179092
case2	0.99593	0.0007	1.0000	0.0038	0.99593	0.179193
case3	0.99651	0.0007	1.0000	0.0038	0.99651	0.17891
case4	0.99569	0.0006	1.0000	0.0038	0.99569	0.17934
case5	0.99926	0.00069	1.0000	0.0039	0.99926	0.137899
case6	1.00022	0.00068	1.0000	0.0039	1.00022	0.137597
case7	0.99832	0.00063	1.0000	0.0039	0.99832	0.137109
case8	0.99708	0.00061	1.0000	0.004	0.99708	0.111351
case9	0.99565	0.00064	1.0000	0.004	0.99565	0.111882
case10	0.99695	0.00064	1.0000	0.0039	0.99695	0.097349
case11	0.99626	0.00063	1.0000	0.0039	0.99626	0.097201
case12	0.99634	0.00065	1.0000	0.0039	0.99634	0.097292
case13	0.99734	0.00065	1.0000	0.0041	0.99734	0.083965
case14	0.99046	0.00073	1.0000	0.0051	0.99046	0.061911
case15	0.99152	0.00077	1.0000	0.0051	0.99152	0.062286
case16	0.99172	0.00072	1.0000	0.0051	0.99172	0.061676
case17	1.00483	0.00073	1.0000	0.0038	1.00483	0.165691
case18	1.00517	0.00074	1.0000	0.0038	1.00517	0.166474
case19	1.00584	0.00071	1.0000	0.0038	1.00584	0.165731
case20	1.00408	0.00082	1.0000	0.0038	1.00408	0.165721
case21	1.00606	0.00084	1.0000	0.0038	1.00606	0.165046
case22	1.00781	0.00066	1.0000	0.0039	1.0078	0.10147
case23	0.99456	0.00073	1.0000	0.004	0.99456	0.195172
case24	0.99488	0.00076	1.0000	0.004	0.99488	0.19449

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
case25	0.99499	0.00072	1.0000	0.004	0.99499	0.195342
case26	0.99848	0.00074	1.0000	0.0039	0.99848	0.150337
case27	0.99915	0.0007	1.0000	0.0039	0.99915	0.150325
case28	0.9973	0.00068	1.0000	0.0039	0.9973	0.150245
case29	0.9993	0.0007	1.0000	0.0039	0.9993	0.150311
case30	0.99698	0.00072	1.0000	0.0039	0.99698	0.120376
case31	0.99813	0.00085	1.0000	0.0039	0.99813	0.119854
case32	0.99729	0.00083	1.0000	0.0039	0.99729	0.120769
case33	0.99549	0.00082	1.0000	0.0039	0.99549	0.120941
case34	0.99601	0.0017	1.0000	0.0039	0.99601	0.120485
case35	0.99654	0.0019	1.0000	0.004	0.99654	0.104687
case36	0.99628	0.0019	1.0000	0.004	0.99628	0.104872
case37	0.99502	0.0019	1.0000	0.004	0.99502	0.104679
case38	0.99636	0.0017	1.0000	0.004	0.99636	0.104449
case39	0.99639	0.0017	1.0000	0.004	0.99639	0.104691
case40	0.99539	0.00093	1.0000	0.004	0.99539	0.104928
case41	0.99649	0.00125	1.0000	0.0041	0.99649	0.090072
case42	0.99545	0.00131	1.0000	0.0041	0.99545	0.089601
case43	0.99459	0.00142	1.0000	0.0041	0.99459	0.089044
case44	0.99125	0.00134	1.0000	0.005	0.99125	0.064508
case45	0.99082	0.00086	1.0000	0.005	0.99082	0.063726
case46	0.98932	0.00085	1.0000	0.005	0.98932	0.064482
case47	1.01095	0.0008	1.0000	0.0042	1.01095	0.188002
case48	1.00649	0.00086	1.0000	0.0042	1.00649	0.187807
case49	1.00631	0.00079	1.0000	0.0042	1.00631	0.188944
case50	1.00952	0.00086	1.0000	0.0041	1.00952	0.113964
case51	1.01266	0.00083	1.0000	0.0041	1.01266	0.114597
case52	1.00759	0.00083	1.0000	0.0041	1.00759	0.11478
lct49-01	0.9923	0.0006	1.0000	0.0034	0.9923	0.294
lct49-02	0.9937	0.0006	1.0000	0.0034	0.9937	0.293
lct49-03	0.9929	0.0006	1.0000	0.0034	0.9929	0.297
lct49-04	0.9931	0.0006	1.0000	0.0034	0.9931	0.3
lct49-05	0.9944	0.0007	1.0000	0.0042	0.9944	0.255
lct49-06	0.9946	0.0007	1.0000	0.0042	0.9946	0.256
lct49-07	0.9932	0.0007	1.0000	0.0042	0.9932	0.253
lct49-08	0.9921	0.0007	1.0000	0.0042	0.9921	0.258
lct49-09	0.9933	0.0006	1.0000	0.0037	0.9933	0.227
lct49-10	0.9946	0.0007	1.0000	0.0037	0.9946	0.227
lct49-11	0.9933	0.0006	1.0000	0.0037	0.9933	0.227
lct49-12	0.9924	0.0007	1.0000	0.0037	0.9924	0.231
lct49-13	0.9935	0.0006	1.0000	0.0036	0.9935	0.271
lct49-14	0.9941	0.0006	1.0000	0.0036	0.9941	0.272
lct49-15	0.9937	0.0006	1.0000	0.0036	0.9937	0.271
lct49-16	0.9938	0.0007	1.0000	0.0036	0.9938	0.254
lct49-17	0.9929	0.0007	1.0000	0.0036	0.9929	0.258
lct49-18	0.997	0.0006	1.0000	0.003	0.997	0.251

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
leust1	1.01182	0.00101	0.9991	0.0029	1.012731	0.05186
leust21	0.99855	0.00058	1.0038	0.004	0.99477	0.02513
leust22	0.99659	0.00064	1.0024	0.0037	0.994204	0.0283
leust23	1.0009	0.0006	1.0024	0.0044	0.998504	0.02684
lst3-1	0.9993	0.0004	0.9997	0.0039	0.9996	0.0186
lst3-2	0.9971	0.00038	0.9993	0.0042	0.997798	0.0166
lst3-3	1.0015	0.00037	0.9995	0.0042	1.002001	0.0164
lst3-4	0.9954	0.00038	0.9995	0.0042	0.995898	0.0162
lst3-5	0.999	0.00031	0.9997	0.0048	0.9993	0.0133
lst3-6	0.9992	0.0003	0.9999	0.0049	0.9993	0.0129
lst3-7	0.9972	0.0003	0.9994	0.0049	0.997799	0.0127
lst3-8	1.0008	0.00025	0.9993	0.0052	1.001501	0.0114
lst3-9	0.9973	0.00025	0.9996	0.0052	0.997699	0.0114
lst8_72	1.0038	0.0002	0.9999	0.0014	1.0039	0.0152
lst8_74	1.0023	0.0002	1.0002	0.0015	1.0021	0.0154
lst8_76	1.0028	0.0002	0.9999	0.0014	1.0029	0.0153
lst8_78	1.004	0.0002	0.9999	0.0014	1.0041	0.0153
lst9_92	1.0018	0.0005	0.9998	0.0014	1.002	0.0155
lst9_93	1.0021	0.0002	0.9999	0.0014	1.0022	0.0157
lst9_94	1.0022	0.0002	0.9999	0.0014	1.0023	0.0158
RUN133	1.0033	0.0002	0.9992	0.001	1.004103	0.0183
RUN142	1.0042	0.0003	0.9996	0.001	1.004602	0.0187
RUN143	1.0045	0.0003	0.9996	0.001	1.004902	0.0188
RUN144	1.0033	0.0003	0.9997	0.001	1.003601	0.0187
RUN145	1.0038	0.0003	0.9992	0.001	1.004604	0.0187
RUN146	1.0037	0.0003	0.9996	0.001	1.004102	0.0186

The set of normalized k_{eff} values is first tested for trending against the spectral parameter AENCF (e.g., average energy of a neutron causing fission) using the build-in regression analysis tool from the Excel software.

