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MCNP Criticality Validation and Bias for LEU System

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Abstract: The bias in MCP calculations was evaluated for low enriched uranium (LEU) systems typical of N reactor fuel. A formula that includes the bias and its uncertainties is given to ensure that LEU systems are safely subcritical.

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MCNP CRITICALITY VALIDATION AND BIAS FOR LEU SYSTEMS

1.0 INTRODUCTION

An evaluation of K Basin criticality by Wittekind (1992) includes a validation of the Monte Carlo code MCNP (Carter 1991) used in the study. Comparisons were made to several criticality experiments and to other criticality codes, specifically the WIMS (versions D and E) code (WIMS 1992). The comparisons provide good support for the use of MCNP in low-enriched uranium (LEU) systems typical of N Reactor fuel in the K basins.

The purpose of this report is to reexamine the experimental support for the validation and to determine a calculational bias to be used in further criticality evaluations. New validation calculations are not undertaken.

Two experiments reported by Wittekind are considered here: an early report on UO_3-H_2O solutions (Neeley and Handler 1961), and a lattice experiment using actual MKIA N reactor fuel elements (Brown et al. 1965). A third experiment performed by Douglas United Nuclear in the 105 N Fuel Storage Basin (Neilson and Toffer 1975) reported k_{eff} values that were often well below the MCNP results. Finally results from a benchmark experiment using 2.35% enriched fuel (Briggs et al. 1992) are included.

The experimental results are considered in the next section, and a statistical analysis is performed in Section 3.0. Results and recommendations are given in Section 4.0.

2.0 EXPERIMENTAL RESULTS

2.1 UO_3-H_2O Solution Measurements

The homogeneous wet uranium UO_3-H_2O solution experiments consisted of 12 measured values for three different enrichments and a range of hydrogen to uranium (H/U) ratios from 3.73 to 7.45. The results were reported as k_∞ and are compared by Wittekind to the MCNP results in Figure 1 which is taken directly from Wittekind's report (Wittekind 1992). The comparisons show that MCNP values are in good agreement with the experimental results and correctly follow the variations in k_∞ both as a function of enrichment and the H/U ratio. Table 1 gives numerical values for both the experiment and MCNP. All values used here for this experiment were taken directly from Wittekind (1992); the experimental report (Neeley and Handler 1961) was not reviewed.

Figure 1. MCNP Calculated k_{inf} for Homogeneous UO_3-H_2O System. HW-70310 Experiments Modeled.

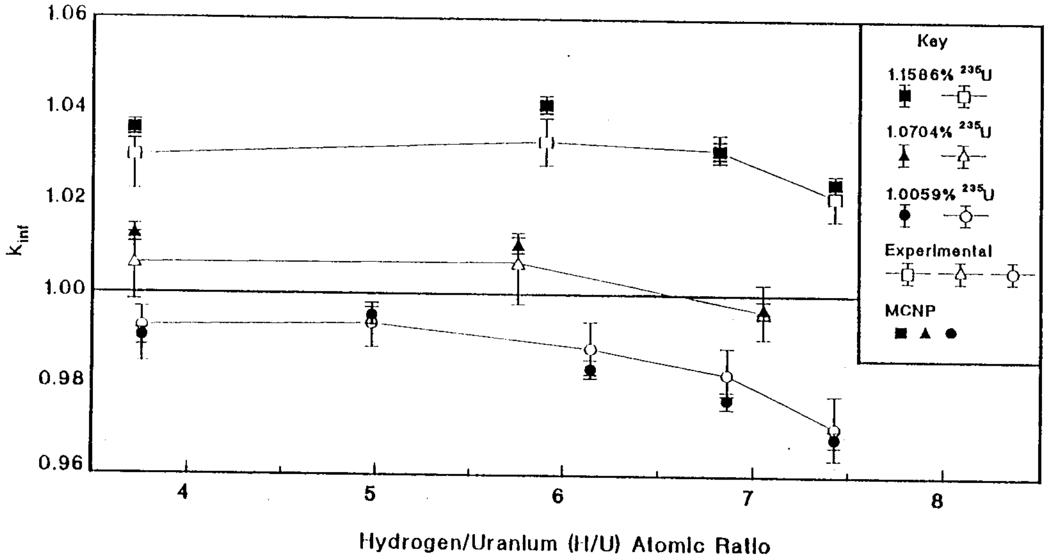


Table 1. MCNP Calculations (Wittekind 1992) and Experimental Results (Neeley and Handler 1961) for Homogeneous UO_3-H_2O Systems. The values are taken directly from Wittekind (1992).

