Appendix 1:

NETCO Report No. 901-02-05

Benchmarking Computer Codes for Calculating the Reactivity State of Spent Fuel Storage Racks, Storage Casks and Transportation Casks.

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Review/Approval Record

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1.0 Introduction

This report documents the results of benchmark calculations of three computer codes used to compute the reactivity state of nuclear fuel assemblies in close-packed arrays. Such close-packed arrays include high density spent fuel storage racks, dry storage casks and casks for transporting nuclear fuel. The three computer codes, which were benchmarked and validated are:

- KENO V.a, which is a module of SCALE 5[1]
- MCNP5[2]
- CASMO-4[3]

Earlier versions of KENO and CASMO have been previously benchmarked and validated by NETCO.[4,5]

To benchmark and validate the codes for spent fuel racks and cask evaluations, KENO and MCNP were used to simulate a series of critical experiments. The calculated eigenvalues (k_{eff}) were then compared with the critical condition (k_{eff} = 1.0) to determine the bias inherent in the calculated values. For the KENO V.a calculation, the 238 energy group ENDF/B-V cross-section library was used. For the MCNP5 calculations, the continuous energy cross-section library based on ENDF/B-VI was used.

After determining the inherent biases associated with KENO V.a and MCNP5, both KENO V.a and CASMO-4 (with its own 70 energy group cross-section library) were used to model central arrays of select critical experiments. It is noted that CASMO-4 models an infinitely repeating array of fuel assemblies and is generally used to generate cross-sections for core simulator models. As such, it does not lend itself directly to finite arrays of fuel racks surrounded by a reflector, as is the case in the critical experiments considered. Accordingly, the central fuel arrays of five critical experiments were modeled as infinite arrays with both KENO V.a and CASMO-4. A comparison of the KENO V.a and CASMO-4 eigenvalues provides a means to determine the CASMO-4 bias.

For the purposes of benchmarking, a set of five Babcock and Wilcox (B&W) critical experiments (XIII, XIV, XV, XVII, and XIX)[6], were selected because they closely represent typical fuel/rack geometries with neutron absorber panels. In addition, the International Committee on the Safety of Nuclear Installations (CSNI) identified a sequence of benchmark problems[7] that closely replicate both fuel/rack and fuel/cask geometries, and included typical LW enrichments and $H/^{235}U$ ratios. The resulting models are representative of most fuel storage rack and fuel cask configurations used today.

All work completed for the benchmarking calculations was carried out under NETCO's Quality Assurance Program[8]. The methods employed have been patterned to comply with industry accepted standards[9,10,11] and with accepted industry criticality references[12, 13, 14, 15, 16].

2.0 BENCHMARKING - STANDARD PROBLEMS AND CONFIGURATION CONTROL

2.1 SCALE-5 and MCNP5 Configuration Control

The binary executable codes and associated batch files were provided by RSICC on CD-ROM for use on Intel Pentium based micro-computers running under the Windows operating system. In this form, the programs can not be altered or modified. In addition to the binary executable codes, there are several supporting files which contain cross-section sets, etc. The file name, file size, and creation date for each executable file is given in Appendix A*. Prior to executing either code sequence, the user will verify the file names, creation dates, and sizes to insure that they have not been changed. Appendix B contains two CD-ROMs, which include the as-received versions of all files required to execute these programs. In all applications described in this report and for all subsequent applications, the files listed in Appendix A are to be used. This appendix is not provided in the non-proprietary version of this report.

2.2 Sample Problems

A suite of input files with their corresponding output files were provided with each code. The input file names and batch files used to execute them are listed in Appendix A. These were executed on NETCO's host computer via batch files provided by RSICC and the resulting output files compared to those provided by RSICC on CD-ROM. Except for the date and time of execution stamps, the respective output files were identical. Each code uses a pseudo-random number generator that is initiated with a default seed value. Since the default value was used in each case, the sequences of random numbers were the same, leading to identical calculations. This verifies that the as-received versions of both codes are identical to the versions documented in the User's Manuals[1,2].

*(Appendices A, B, C, D and E are included in the proprietary version of this report.)