The linear regression is performed using the regression tool from Excel's menu by selecting the normalized k_{eff} (k_{norm}) as the y variable and the AENCF values as x variable. The full output of the regression tool contains statistics regarding validity of a trend, such as the coefficient of determination (r^2), standard error, t stat, etc., and is given below:

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.342757487
R Square	0.117482695
Adjusted R Square	0.108094213
Standard Error	0.004940048
Observations	96

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.000305	0.000305	12.51349	0.00063
Residual	94	0.002294	2.44E-05		
Total	95	0.002599			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.000851516	0.000875	1144.08	1.4E-196	0.999115	1.002588
X Variable 1	-0.02056151	0.005813	-3.53744	0.00063	-0.0321	-0.00902

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 17 (Section 5.3). Since the coefficient of determination (r^2) is low and the absolute value of t-stat (renamed T in Table 17) is greater than $t_{0.025,94}$, the linear trend is debatable and an analysis of the residuals is necessary.

For a valid trend, the residuals (see Section 2) need to be normally distributed and with a mean of 0. The residuals are calculated by the regression tool in Excel (corresponding option need to be activated at the beginning of the process). Normality test of residuals is performed by applying the Anderson-Darling A^2 test (Reference 8, p. 372). The Anderson-Darling A^2 normality test consists of the following six steps:

1. The residuals, $X_{(i)}$, are arranged in ascending order,
   $X_{(1)} \le \cdots \le X_{(n)}$
2. The standardized values are calculated by using,
   $$y_{(i)} = \frac{X_{(i)} - X_{(avg)}}{S}$$
   where $X_{(avg)}$ is the average of the residual values and S is the standard deviation for the values.
3. P_i for i=1,......,n is calculated by the following formula,
   $$P_i = \Phi(Y_{(i)}) = \int_{-\infty}^{Y_{(i)}} \frac{e^{-t_2^2}}{\sqrt{2\pi}}\,dt$$
   here $\Phi(y)$ represents the cumulative distribution function (cdf) of the standard normal distribution and P_i is the cumulative probability corresponding to the standard value $Y_{(i)}$. The value of P_i can be found from standard normal tables or can be calculated using built in functions of spreadsheet programs such as Excel (i.e., NORMDIST).
4. The Anderson-Darling A^2 statistic is computed using,
   $$A^2 = \sum_{i=1}^{n} [(2i-1)\{\log P_i + \log(1-P_{n+1-i})\}/n] - n$$
   where log is log base e.
5. The modified statistics is calculated using,
   $A^* = A^2(1.0 + 0.75/n + 2.25/n^2)$

6. The null hypothesis of normality is rejected if A^* exceeds 0.752 at the 0.05 significance level.

The standardized residuals calculated in step 2 above as a function of AENCF are shown in Figure A.III-1.

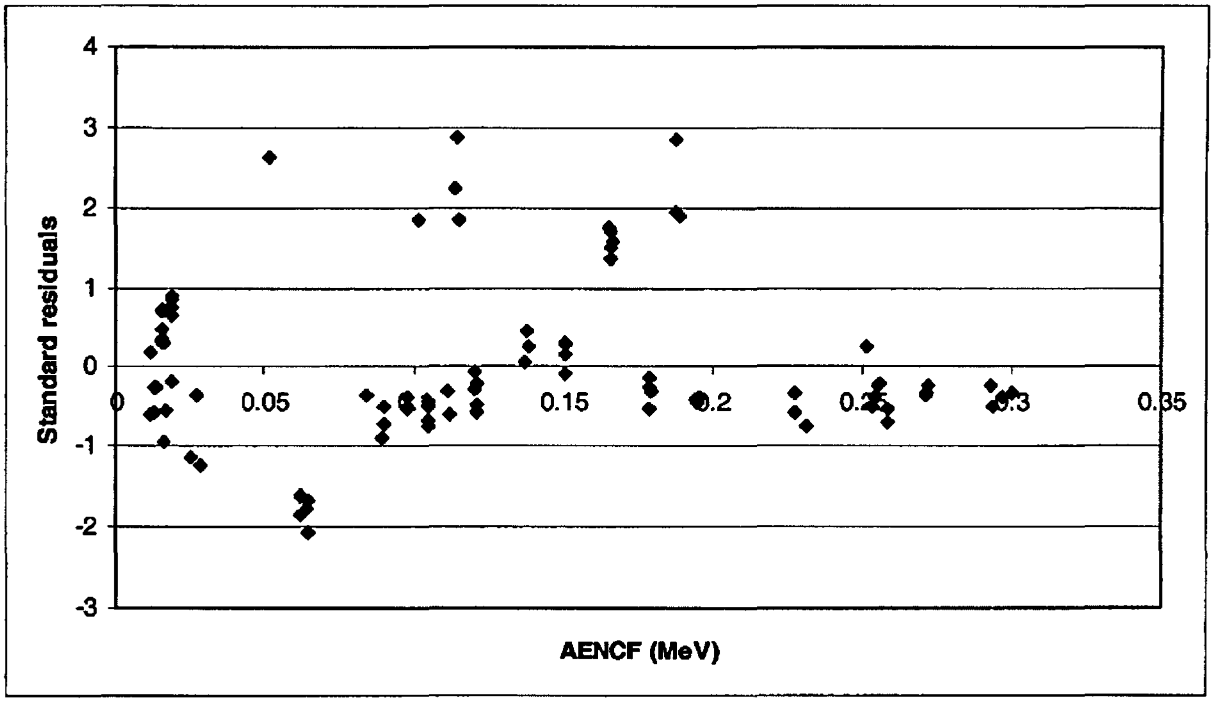

Figure A.III-1. Plot of Standardized Residuals for LEU Cases.

The Anderson-Darling A^2 test for the residuals results in $A^2 = 3.516$ and $A^* = 3.544$. Since $A^* > 0.752$, the residuals are not normally distributed. Inspection of Figure A.III-1 shows that the residuals are not evenly distributed by exhibiting a visible pattern. Both these results, together with the weak trending parameters identified earlier indicate that the linear trending is not valid.

Since no trend with AENCF could be identified, according to the methodology presented in Section 2, an Anderson-Darling A^2 test is performed on the normalized k_{eff} values. The calculation steps are similar to the one outlined above for the residuals the only difference being that the normalized k_{eff} values are used instead of the residuals.

The Anderson-Darling A^2 test for the pool of k_{eff} data results in $A^2 = 1.854$ and A^* is 1.869. The pool of data is not normal because $A^* > 0.752$. Since the set of values is not normally distributed the non-parametric distribution free tolerance limit (DFTL) applies (Section 2). Based on Equation 6, the percent confidence that 95% of the keff population is above the lowest value observed is $\beta = 99.3\%$. Using the data from Table 2, the non-parametric margin (NPM) is 0 for this particular situation.