Enrichment	H/U	MCNP	Experiment	Exp.Uncert.
1.0059	3.772	0.9898	0.9920	0.0060
1.0059	4.999	0.9945	0.9925	0.0050
1.0059	6.614	0.9830	0.9875	0.0058
1.0059	6.881	0.9761	0.9821	0.0054
1.0059	7.449	0.9680	0.9702	0.0070
1.0704	3.728	1.0125	1.0063	0.0070
1.0704	5.778	1.0103	1.0064	0.0080
1.0704	7.075	0.9964	0.9957	0.0061
1.1586	3.728	1.0358	1.0298	0.0060
1.1586	5.926	1.0412	1.0330	0.0051
1.1586	6.838	1.0311	1.0313	0.0032
1.1586	7.449	1.0240	1.0209	0.0051

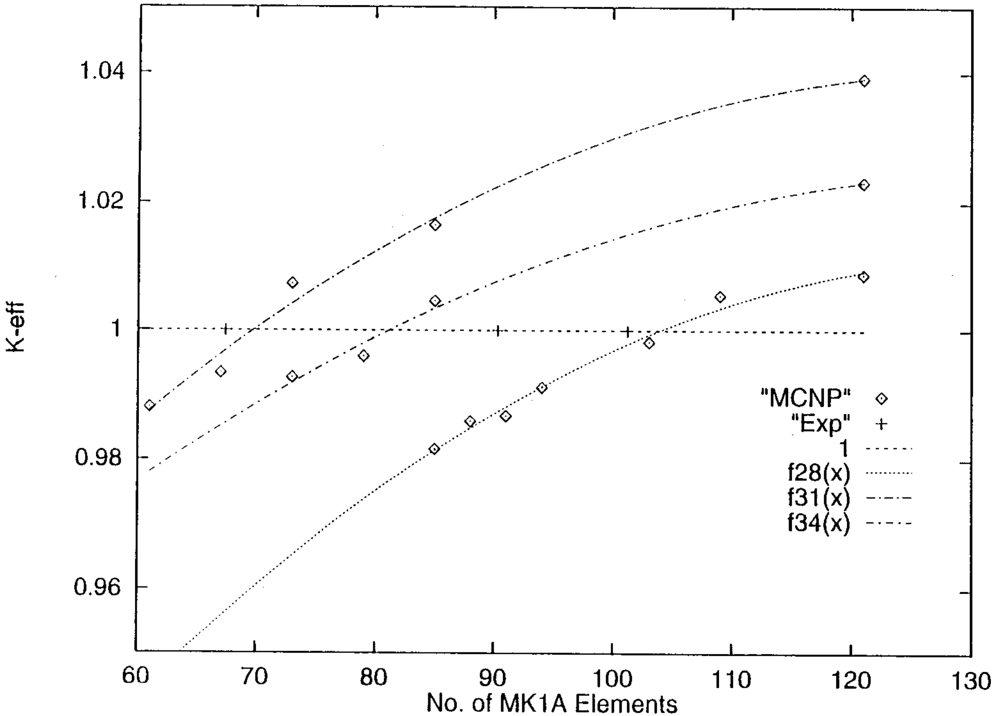
2.2 MKIA Lattice Experiment

A set of criticality measurements was made using a lattice of actual N Reactor MKIA fuel elements (Brown et al. 1965). These results have the advantage that they are representative of actual N reactor fuel configurations, with fuel elements of metallic uranium with density close to 18.64 g/cm^3. However, experimental uncertainties were not reported either in the initial report or by Wittekind (1992). For this reason, the original report was reviewed with the intent to determine the validity of the results and to obtain semi-quantitative uncertainties.

The experiment consisted of three distinct types of measurements (exponential pile, neutron multiplication, and pulsed-neutron) and two fuel lattice configurations (MKIA outers and tube-in-tube). Several different lattices pitches were also included.