Examination of the sample input decks shows that the run modules in batch files exercise all of the code options used by this benchmarking exercise. Before and after each subsequent use of each code, one set of sample input modules are executed and the output files compared to the sample output files to verify that no system degradation has occurred. (All of these files are contained in Appendix B* at the end of this report). This appendix is not provided in the non-proprietary version of this report.

2.3 CASMO-4 Configuration Control

The version of CASMO-4 used for these analyses was developed for a RISCC workstation. Version 2.05.01 of CASMO-4 was used for this benchmarking work and subsequent users of CASMO-4 for NETCO will verify that Version 2.05.01 is being used. CASMO-4 and all versions are controlled by Studsvik of America under their Quality Assurance Program[17]. If a different version of CASMO-4 is used by NETCO for any subsequent analyses, the CASMO-4 analyses in Section 3.2 shall be repeated with the version in use.

*(Appendices A, B, C, D and E are included in the proprietary version of this report.)

3.0 BENCHMARK MODELING OF LWR CRITICAL EXPERIMENTS

An index of input and output files for each experiment modeled is contained in Appendices C* and D*. For each experiment, the input and output files are on 3.5 inch 1.44 MB diskettes which are also contained in Appendices C and D. Appendix E* contains the calculation notebook for this project and represents a permanent record of all hand calculations performed during input preparation. All input parameters are fully traceable to the appropriate source documents. These appendices are not provided in the non-proprietary version of this report.

3.1 BENCHMARKING OF SCALE-5 and MCNP5

The B&W experiments[6] include twenty (20) water moderated LWR fuel rod cores and close-packed critical LWR fuel storage arrays. Of these, five (5) used boron carbide/aluminum cermet poison plates (BORAL) in the closest possible packing geometry representing a 3x3 array of LWR fuel assemblies in high density fuel storage racks. These five (5) experiments have been modeled, as they most closely represent LWR fuel in high density fuel storage racks and cask configurations with neutron absorber panels. Table 3-1 summarizes some of the model parameters, including U-235 enrichment, moderator-to-fuel ratio and absorber macroscopic absorption cross-section.

The Committee on the Safety of Nuclear Installations (CSNI) has published a selection of critical experiments[7], which are a sequence of exercises arranged in order of increasing complexity, introducing one new parameter into the geometry and materials at a time. They were selected specifically to validate calculational methods for criticality safety assessments. The fuel is designed to simulate LWR fuel, is water moderated, and the lattices include BORAL plates between assemblies when neutron poisons are

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included. The sequence starts with Experiment 1-1, a single array of 20x18, 2.35 w/o ^{235}U rods with a water reflector all around. Experiments 1-2-1 and 1-2-2 are also single water reflected arrays but are at a higher enrichment (4.74 w/o ^{235}U) and are at undermoderated (1-2-1) and optimum moderation (1-2-2) conditions. Experiment 2-1 has three square arrays of 2.35 w/o ^{235}U fuel separated by BORAL neutron absorber plates. Experiment 2-2 has a 2x2 array of four 4.74 w/o ^{235}U rod arrays also separated by BORAL plates. Experiments 3-A-1 and 3-B-1 are similar to experiment 2-1 but include, respectively, lead and steel reflecting walls. Experiment 3-A-2 is similar to Experiment 2-2 but also has a lead reflecting wall.

In each MCNP5 model of the criticals, 4,000,000 neutrons in 2,000 generations were tracked. In each KENO model of the criticals, at least 20,000,000 neutrons in at least 10,000 generations were tracked. The output files were always checked to insure that the fission source distribution had converged. A summary of the distribution of k_{eff} over all generations is automatically plotted in the output files and shows them to be approximately normally distributed. Thus, normal one-sided tolerance limits with appropriate 95% probability / 95% confidence factors (95/95) can be used. The calculated results for each critical experiment are given in Table 3-2, including the calculated k_{eff}, the one-standard-deviation statistical uncertainty of k_{eff}, denoted by σ, and the bias with respect to the critical state k_{eff} = 1.0.