The lower bound tolerance limit (LBTL) is defined as (see Equation 7, Section 2):

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM)
where:

Based on the values given in Table A.III-1 the minimum normalized k_{eff} is 0.9893. Since the smallest k_{eff} is less than 1 the total (code run combined with benchmark) sigma associated with this k_{eff} is used which is $0.0051 = (0.005^2+0.00085^2)^{1/2}$. Due to the size of the data pool the NPM is zero as showed above. The lower bound tolerance limit is calculated as:

LBTL = f = 0.9893 - 0.0051=0.9842

ATTACHMENT IV: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing Uranium and Plutonium Fissile Isotopes

This attachment presents additional information about the steps performed (Section 5.4) in the calculation of the lower bound tolerance limit including trending analysis and normality tests. The purpose is to provide to an individual reviewer all information necessary to replicate the current results by developing spreadsheets (in Excel or similar commercial software) independent of the originator. The k_{eff} data set used in this calculation contains the k_{eff} values calculated with MCNP for the critical benchmark experiments selected for external configurations containing uranium and plutonium fissile isotopes (Table 18, Section 5.4). The data set for the benchmark cases relevant to external configurations containing mixed uranium and plutonium has a size of n= 120 cases.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} values calculated with MCNP (k_{calc}) was done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations. These values are included in Table A.IV-1 together with the data from Table 18.

Table A.IV-1. Summary of k_{eff} Data on Criticality Benchmark Experiments for External Configurations Containing Uranium and Plutonium Fissile Isotopes

Experiment/Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark-Model k_{eff}	Benchmark Sigma, σ_{exp}	$k_{norm}=k_{calc}/k_{exp}$	AENCF (MeV)
c1_mc50	0.97642	0.00071	1.0042	0.0058	0.972336	0.070929
c2_mc50	0.97698	0.0007	1.0042	0.0058	0.972894	0.071208
c3_mc50	0.97429	0.0007	1.0042	0.0058	0.970215	0.070838
c4_mc50	0.98038	0.00067	1.0042	0.0058	0.97628	0.070862
c5_mc50	0.97563	0.00069	1.0042	0.0058	0.971549	0.071014
c6_mc50	0.98054	0.00072	1.0042	0.0058	0.976439	0.07137
c7_mc50	1.03527	0.00063	1.0023	0.0036	1.032894	0.026793
c8_mc50	1.03085	0.00061	1.0023	0.0036	1.028484	0.026382
c9_mc50	1.02805	0.00064	1.0023	0.0036	1.025691	0.026685
c10_mc50	1.02766	0.00064	1.0023	0.0036	1.025302	0.026786
c11_mc50	1.02639	0.00063	1.0023	0.0036	1.024035	0.026489
c12_mc50	1.02873	0.00065	1.0023	0.0036	1.026369	0.026623
c13_mc50	1.03723	0.00065	1.0023	0.0036	1.03485	0.0266
c14_mc50	1.02308	0.00073	1.0002	0.0027	1.022875	0.046391
c15_mc50	1.02342	0.00077	1.0002	0.0027	1.023215	0.04644
c16_mc50	1.01943	0.00072	1.0002	0.0027	1.019226	0.0463
c17_mc50	1.01881	0.00073	1.0002	0.0027	1.018606	0.045704
c18_mc50	1.01723	0.00074	1.0002	0.0027	1.017027	0.045911
c19_mc50	1.01673	0.00071	1.0002	0.0027	1.016527	0.045601
c20_mc50	1.01733	0.00082	1.0004	0.0037	1.016923	0.057147
c21_mc50	1.01595	0.00084	1.0004	0.0037	1.015544	0.058073
c22_mc50	1.0129	0.00081	1.0004	0.0037	1.012495	0.057085

c23_mc50	1.01078	0.00073	0.9997	0.0049	1.011083	0.038802
c24_mc50	1.0122	0.00076	0.9997	0.0049	1.012504	0.038649
c25_mc50	1.01115	0.00072	0.9997	0.0049	1.011453	0.038387
c26_mc50	1.00919	0.00074	0.9997	0.0049	1.009493	0.038186
c27_mc50	1.0089	0.0007	0.9997	0.0049	1.009203	0.037983
c28_mc50	1.01042	0.00068	0.9997	0.0049	1.010723	0.03806
c29_mc50	1.01129	0.0007	0.9997	0.0049	1.011593	0.037569
c30_mc50	1.009	0.00072	0.9997	0.0049	1.009303	0.03793
c31_mc50	0.99634	0.00085	1.0007	0.0052	0.995643	0.049337
c32_mc50	0.99696	0.00083	1.0007	0.0052	0.996263	0.049016
c33_mc50	0.99349	0.00082	1.0007	0.0052	0.992795	0.049798
81-1-B5	1.00028	0.0017	1.0002	0.0037	1.00008	0.456722
81-1AB5	0.99907	0.0019	1.0002	0.0032	0.99887	0.45051
81-2-B5	1.00399	0.0019	1.0005	0.0025	1.003488	0.379954
81-3-b5	1.00939	0.0019	1.0000	0.0025	1.00939	0.340488
81-4-b5	1.01653	0.0017	1.0001	0.0025	1.016428	0.217775
81-5-b5	1.01628	0.0017	1.0003	0.0025	1.015975	0.214455
case1	1.02857	0.00093	0.9986	0.0041	1.030012	1.701859
case2	1.01876	0.00125	1.0000	0.0068	1.01876	0.633149
case3	1.01495	0.00131	0.999	0.0067	1.015966	0.275288
case4	0.98531	0.00142	1.0000	0.0066	0.98531	0.287764
case5	1.00838	0.00134	0.9989	0.0072	1.00949	0.099934
case1	1.03181	0.00086	0.999	0.0046	1.032843	1.045771
case2	1.03092	0.00085	0.999	0.0046	1.031952	1.030255
case3	1.02529	0.0008	0.999	0.0046	1.026316	1.008902
case4	1.01988	0.00086	0.999	0.0046	1.020901	0.980677
case5	1.01394	0.00079	0.999	0.0046	1.014955	0.943255
case6	1.01683	0.00086	1.0000	0.0075	1.01683	0.437694
case7	1.01826	0.00083	1.0000	0.0075	1.01826	0.433389
case8	1.01765	0.00083	1.0000	0.0075	1.01765	0.423376
case9	1.01892	0.0009	1.0000	0.0075	1.01892	0.413717
case10	1.02824	0.00086	1.0000	0.0073	1.02824	0.183574
case11	1.02481	0.00089	1.0000	0.0073	1.02481	0.187186
case12	1.02504	0.00083	1.0000	0.0073	1.02504	0.191855
case13	1.02196	0.00097	1.0000	0.0073	1.02196	0.193165
case14	1.0268	0.00092	1.0000	0.0073	1.0268	0.193259
case15	1.02238	0.0009	1.0000	0.0073	1.02238	0.193815
case16	1.01882	0.00089	1.0000	0.0073	1.01882	0.191721
case17	1.00622	0.00086	0.9988	0.0055	1.007429	0.196312
case18	1.00713	0.00083	0.9988	0.0055	1.00834	0.204026
case19	1.00682	0.00088	0.9988	0.0055	1.00803	0.204044
case20	1.00782	0.00092	0.9988	0.0055	1.009031	0.205974
case21	1.00749	0.00089	0.9988	0.0055	1.0087	0.206285
case22	1.01175	0.00087	0.9988	0.0055	1.012966	0.203775
case23	1.00579	0.0009	1.0000	0.0068	1.00579	0.076988
case24	1.00895	0.00088	1.0000	0.0068	1.00895	0.076998
case25	1.00813	0.0009	1.0000	0.0068	1.00813	0.077666
case26	1.01027	0.00095	1.0000	0.0068	1.01027	0.077373
case27	1.00895	0.00089	1.0000	0.0068	1.00895	0.077622