The primary results used by Wittekind for the MCNP validation tests were taken from the exponential measurements for the tube-in-tube geometries. Expressed as the number of MKIA fuel elements to reach k_{eff}=1, this gave three experimental values, 101.2, 67.4, and 90.3 corresponding to lattice pitches of 2.8 in., 3.1 in., and 3.4 in. The corresponding metric values are 7.112 cm, 7.874 cm, and 8.636 cm. These experimental values are shown on Figure 2 along

Figure 2. MCNP Calculations of k_{eff} for MK1A Lattices Compared to Experimental Results from (Brown et al. 1965)



with the corresponding MCNP calculations made by Wittekind. The calculated values of k_{eff} are taken directly from Table 6-5 in Wittekind (1992). Representative MCNP statistical uncertainties are 2 mk. The 3.1 in. lattice is most reactive and is between the two other two lattice pitches.

To compare the experimental and calculated values, quadratic regression curves were fitted to the calculated points. As seen in Figure 2, the MCNP k_{eff} values corresponding to the same number of MKIA elements are slightly below the measured values for the 2.8 in. and 3.1 in. pitches and high for the 3.4 in. result.Ratios of the MCNP-fitted curves to the experimental values were found for the three lattice pitches. These ratios are 0.9979, 0.9968, and 1.0077 for the lattice pitches 2.8 in., 3.1 in., and 3.4 in. respectively.

Uncertainties

Experimental uncertainties were not reported for the measured values. Nevertheless a review of the experimental report (Brown et al. 1965) provides some useful information. The estimated number of critical tubes for the enriched outer tubes were determined separately by both neutron multiplication and by exponential pile measurements for two lattice pitches, 2.8 in. and 3.1 in. The exponential pile (or buckling) measurements are based on the falloff of the neutron flux as a function of z while the neutron multiplication measurements represent an extrapolation of the inverse count-rate to zero. The two measurements differ by 1 tube for the 2.8 in. lattice and by 3.5 tubes for the 3.1 in. lattice. Based on the given graphs, a qualitative estimate of the extrapolation error for the multiplication measurements is roughly three or four tubes (1-sigma), a result reasonably consistent with the separate agreement with the exponential measurements.

Neutron multiplication measurements were not reported for the tube-in-tube measurements used by Wittekind. However the experimental setup and measurements were the same as for the enriched outer tubes. Given the overall consistency of the results and giving consideration to the difficulties in assessing extrapolation errors, a relatively large value of ±5 tubes was chosen to reflect the uncertainty in the critical number of tubes.

The corresponding uncertainty in k_{eff} can be obtained by reference to Figure 2. The three displayed curves have slopes close to 0.001 for points near the measurements. Thus an uncertainty of ±5 tubes corresponds to an uncertainty of ±0.005 in k_{eff}.

Subcriticality of Low Enriched Systems

It is worth noting that the small $\Delta k/\Delta N$ slope implies a small change in Δk for a fairly large change ΔN in the number of MKIA tubes. For example, to move from a subcritical value of k_{eff}=0.98 to a value of 1.0 requires the addition of roughly 20 fuel elements.

2.3 Benchmark Experiment for 2.35% Enriched Lattice

A set of measurements not included in Wittekind's validation is documented for benchmark experiments performed at Pacific Northwest Laboratories critical mass laboratory and designated as LEU-COMP-THERM-001 (Briggs et al. 1992). Results are given for eight water-moderated UO_2 (2.35% enriched) lattices, mostly grouped in three clusters. The theoretical density of uranium oxide fuel, UO_2 is 10.96 g/cm^3 which calculates to a maximum effective uranium density (taking into account the presence of $U^{238}O_2$) of 9.66 g/cm^3.

Although the enrichment is about twice that of the N Reactor fuel, the benchmark report includes a very detailed analysis of the experimental uncertainties. The reported benchmark value for k_{eff} is 0.9998±0.0031. (The value less than one accounts for a small correction from acrylic lattice plates omitted from the model.) The experimental uncertainties are primarily due to lattice characteristics: enrichment, fuel diameter, and pitch.

The benchmark report also includes MCNP results with statistical errors for comparison (≈1.6 mk). Resulting values are reproduced in Table 2. Three cases for which MCNP input models were already constructed were recalculated on local computers. The results for Cases 1, 2, and 4 are 0.9974.±.00076, 0.9950±.00089, and 0.9964±.00081 respectively. The three recalculated values are biased low with an average bias of -3.5 mk which compares well with an average bias of -3.2 mk for the eight benchmark calculations.

Table 2. MCNP calculations for benchmark LEU-COMP-THERM-001 as reported in Briggs et al.(1992).

Case Number	Number of Clusters	Cluster Dimensions (No. of rods, X x Y)	MCNP
1	1	20 x 18.08	0.9987±.0016
2	3	20 x 17	0.9977±.0017
3	3	20 x 16	0.9956±.0016
4	3	20 x 16 (center) 22 x 16 (two outer)	0.9992±.0014
5	3	20 x 15	0.9970±.0016
6	3	20 x 15 (center) 24 x 15 (two outer)	0.9955±.0015
7	3	20 x14	0.9968±.0017
8	3	19 x 16	0.9921±.0015

3.0 STATISTICAL ANALYSIS

The three sets of results are conveniently compared in Figure 3 where the ratios of the MCNP values to the corresponding measured values are shown. (The abscissa is an arbitrary index that delineates the distinct measurements.) The first 12 points represent the homogeneous UO_3-H_2O solution results; the second set of 3 points represents the metallic uranium MKIA lattice measurements; and the final set of 8 points represents the 2.35% enriched uranium oxide benchmark values. (Note that for values this close to unity, the difference between the calculation to measurement ratio, C/E, and one is nearly equivalent to the absolute difference, C/E-1≈C-E.)

These data can now be used to determine a calculational bias, b, defined by

$$k_{calc}=k_{eff}+b$$

where k_{calc} represents the calculated estimate of k_{eff}.

Following standard practice (see Macklin and Miller (1991) for example), a lower tolerance limit b_L is established such that one is 95% confident that 95% of the population is above the limit. The non-central t-distribution gives a prescription (Resnikoff and Lieberman 1956) for this limit:

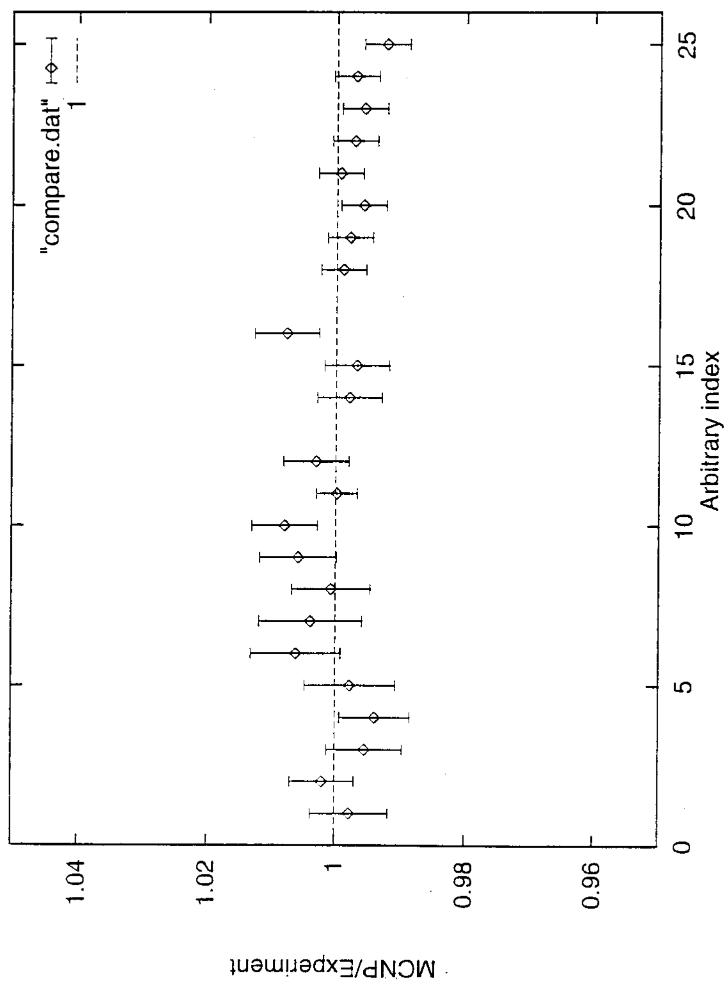
$$b_L=b_{ave}-K_b s_b$$

where b_{ave} is the mean value and s_b is the corresponding sample variance. The multiplier K_b may be found from statistical tables of the non-central t-distribution and depends on the number of degrees of freedom (DOF) for the supporting measurements.