case28	1.00954	0.00089	1.0000	0.0068	1.00954	0.077736
case29	1.01038	0.00088	1.0000	0.0068	1.01038	0.078493
pnl3187	0.9976	0.0012	1.0000	0.0016	0.9976	0.0417
pnl3391	0.9943	0.0012	1.0000	0.0016	0.9943	0.0411
pnl3492	0.9975	0.0012	1.0000	0.0016	0.9975	0.0431
pnl3593	0.9973	0.0011	1.0000	0.0016	0.9973	0.0459
pnl3694	1.0026	0.0012	1.0000	0.0016	1.0026	0.0445
pnl3795	1.0017	0.0012	1.0000	0.0016	1.0017	0.04
pnl3896	1.0024	0.0012	1.0000	0.0016	1.0024	0.0232
pnl3897	1.0045	0.0011	1.0000	0.0016	1.0045	0.0142
pnl3898	1.0029	0.001	1.0000	0.0016	1.0029	0.0299
pnl3808	1.002	0.0011	1.0000	0.0016	1.002	0.0213
pnl3999	1.0092	0.0011	1.0000	0.0052	1.0092	0.0296
pnl5300	1.008	0.0011	1.0000	0.0052	1.008	0.0288
pnl1158	1.0069	0.0007	1.0000	0.0024	1.0069	0.0038
pnl1159	1.0074	0.0006	1.0000	0.0024	1.0074	0.0037
pnl1161	1.0079	0.0007	1.0000	0.0024	1.0079	0.0061
awre1	1.0147	0.001	0.9985	0.002	1.016224	0.0315
awre2	1.0157	0.0012	0.996	0.002	1.019779	0.0315
awre3	1.012	0.0012	0.9935	0.002	1.018621	0.032
awre4	1.0051	0.0012	0.9909	0.002	1.01433	0.0319
awre5	1.0085	0.001	0.9981	0.0022	1.01042	0.0104
awre6	1.0107	0.001	0.9959	0.0022	1.014861	0.0104
awre7	1.008	0.001	0.9935	0.0022	1.014595	0.0105
awre8	1.0128	0.0008	0.9988	0.0025	1.014017	0.0069
awre9	1.0094	0.0009	0.9958	0.0025	1.013657	0.0066
awre10	1.0102	0.0008	0.9964	0.0025	1.01385	0.0066
pnl1577	0.9958	0.0012	1.0000	0.0033	0.9958	0.0589
pnl1678	0.9974	0.0012	1.0000	0.0033	0.9974	0.0504
pnl1783	0.9992	0.0012	1.0000	0.0078	0.9992	0.0534
pnl1868	1.0039	0.0013	1.0000	0.0078	1.0039	0.0343
pnl1969	1	0.0012	1.0000	0.0033	1	0.0334
pnl2070	0.9996	0.0014	1.0000	0.0033	0.9996	0.0377
pnl2565	1.0015	0.0012	1.0000	0.0033	1.0015	0.0129
pnl2666	1.0018	0.0011	1.0000	0.0033	1.0018	0.0117
pnl2767	1.0061	0.0011	1.0000	0.0078	1.0061	0.0123
msl5-63	0.9877	0.0008	1.0000	0.0037	0.9877	0.013
msl5-64	1.0045	0.0007	1.0000	0.0037	1.0045	0.012
msl5-71	1.0032	0.0008	1.0000	0.0037	1.0032	0.033
msl5-72	1.0001	0.0008	1.0000	0.0037	1.0001	0.032
msl5-74	0.9922	0.0009	1.0000	0.0037	0.9922	0.037
msl5-75	0.9898	0.0009	1.0000	0.0037	0.9898	0.059
msl5-76	0.9974	0.0007	1.0000	0.0037	0.9974	0.049
C1	0.99921	0.00058	1.0000	0.0011	0.99921	0.035197
C2	1.00179	0.00057	1.0000	0.001	1.00179	0.037482
C3	1.00247	0.00053	1.0000	0.0012	1.00247	0.037964
C4	1.00409	0.00048	1.0000	0.0016	1.00409	0.039617
C5	1.00392	0.0005	1.0000	0.0011	1.00392	0.040463

C6	1.00214	0.00049	1.0000	0.0014	1.00214	0.040442

The set of normalized k_{eff} values is tested for trending against the spectral parameter AENCF (e.g., average energy of a neutron causing fission) using the build-in regression analysis tool from the Excel software.

The linear regression is performed using the regression tool from Excel's menu by selecting the normalized k_{eff} (k_{norm}) as the "y" variable and the AENCF values as "x" variable. The full output of the regression tool contains statistics regarding validity of a trend, such as the coefficient of determination (r^2), standard error, t-stat, etc., and is given below:

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.331868938
R Square	0.110136992
Adjusted R Square	0.10259578
Standard Error	0.012443284
Observations	120

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.002261	0.002261	14.60468	0.000213
Residual	118	0.018271	0.000155		
Total	119	0.020532			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.006210407	0.001309	768.9507	3.7E-220	1.003619	1.008802
X Variable 1	0.016779889	0.004391	3.821607	0.000213	0.008085	0.025475

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 21 (Section 5.4). Since the coefficient of determination (r^2) is low and the absolute value of t-stat (renamed T in Table 21) is greater than $t_{0.025,118,}$ the linear trend is debatable and an analysis of the residuals is necessary.

For a valid trend, the residuals (see Section 2) need to be normally distributed and with a mean of 0. The residuals are calculated by the regression tool in Excel (corresponding option need to be activated at the beginning of the process). Normality test of residuals is performed by applying the Anderson-Darling A^2 test (Reference 8, p. 372). The Anderson-Darling A^2 normality test consists of the following six steps:

1. The residuals, $X_{(i)}$, are arranged in ascending order,
   $X_{(1)} \leq \cdots \leq X_{(n)}$

2. The standardized values are calculated by using,

   $$y_{(i)} = \frac{X_{(i)} - X_{(avg)}}{S}$$

   where $X_{(avg)}$ is the average of the residual values and S is the standard deviation for the values.
3. P_i for i=1,......,n is calculated by the following formula,

   $$P_i = \Phi(Y_{(i)}) = \int_{-\infty}^{Y_{(i)}} \frac{e^{-t^2_2}}{\sqrt{2\pi}}\,dt$$

   here Φ(y) represents the cumulative distribution function (cdf) of the standard normal distribution and P_i is the cumulative probability corresponding to the standard value $Y_{(i)}$. The value of P_i can be found from standard normal tables or can be calculated using built in functions of spreadsheet programs such as Excel (i.e., NORMDIST).
4. The Anderson-Darling A^2 statistic is computed using,

   $$A^2 = \sum_{i=1}^{n} [(2i-1)\{\log P_i + \log(1-P_{n+1-i})\}/n] - n$$

   where log is log base e.
5. The modified statistics is calculated using,

   $$A^* = A^2(1.0 + 0.75/n + 2.25/n^2)$$
6. The null hypothesis of normality is rejected if A^* exceeds 0.752 at the 0.05 significance level.

The standardized residuals calculated in step 2 above as a function of AENCF are shown in Figure A.IV-1.