<u>Application</u>

The application of these statistical rules requires some judgement since there is not a unique way to analyze the data. One possibility is to pool the data, treating each measurement as an independent value and using the sample variance as an estimate of the uncertainty. There are several concerns with this approach. First there is no assurance, at least for the present study, that the data are independent. Secondly, it ignores useful information contained in the estimated uncertainties. For example, one subset of the data could have fewer values that would reduced its weight even though it had smaller prior uncertainties. The relation of a given set of measurements to the desired conditions (such as similar enrichments or uranium density) is also ignored. Finally, the variations in the C/E values arises from a variety of separate sources that may not be adequately sampled. In statistical terms, the number of degrees of freedom associated with the measurements is difficult to determine. Here the three separate sets of measurements, which represent distinct experimental conditions, are first considered individually. They are

Figure 3. Ratio of MCNP Calculations to Experimental Values for Low-Enriched Systems



then considered jointly with due consideration of their overall consistency and relevance. The results are summarized in Table 3 below which shows the average bias, b_{ave}, and the associated sample variance (expressed as a standard deviation, s_b) for each of the three individual data sets and for the pooled total set of data. The average assigned experimental uncertainty, σm-ave, is shown for comparison.

Table 3. Statistical MCNP Bias Results for Three Experiments and the Pooled Data.

Description	n	b_{ave}, mk	s_b, mk	σ_{m-ave}, mk	sb/σ_{m-ave}
UO_3-H2O soln.	12	1.2	4.4	5.8	0.76
MKIA elements	3	0.8	6.0	5.0	1.20
Benchmark exp.	8	-3.2	2.2	3.5	0.64
Pooled data	23	-0.4	3.8	4.9	0.78

The MCNP calculations are biased slightly high for the first two sets of experimental values but well within the sample standard deviation. The benchmark calculations for the 2.35% enriched oxide fuel are biased low (see also Figure 2) but are within the assigned average experimental uncertainty. The bias is somewhat larger than the sample standard deviation, however this value could easily be low if the values are correlated as appears to be the case from Figure 2.

As shown by the last column in Table 3, the uncertainties as determined from the sample variance are in reasonable agreement with the prior assigned experimental uncertainties. Since the sample variance is distributed as chi-square, this comparison could be made more quantitative; however, the difficulty in determining the associated degrees of freedom reduces the value of doing so.

Based on the results in Table 3, the pooled bias of b_{ave}= -0.4 mk was chosen for final result. This choice includes the lower values of the benchmark data giving a conservative result. A standard deviation of s_b=5.0 mk was chosen in favor of the somewhat lower value of 3.8 mk associated with pooled sample variance. The latter value assumes that all the data points are independent, while the larger value is generally consistent with the results in Table 3.

Finally, a value of the multiplier, K_b is detemined. A precise value for K_b can only be determined for a known number of degrees-of-freedom. Nevertheless for a 95/95 tolerance limit, standard non-central t-distribution tables show that K_b ranges from 2.4 to 1.9 as the DOF range from 20-100. Given that a somewhat conservative value was already chosen for s_b, a conventional and rounded value of K_b=2.0 is a good practical choice.

The final result for the lower tolerance limit of the bias (calculated to two significant figures and rounded up to be conservative) is

$$\begin{aligned} b_L &= -0.4 - (2)(5.0) \\ &= -11 \text{ mk} \end{aligned}$$

Therefore, +11 mk should be added to MCNP criticality computed results prior to checking for other prescribed limits.

To account for Monte Carlo statistical uncertainties, an additional value 1.645 σ_c is added in quadrature to the bias uncertainty. This means that the MCNP Monte Carlo statistical uncertainties are not correlated to the uncertainty in the bias when compared to experiment, a reasonable assumption The value of 1.645 is the number of standard deviations in the standard normal distribution required to yield 95 % confidence in the calculation. For example, a value of σ_c=2.0 mk would yield a combined limit of:

$$-0.4-[10^2+(1.645\text{x}2)^2]^{1/2} = -10.9 \text{ mk}.$$

4.0 RESULTS AND RECOMMENDATIONS

The results are summarized by

$$k_{calc}+0.0004+\sqrt{0.010^2+(1.645\sigma_{calc})^2} < k_{limit}$$

where k_{calc} and σ_{calc} represent the calculated value for k_{eff} and its standard deviation respectively. The limit, k_{limit}, is an established limiting value. The multiplier of 1.645 ensures that 95% of the Monte Carlo population is bounded by the limit and assumes that there is no uncertainty in the standard deviation, σ_{calc}. It can be obtained from tables of the normal distribution; alternately it also corresponds to the non-central t-distribution multiplier for an infinite number of degrees of freedom.

A value of σ_{calc} that is larger than that accepted by almost all criticality calculations done by specialists using MCNP is 0.004 k. For this value, the bias limit would be:

$$k_{calc}+0.0004+\sqrt{0.010^2+(1.645*0.004)^2} < k_{limit}$$

$$k_{calc} < k_{limit} - 0.013k$$

so

$$k_{calc} + 0.013k < k_{limit}$$

All resulting values are rounded up to be conservative.

Using the above calculated bias value means that the k_{calc} computed from a new MCNP run would have to be below k_{limit} - 0.013 k in meeting the allowable limit on k_{eff}. For a k_{limit} of 0.95, k_{calc} would have to be less than 0.937 to be within acceptable limits. If this particular value is used for the acceptable limit, the σ_{calc} must be less than 0.004 for each calculation. Table 4. gives other calculated biases for given values of σ_{calc} that could be used to designate an acceptable limit on the k_{eff} computed by MCNP.

Table 4. Biases calculated from given σ_{calc}

bias

σ_{calc} (k)	bias limit (b_L) (k)
0.001	-0.011
0.002	-0.011
0.003	-0.012
0.004	-0.013
0.005	-0.013
0.006	-0.015
0.007	-0.016

For most situations, the dominant correction is the 10 mk correction arising from the uncertainty in the bias analysis, scatter in the calculation of k_{eff} for the benchmark cases. The bias of -0.4 mk is not significantly different from zero.

The widespread use of MCNP in a variety of situations adds a measure of confidence to these results significantly beyond the quantitative aspects reported here.

Additional work that could be done within the context of the present study includes surveying additional experimental results and to independently recreate and apply the MCNP 2.35%-enriched oxide fuel benchmark models. However, this would represent a significant increase in work scope.

A theoretical assessment of the relevance of the results for the higher-enriched experiments could also be carried out.

5.0 PEER REVIEW

This document was peer reviewed for three aspects; general, MCNP technics (Carter 1996) and statistical validity (Kline 1996).

5.1 GENERAL PEER REVIEW

The general review was done for technical content and adequacy by Warren D. Wittekind of Criticality and Shielding. His comments follow:

A bias calculation should be appropriate for the application intended.

The bias calculation performed in 1992 (Wittekind 1992) was for solid metallic uranium in a uranium bearing solution. This study broadens the application to all low enriched uranium systems by including a 2.35 wt% uranium oxide fuel case which has a uranium density midway between homogeneous solutions and metallic uranium slugs. The bias limitation is the precision of the historical criticality experiments and not the precision of present day computer calculations. The emphasis on criticality experiments has diminished in recent years while progress in computer performance, especially speed, which reduces the Monte Carlo statistical uncertainty, has progressed rapidly.

There are assumptions in these statistical bias calculations which reflect the author's values of how much to weight the various benchmark experimental classes. The assumption which led to b_L = -0.4 mK and with the 95% confidence interval (single sided) of 10 mK are conservative, and reasonable and defensible.

5.2 MCNP TECHNICS PEER REVIEW

This document was reviewed by Lee L. Carter of the Criticality and Shielding Group for proper use of the MCNP computer code. His comments follow:

I have reviewed this report and am in agreement with the approach and recommendation obtained for the bias and the uncertainty in the bias; i.e., as given by the inequality at the beginning of section 4.0. This EDT does not mention that the MCNP calculations were made using ENDF/B-V cross sections at 300 degrees K. This is important since the validation is specifically for those cross sections as utilized by MCNP.