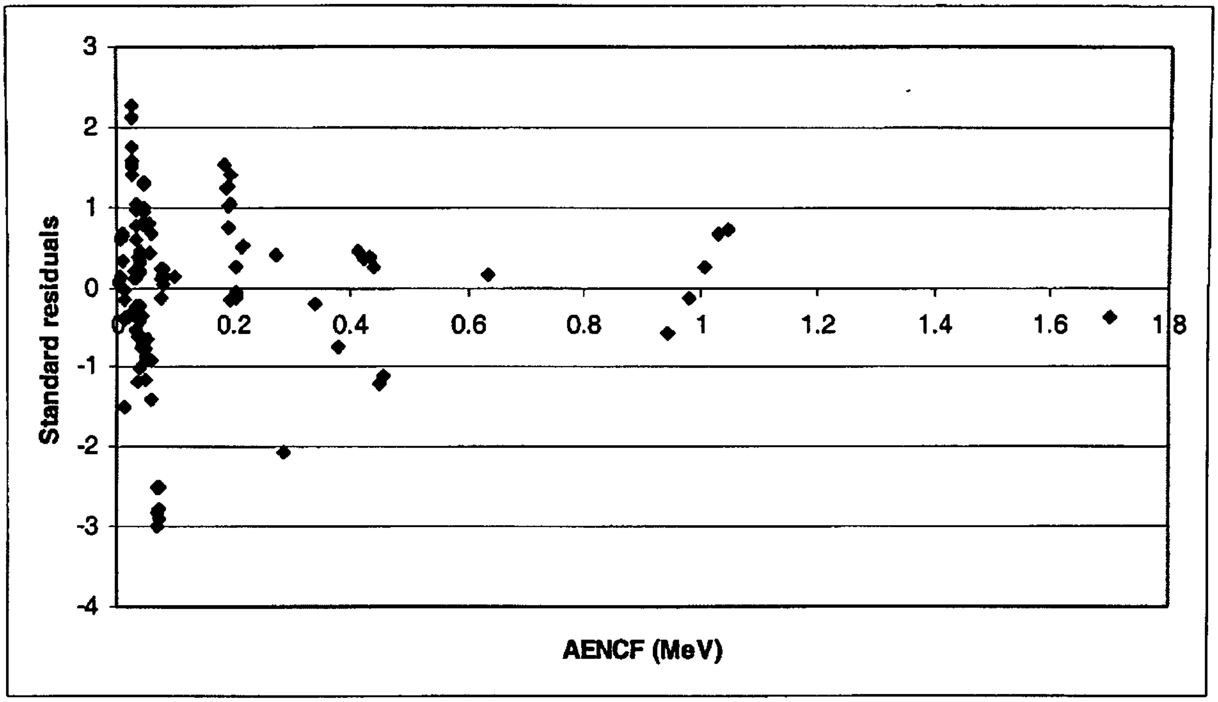

Figure A.IV-1. Plot of Standardized Residuals for Uranium and Plutonium Mixed Cases.

The Anderson-Darling A^2 test for the residuals results in $A^2 = 1.415$ and $A^* = 1.424$. Since $A^* > 0.752$, the residuals are not normally distributed. Inspection of Figure A.IV-1 shows that the residuals are not evenly distributed by exhibiting a visible pattern. Both these results, together with the weak trending parameters identified earlier indicate that the linear trending is not valid.

Since no trend with AENCF could be identified, according to the methodology presented in Section 2, an Anderson-Darling A^2 test is performed on the normalized k_{eff} values. The calculation steps are similar to the one outlined above for the residuals the only difference being that the normalized k_{eff} values are used instead of the residuals.

The Anderson-Darling A^2 test for the pool of k_{eff} data results in $A^2 = 0.889$ and A^* is 0.894. The pool of data is not normal because $A^* > 0.752$. Since the set of values is not normally distributed the non-parametric distribution free tolerance limit (DFTL) applies (Section 2). Based on Equation 6, the percent confidence that 95% of the keff population is above the lowest value observed is $\beta = 99.9\%$. Using the data from Table 2, the non-parametric margin (NPM) is 0 for this particular situation.

The lower bound tolerance limit (LBTL) is defined as (see Equation 7, Section 2):

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM)
where:

Based on the values given in Table A.IV-1 the minimum normalized k_{eff} is 0.9702. Since the smallest k_{eff} is less than 1 the total (code run combined with benchmark) sigma associated with this k_{eff} is used, which is $0.00584 = (0.0058^2+0.0007^2)^{1/2}$. Due to the size of the data pool the NPM is zero as showed above. The lower bound tolerance limit is calculated as:

$$LBTL = f = 0.9702 - 0.0058 = 0.9644$$

ATTACHMENT V: Detailed Calculations on MCNP k_{eff} Values for Critical Benchmark Experiments Selected for External Configurations Containing ^{233}U

This attachment presents additional information about the steps performed (Section 5.5) in the calculation of the lower bound tolerance limit including trending analysis and normality tests. The purpose is to provide to an individual reviewer all information necessary to replicate the current results by developing spreadsheets (in Excel or similar commercial software) independent of the originator. The k_{eff} data set used in this calculation contains the k_{eff} values calculated with MCNP for the critical benchmark experiments selected for external configurations containing uranium and plutonium fissile isotopes (Table 22, Section 5.5). The data set for the benchmark cases relevant to external configurations containing ^{233}U has a size of n= 83 cases.

For the critical benchmark experiments that were slightly super or subcritical, an adjustment to the k_{eff} values calculated with MCNP (k_{calc}) was done by normalizing the MCNP calculated (k_{calc}) value to the experimental value (k_{exp}). Unless otherwise mentioned, the normalized k_{eff} values (k_{norm}) have been used in all subsequent calculations. These values are included in Table A.V-1 together with the data from Table 22.

Table A.V-1. Summary of k_{eff} Data on Criticality Benchmark Experiments for External Configurations Containing ^{233U}

Experiment/ Case	MCNP Calculated k_{eff}	MCNP Sigma, σ_{calc}	Benchmark -Model k_{eff}	Benchmark Sigma, σ_{exp}	k_{norm}=k_{calc}/ k_{exp}	AENCF (MeV)	H/X
ust001-1	1.0018	0.0005	1.0000	0.0031	1.0018	0.0038	1530.92
ust001-2	1.0004	0.0006	1.0005	0.0033	0.9999	0.0041	1471.08
ust001-3	0.9994	0.0006	1.0006	0.0033	0.998801	0.0043	1419.48
ust001-4	0.9989	0.0006	0.9998	0.0033	0.9991	0.0043	1369.11
ust001-5	0.9987	0.0006	0.9999	0.0033	0.9988	0.0043	1324.91
ust02-04	1.0103	0.0011	1.004	0.0087	1.006275	0.026	119
ust02-05	0.9973	0.0011	1.004	0.0087	0.993327	0.0214	149.2
ust02-08	1.0113	0.001	1.004	0.0087	1.007271	0.0173	192.2
ust02-10	1.0096	0.0011	1.004	0.0087	1.005578	0.0138	246
ust02-11	1.0126	0.001	1.004	0.0087	1.008566	0.0115	295.7
ust02-12	1.0006	0.001	1.004	0.0087	0.996614	0.01	354.7
ust02-14	0.9875	0.0009	1.004	0.0087	0.983566	0.0098	393.6
ust02-15	1.0026	0.001	1.004	0.0087	0.998606	0.0083	458.9
ust02-17	0.9897	0.0009	1.004	0.0087	0.985757	0.0072	579.5
ust02-18	1.0029	0.0008	1.004	0.0087	0.998904	0.0066	628.3
ust02-19	1.0102	0.0008	1.004	0.0087	1.006175	0.0056	752.6
ust02-22	0.9967	0.0011	1.004	0.0087	0.992729	0.0356	83.9
ust02-24	0.9976	0.0012	1.004	0.0087	0.993625	0.049	57.1
ust02-34	1.0038	0.0011	1.004	0.0087	0.999801	0.0223	144.2
ust02-35	1.0103	0.0009	1.004	0.0087	1.006275	0.0155	212.1
ust02-36	1.0115	0.0009	1.004	0.0087	1.00747	0.0096	377.9
ust02-38	1.0097	0.0008	1.004	0.0087	1.005677	0.0075	512.6
ust03-40	1.008	0.001	0.9995	0.0087	1.008504	0.0387	74.1