5.3 STATISTICAL VALIDITY PEER REVIEW

This document was reviewed by Niall W. Kline of the Information and Scientific Systems Group, Lockheed Martin Services, Inc. for proper statistical treatment of the data. His comments follow:

Introduction

Estimation of calculational bias with the MCNP code proceeds by collecting a sample of bias realizations. Each bias realization, b, is determined by

$$b = k_{calc} - k_{eff} ,$$

where k_{eff} is a measured value from a physical experiment and k_{calc} is the analagous value determined from simulation of the physical experiment with the MCNP code. The intent is to obtain a sample from which to estimate the bias b that is inherent in using the MCNP code.

The sample used for this purpose in Section 3 is constructed of three subsamples. Each subsample is a set of realizations of b that is determined from a set of related physical experiments. Issues regarding independence, sufficiency and convergence in relation to the sample and subsamples are raised in discussion of statistical estimates in Section 3. The purpose here is to provide some input to the resolution of those issues.

Sample Independence

Ideally the full sample should be a random sample; i.e., the realizations should be independent and identically distributed. Independence means that the value of any realization of b does not depend on the value of any other realization of b. The measurements of k_{eff} taken from the physical experiments are related in that the experiments are related and the values of k_{calc} determined from simulations of the experiments are similarly related, but there is no correlation reported with the data and hence for the present purposes the realizations of bias are assumed to be independent. Under the assumption of independence, the number of degrees of freedom is equal to the sample size.

Sample Homogeneity

The realizations of bias should also be identically distributed, meaning that all of the realizations are from one homogeneous population. Display of the full sample in Figure 3 appears to suggest the possibility of subpopulations. Letting b_x denote a realization of bias from the U03-H20 solution data (n_x=12) and b_y denote a realization from the benchmark experiment data (n_y=8), the b_x sample mean and sample standard deviation are μ_x=0.001225 and S_x=0.00446 and the b_y sample mean and sample standard deviation are μ_y=-0.003225 and S_y=0.00223 (cf. Table 3). Note that μ_y is in the interval from μ_x to $\mu_x - S_x$, but μ_x is not in the interval from μ_y to $\mu_y + S_y$.

Homogeneity has been formalized as a null hypothesis (H_o: $F_x = F_y$, where F_x and F_y denote the distribution functions of the b_x and b_y subsamples respectively), and tested with both the Runs test and the Rank-Sum test. Details of the Runs and Rank-Sum tests can be found in most texts on mathematical statistics. Using small Type I error, 0.01 = Pr(Type I error) = the probability of rejecting the null hypothesis when it is true, then both the Runs test and the Rank-Sum test fail to reject the null hypothesis. This supports the homogeneity supposition and use of the "pooled" sample.

Estimator

The estimator of a lower bound on bias is taken to be

$$b_L = b_{ave} - K_b S_b,$$

where b_{ave} is the sample mean of the pooled sample (n=23),

S_b is the sample standard deviation of the pooled sample,

and K_b is the 95th percentile from the non-central t distribution.

Based on work by Dyer et al (1991), b_L is a lower limit on a 95% single-sided, uniform width, closed-interval, lower tolerance band (LTB). In other terms, at least 95% of the biases realized with the MCNP code are expected to be greater than b_L, with 95% confidence.

Sufficiency

Broadly, an estimator is defined to be statistically sufficient if it preserves the information contained in the sample data. While the estimator

b_L isn't necessarily insufficient, the estimator is supplemented hueristically to account for apparent (unquantified) experimental variation and Monte Carlo statistical uncertainty. The final form shown in Section 4 is more conservative; i.e., the final lower limit includes at least 95% of the biases realized with the MCNP code.

Convergence

Although the full sample size, n=23, is not small, neither is it a large sample. Investigation of adequacy of the sample in terms of both size and variation (degrees of freedom) is beyond the scope of this initial review effort.

Conclusions

Construction of a reasonable initial sample and estimation of a lower limit on at least 95% of the biases that are expected to be realized in use of the MCNP code has been undertaken with due consideration to concerns for stochastic independence of the sample and statistical sufficiency of the estimator. As part of this review investigation it has also been determined that the initial sample can satisfy a condition of homogeneity. Supplementation of the sample to provide indication of convergence of sample mean and variance estimates would be a useful extension of the present work.

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