ust03-41	1.026	0.0011	0.9991	0.0151	1.026924	0.0397	74.1
ust03-42	1.0044	0.0011	1.0007	0.0087	1.003697	0.04	74.1
ust03-45	1.014	0.0011	1.0015	0.0126	1.012481	0.061	45.9
ust03-55	1.0197	0.0011	1.0006	0.0122	1.019089	0.0693	39.4
ust03-57	1.0244	0.001	1.0012	0.0087	1.023172	0.0209	154
ust03-58	1.0167	0.001	1.0016	0.0087	1.015076	0.0138	250.1
ust03-61	1.0133	0.001	1.0016	0.0087	1.011681	0.0108	328.7
ust03-62	1.0107	0.001	1.0018	0.0087	1.008884	0.0095	395.3
ust03-65	1.0073	0.0008	1.0008	0.0087	1.006495	0.0056	774.7
ust04-03	1.0086	0.0011	1.0039	0.0088	1.004682	0.0257	119
ust04-06	1.0113	0.001	1.0034	0.0086	1.007873	0.0208	149.2
ust04-20	1.0006	0.0011	1.0041	0.0089	0.996514	0.0353	83.9
ust04-25	0.9936	0.0011	1.0051	0.0089	0.988558	0.0493	57.14
ust04-27	1.0119	0.0011	1.002	0.0105	1.00988	0.0479	57.14
ust04-28	1.0063	0.0011	1.002	0.0104	1.004291	0.0425	66.42
ust04-30	0.9988	0.0011	1.0037	0.009	0.995118	0.043	66.42
ust04-33	1.0087	0.0011	1.002	0.0102	1.006687	0.0215	144.23
ust05-01	1.0054	0.0009	1.0000	0.004	1.0054	0.0094	405
ust05-02	1.0075	0.0009	1.0000	0.0049	1.0075	0.0078	514
ust008	0.9986	0.0004	1.0006	0.0029	0.998001	0.003	1983.7
m35	1.023	0.0008	1.0000	0.0035	1.023	0.0576	68.78
m36	1.0113	0.0008	1.0000	0.0035	1.0113	0.0583	68.78
m37	0.9996	0.0008	1.0000	0.0035	0.9996	0.0588	68.78
m38	1.0011	0.0008	1.0000	0.0035	1.0011	0.0584	68.78
m45	1.0186	0.0011	1.0000	0.0035	1.0186	0.059	68.78
m61	1.0228	0.0008	1.0000	0.0035	1.0228	0.0345	120.86
m62	1.0132	0.0008	1.0000	0.0035	1.01322	0.0346	120.86
m63	0.9988	0.0008	1.0000	0.0035	0.99875	0.0352	120.86
m65	0.9939	0.0008	1.0000	0.0035	0.99386	0.0350	120.86
m77	0.9939	0.0011	1.0000	0.0035	0.99391	0.0358	120.86
m78	0.9932	0.0011	1.0000	0.0035	0.99324	0.0358	120.86
m79	0.9929	0.0011	1.0000	0.0035	0.99288	0.0355	120.86
hcm-1	1.0027	0.001	1.0000	0.0059	1.0027	0.1045	48.96
hcm-2	1.0059	0.0011	1.0012	0.0059	1.004694	0.1053	30.6
hcm-5	0.9963	0.001	0.9985	0.0056	0.997797	0.7833	0
hcm-6	0.9899	0.001	0.9953	0.0056	0.994575	0.7962	0
hcm-7	0.9949	0.001	0.9997	0.0038	0.995199	0.8015	0
hcm-8	0.9915	0.0011	0.9984	0.0052	0.993089	0.6872	1.34
hcm-9	0.9931	0.0011	0.9983	0.0052	0.994791	0.6536	2.05
hcm-10	0.9941	0.001	0.9979	0.0052	0.996192	0.6494	2.05
hcm-11	0.9934	0.0011	0.9983	0.0052	0.995092	0.6385	2.73
hcm-12	0.996	0.0011	0.9972	0.0052	0.998797	0.6358	2.73
hcm-13	0.9977	0.0011	1.0032	0.0053	0.994518	0.6309	3.45
hcm-15	0.9949	0.0011	1.0083	0.005	0.98671	0.4671	8.85
hcm-16	0.9926	0.0011	1.0001	0.0046	0.992501	0.4692	8.85
hcm-17	1.0012	0.0011	0.9997	0.0046	1.0015	0.4647	12.22
hcm-18	1	0.001	1.0075	0.0046	0.992556	0.4625	14.88
hcm-19	1	0.0011	1.0039	0.0047	0.996115	0.5191	6.4
hcm-20	1.0051	0.0015	1.006	0.0065	0.999105	0.5357	1.556

hcm-21	1.0046	0.0016	1.0026	0.0064	1.001995	0.5378	1.556
hcm-22	0.9995	0.0016	1.0013	0.0064	0.998202	0.5371	1.556
hcm-23	1.0056	0.0015	0.9995	0.0053	1.006103	0.535	1.556
hcm-24	1.0003	0.0016	1.002	0.0053	0.998303	0.5352	1.556
hcm-25	0.997	0.0014	0.9983	0.0053	0.998698	0.5333	1.556
hcm-26	1.0001	0.0015	0.9998	0.0053	1.0003	0.5283	1.556
hcm-27	0.9978	0.0016	0.9991	0.0053	0.998699	0.5302	1.556
hcm-28	1.0033	0.0015	1.0037	0.0053	0.999601	0.541	1.556
hcm-29	0.9998	0.0014	0.9992	0.0052	1.0006	0.5401	1.556
hmt001	1.0097	0.0010	1.001	0.006	1.008691	0.0215	n/a
hmt14	1.0125	0.0004	0.9939	0.0015	1.018744	0.0233	n/a

The set of normalized k_{eff} values is tested for trending against the spectral parameter AENCF and H/X using the build-in regression analysis tool from the Excel software.

The linear regression is performed using the regression tool from Excel's menu by selecting the normalized k_{eff} (k_{norm}) as the "y" variable and the AENCF and H/X values as "x" variable. The full output of the regression tool contains statistics regarding validity of a trend, such as the coefficient of determination (r^2), standard error, t-stat, etc., and is given below for the analysis done on H/X:

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.047997
R Square	0.002304
Adjusted R Square	-0.010824
Standard Error	0.008793
Observations	78

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	1.36E-05	1.36E-05	0.175487	0.676462517
Residual	76	0.005876	7.73E-05		
Total	77	0.005889			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.002416	0.001172	855.1957	3.9E-153	1.000081648	1.004751
X Variable 1	-1.02E-06	2.43E-06	0.418911	0.676463	-5.8515E-06	3.82E-06

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 25 (Section 5.5). The coefficient of determination (r^2) is very low and the absolute value of t-stat (renamed T in Table 25) is lower than $t_{0.025,81}$, indicating no trend with H/X.

The full output of the regression tool contains statistics regarding validity of a trend, such as the coefficient of determination (r^2), standard error, t-stat, etc., and is given below for the analysis done on H/X:

SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.357467
R Square	0.127783
Adjusted R Square	0.117015
Standard Error	0.008257
Observations	83

ANOVA

	df	*SS*	*MS*	*F*	*Significance F*
Regression	1	0.000809	0.000809	11.86677	0.000908
Residual	81	0.005523	6.82E-05		
Total	82	0.006332			

	Coefficients	*Standard Error*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*
Intercept	1.004499	0.001124	893.5477	1.6E-163	1.002262	1.006736
X Variable 1	-0.0121	0.003512	-3.44482	0.000908	-0.01908	-0.00511

The values of the intercept, slope, r^2, t-stat and P-value for slope have been transferred in Table 25 (Section 5.5). Since the coefficient of determination (r^2) is low and the absolute value of t-stat (renamed T in Table 25) is greater than $t_{0.025,83,}$ the linear trend is debatable and an analysis of the residuals is necessary.

For a valid trend, the residuals (see Section 2) need to be normally distributed and with a mean of 0. The residuals are calculated by the regression tool in Excel (corresponding option need to be activated at the beginning of the process). Normality test of residuals is performed by applying the Anderson-Darling A^2 test (Reference 8, p. 372). The Anderson-Darling A^2 normality test consists of the following six steps:

7. The residuals, $X_{(i)}$, are arranged in ascending order,
   $X_{(1)} \leq \cdots \leq X_{(n)}$
8. The standardized values are calculated by using,
   $$y_{(i)} = \frac{X_{(i)} - X_{(avg)}}{S}$$
   where $X_{(avg)}$ is the average of the residual values and S is the standard deviation for the values.

9. P_i for i=1,......,n is calculated by the following formula,

   $$P_i = \Phi(Y_{(i)}) = \int_{-\infty}^{Y_{(i)}} \frac{e^{-t^2_2}}{\sqrt{2\pi}}\, dt$$

   here Φ(y) represents the cumulative distribution function (cdf) of the standard normal distribution and P_i is the cumulative probability corresponding to the standard value $Y_{(i)}$. The value of P_i can be found from standard normal tables or can be calculated using built in functions of spreadsheet programs such as Excel (i.e., NORMDIST).
10. The Anderson-Darling A^2 statistic is computed using,

    $$A^2 = \sum_{i=1}^{n} \left[(2i-1)\{\log P_i + \log(1-P_{n+1-i})\}/n\right] - n$$

    where log is log base e.
11. The modified statistics is calculated using,

    $$A^* = A^2(1.0 + 0.75/n + 2.25/n^2)$$
12. The null hypothesis of normality is rejected if A^* exceeds 0.752 at the 0.05 significance level.

The standardized residuals calculated in step 2 above as a function of AENCF are shown in Figure A.V-1.

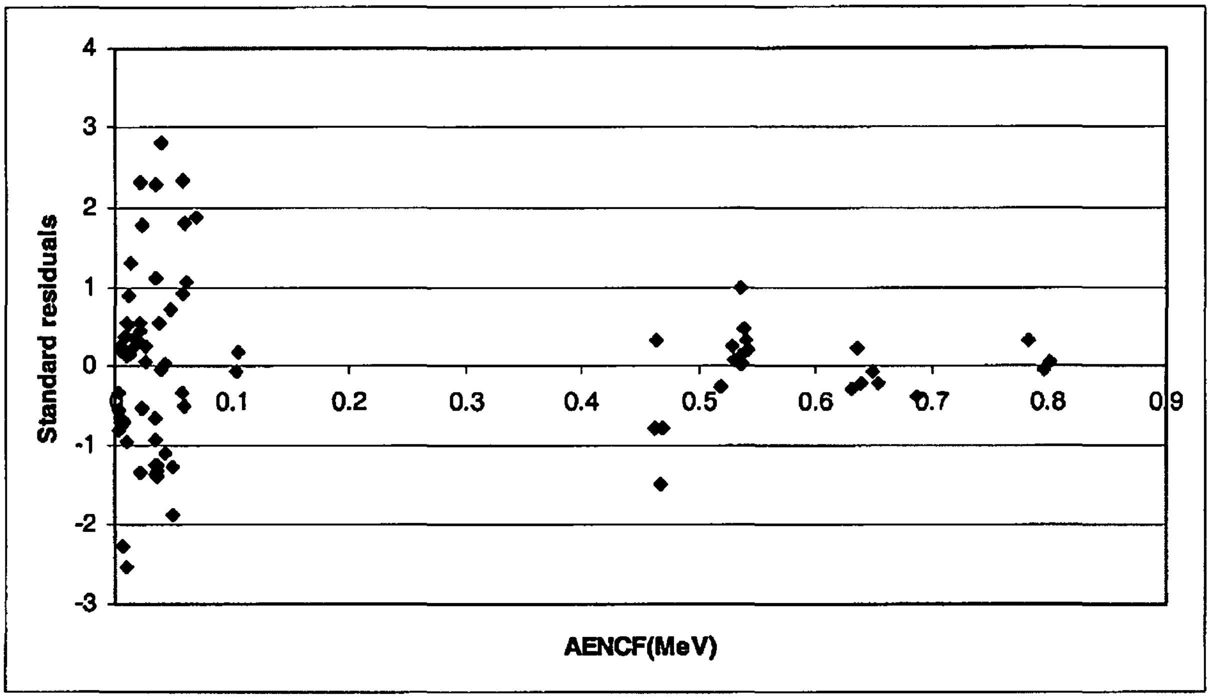

Figure A.V-1. Plot of Standardized Residuals for Uranium and Plutonium Mixed Cases.

The Anderson-Darling A^2 test for the residuals results in A^2= 1.035 and A^* is 1.044. Since A^* > 0.752, the residuals are not normally distributed. Inspection of Figure A.V-1 shows that the residuals are not evenly distributed by exhibiting a visible pattern. Both these results, together with the weak trending parameters identified earlier indicate that the linear trending is not valid.

Since no trend with AENCF could be identified, according to the methodology presented in Section 2, an Anderson-Darling A^2 test is performed on the normalized k_{eff} values. The calculation steps are similar to the one outlined above for the residuals the only difference being that the normalized k_{eff} values are used instead of the residuals.

The Anderson-Darling A^2 test for the pool of k_{eff} data results in $A^2 = 1.128$ and A^* is 1.138. The pool of data is not normal because $A^* > 0.752$. Since the set of values is not normally distributed the non-parametric distribution free tolerance limit (DFTL) applies (Section 2). Based on Equation 6, the percent confidence that 95% of the k_{eff} population is above the lowest value observed is $\beta = 98.6\%$. Using the data from Table 2, the non-parametric margin (NPM) is 0 for this particular situation.

The lower bound tolerance limit (LBTL) is defined as (see Equation 7, Section 2):

Lower bound tolerance limit = Smallest k_{eff} value – Uncertainty for smallest k_{eff} – Non-parametric Margin (NPM)

Based on the values given in Table A.V-1 the minimum normalized k_{eff} is 0.9835. Since the smallest k_{eff} is less than 1 the total (code run combined with benchmark) sigma associated with this k_{eff} is used, which is $0.0087 = (0.0087^2+0.0009^2)^{1/2}$. Due to the size of the data pool the NPM is zero as showed above. The lower bound tolerance limit is calculated as:

$\text{LBTL} = f = 0.9835 - 0.0087 = 0.9748$

ATTACHMENT VI: CLREG V1.0 Software Validation and Verification

Installation and validation of CLReg is performed according to Reference 11. There are 5 test cases that are described in Section 6.1 of Reference 11. The acceptance criteria in Section 6.2 of Reference 11 state that the results obtained by the installed version of CLReg should agree to within ± 0.0005 for installation and ± 0.001 for validation.

The CLReg code was installed and the test cases executed per the instructions provided in Reference 11. Note that installation required only copying the executable from the CLReg distribution to a folder on a personal computer. No modification was necessary.

The test method has been applied as described in Section 6.5 of Reference 11. All cases passed the acceptance criteria for installation and validation. The test log is shown in table A.VI-1.

Table A.VI-1 TEST LOG for CLReg Installation

Date	Initials	Test Case	Pass (P)/Fail (F)	Comment
6/15/2004	MS	Test01	P	None
6/15/2004	MS	Test02	P	None
6/15/2004	MS	Test03	P	None
6/15/2004	MS	Test04	P	None
6/15/2004	MS	Test05	P	None

The relevant output and utility files for the test cases are listed below.

File Name	Date	Comment
T1testout.csv	06/15/2004	Output for Test Case 01
T1testout.utl	06/15/2004	Utility file for Test Case 01
T2testout.csv	06/15/2004	Output for Test Case 02
T2testout.utl	06/15/2004	Utility file for Test Case 02
T3testout.csv	06/15/2004	Output for Test Case 03
T3testout.utl	06/15/2004	Utility file for Test Case 03
T4testout.csv	06/15/2004	Output for Test Case 04
T4testout.utl	06/15/2004	Utility file for Test Case 04
T5testout.csv	06/15/2004	Output for Test Case 05
T5testout.utl	06/15/2004	Utility file for Test Case 05

The files have been uploaded into the COLD server and are included in the COLD listing presented in Section 7.

ATTACHMENT VII: MCNP 4B2 Software Installation and Verification on the on the PA-RISC HP/UX workstations designated gr0 and gr1

Purpose and Objective

The purpose of this appendix is to provide verification and documentation of MCNP 4B2 on the PA-RISC HP/UX workstations designated gr0 and gr1.

MCNP is an externally supplied code that comes with a manual that fully describes the input, output and functionality of the code.

MCNP was installed on gr0 and gr1 and passed the vendors test cases on each. FANP procedure 0402-01 (Reference 3), Section VII.B.1 requires these programs be verified. The documentation is authored by the vendor (Reference 1). Verification for the purposes of the present calculation (validation of consistent output across platforms) was carried by running two test cases as described below. The version of MCNP documented here has previously been independently qualified for the same platform for use under the OCRWM procedures.

Installation and Verification

MCNP 4B2 was used to evaluate 29 validation test problems that were delivered with MCNP code. The test cases include input decks and Los Alamos-generated output and tally files. All 29 test cases were run on gr0 and are documented in the directory 32-5045840-00 on the COLD server (COLD SS) with filenames of inp*xx*o, where the '*xx*' represents the case number.

The UNIX 'diff' command was used to demonstrate that the Los Alamos-generated output/tally files were within the calculated uncertainty of the files generated locally. This indicates that MCNP 4B2 was installed correctly and is functioning as intended.

Additionally, 2 verification cases were run on gr0 and gr1 to serve as validation of consistent output across platforms. These cases, named corei.gr0, corei.gr1 and leuct12_1.gr0 and leuct12_1.gr01 produced matching k_{eff} values on all machines. These files are also located in the 32-5045840-00 directory on COLD SS.

Following is a listing of all the files included in the 32-5045840-00 directory on COLD SS.

corei.grl0
corei.gr1
leuct12_1.gr0
leuct12_1.gr1

inp01o
inp02o
inp03o
inp04o
inp05o
inp06o
inp07o
inp08o

inp09o
inp10o
inp11o
inp12o
inp13o
inp14o
inp15o
inp16o

inp17o
inp18o
inp19o
inp20o
inp21o
inp22o
inp23o
inp24o

inp25o
inp26o
inp27o
inp28o
inp29o

Evaluation of Acceptability

The MCNP 4B2 source code was received from RSICC and compiled without error on gr0 and gr1. The 29 test cases provided with the code yielded results that matched the RSICC-supplied results to acceptable round-off values. Case 25 had the largest differences. However, these were due to the execution of only one batch of particles after restart and a different random number to start. There were insufficient histories to allow convergence of the comparison cases. Thus, the differences are acceptable and do not impact verification results.

Conclusions

MCNP 4B2 was installed and tested on gr0 and gr1. The installation was tested on gr0 using 29 test cases provided with the code. All tests indicate that MCNP 4B2 is correctly installed on gr0, and gr1 and is performing as intended.

AREVA

DESIGN VERIFICATION CHECKLIST

Document Identifier 32 - 5045840 - 00

Title Analysis of Critical Benchmark Experiments for Configurations External to WP

1.	Were the inputs correctly selected and incorporated into design or analysis?	☒ Y	☐ N	☐ N/A
2.	Are assumptions necessary to perform the design or analysis activity adequately described and reasonable? Where necessary, are the assumptions identified for subsequent re-verifications when the detailed design activities are completed?	☒ Y	☐ N	☐ N/A
3.	Are the appropriate quality and quality assurance requirements specified? Or, for documents prepared per FANP procedures, have the procedural requirements been met?	☒ Y	☐ N	☐ N/A
4.	If the design or analysis cites or is required to cite requirements or criteria based upon applicable codes, standards, specific regulatory requirements, including issue and addenda, are these properly identified, and are the requirements/criteria for design or analysis met?	☐ Y	☐ N	☒ N/A
5.	Have applicable construction and operating experience been considered?	☐ Y	☐ N	☒ N/A
6.	Have the design interface requirements been satisfied?	☐ Y	☐ N	☒ N/A
7.	Was an appropriate design or analytical method used?	☒ Y	☐ N	☐ N/A
8.	Is the output reasonable compared to inputs?	☒ Y	☐ N	☐ N/A
9.	Are the specified parts, equipment and processes suitable for the required application?	☐ Y	☐ N	☒ N/A
10.	Are the specified materials compatible with each other and the design environmental conditions to which the material will be exposed?	☐ Y	☐ N	☒ N/A
11.	Have adequate maintenance features and requirements been specified?	☐ Y	☐ N	☒ N/A
12.	Are accessibility and other design provisions adequate for performance of needed maintenance and repair?	☐ Y	☐ N	☒ N/A
13.	Has adequate accessibility been provided to perform the in-service inspection expected to be required during the plant life?	☐ Y	☐ N	☒ N/A
14.	Has the design properly considered radiation exposure to the public and plant personnel?	☐ Y	☐ N	☒ N/A
15.	Are the acceptance criteria incorporated in the design documents sufficient to allow verification that design requirements have been satisfactorily accomplished?	☐ Y	☐ N	☒ N/A
16.	Have adequate pre-operational and subsequent periodic test requirements been appropriately specified?	☐ Y	☐ N	☒ N/A
17.	Are adequate handling, storage, cleaning and shipping requirements specified?	☐ Y	☐ N	☒ N/A
18.	Are adequate identification requirements specified?	☐ Y	☐ N	☒ N/A
19.	Is the document prepared and being released under the FANP Quality Assurance Program? If not, are requirements for record preparation review, approval, retention, etc., adequately specified?	☒ Y	☐ N	☐ N/A

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DESIGN VERIFICATION CHECKLIST

Comments: None.

Verified By:	Mehmet Saglam	M. Saglam	6/28/2004
(First, MI, Last)	Printed / Typed Name	Signature	Date

OCRWM	**SPECIAL INSTRUCTION SHEET** file list 8-14-04 mfc	1. QA: QA Page 1 of 1

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