The overall bias between the calculation eigenvalue and the experiments is calculated as follows. First, the variance-weighted mean is calculated as

$$k_m = \sum_{i=l}^{N} (k_i / \sigma_i^2) / \sum_{i=l}^{N} (1 / \sigma_i^2 \qquad (3\text{-}1)$$

where N = 13 (for the 5 B&W and 8 CSNI criticals), k_i is the SCALE-5 calculated k_{eff} for critical i, and σ_i is the SCALE-5 calculated standard deviation of the distribution of k_{eff} for critical i. The standard deviation around k_m is given by

$$\sigma_m = \left[\frac{1}{N-1} \sum_{i=1}^{N} \left(k_i - k_m\right)^2 \right]^{1/2} \quad (3\text{-}2)$$

The bias is calculated as k_m - 1, and has the same standard deviation as k_m. Based upon the results shown in Table 3-2, it is recommended that the 238 energy group ENDF/B-V library be used in all criticality analyses. For SCALE-5, the resulting mean bias for this library is -0.00782 ± 0.00361. For MCNP5, using the continuous energy cross-section library based on ENDF/B-VI, the resulting variance weighted mean bias is - 0.00574 ± 0.00509.

Correlations of bias with respect to moderator-to-fuel ratio (H / ^{235}U) number density ratio and absorber strength (Σ_a^{th}) were investigated and found to be not significant. The coefficient of determination for bias versus moderator-to-fuel ratio for the 238 group ENDF/B-V library was a negligible 2.6%, whereas for MCNP5 it was 4.1%, indicating that the method bias is not strongly dependent on moderator-to-fuel ratio. In all cases, the bias becomes less negative with decreasing moderator-to-fuel ratio (i.e., increasing enrichment). The coefficient of determination for bias versus absorber strength for the 238 Group ENDF/B-V library was an insignificant 6.1%, while for MCNP5, it was 37.1%. In all cases, the bias becomes less negative with increased absorber strength. These results are illustrated in Figures 3-1 and 3-2, respectively.

Table 3-1: B&W [6] and CSNI [7] Critical Experiments - Design Parameters

Reference	Experiment Number	Absorber Type	Absorber $\ni_a$ [cm^{-1}]	Enrichment w%	$H/^{235}U$ Ratio
6	XIII	BORAL	1.871	2.459	216.43
6	XIV	BORAL	1.460	2.459	216.52
6	XV	BORAL	0.475	2.459	216.52
6	XVII	BORAL	0.293	2.459	216.54
6	XIX	BORAL	0.129	2.459	216.54
7	1-1	none	-	2.35	398.72
7	1-2-1	none	-	4.75	109.44
6	1-2-2	none	-	4.75	228.53
7	2-1	BORAL	30.6	2.35	398.72
7	2-2	BORAL	24.6	4.75	228.53
7	3-A-1	none	-	2.35	398.75
7	3-B-1	none	-	2.35	398.75
7	3-A-2	BORAL	24.6	4.75	228.53

Table 3-2 B&W[6] and CSNI[7] Critical Experiment Results

Reference	Experiment	SCALE 5			MCNP5		
		Keff	sigma	bias	Keff	sigma	bias
6	XIII	0.99341	0.00017	-0.00659	0.99422	0.00035	-0.00578
6	XIV	0.98989	0.00018	-0.01011	0.98997	0.00035	-0.01003
6	XV	0.98623	0.00017	-0.01377	0.98525	0.00035	-0.01475
6	XVII	0.98972	0.00016	-0.01028	0.98846	0.00034	-0.01154
6	XIX	0.99136	0.00018	-0.00864	0.99004	0.00035	-0.00996
7	1-1	0.99048	0.00017	-0.00952	0.99294	0.00032	-0.00706
7	1-2-1	0.99404	0.00020	-0.00596	1.00000	0.00030	0.00000
7	1-2-2	0.99774	0.00020	-0.00226	1.00000	0.00030	0.00000
7	2-1	0.98925	0.00017	-0.01075	0.99164	0.00032	-0.00836
7	2-2	0.99549	0.00020	-0.00451	1.00000	0.00030	0.00000
7	3-A-1	0.99390	0.00018	-0.00610	0.99012	0.00033	-0.00988
7	3-B-1	0.99287	0.00017	-0.00713	0.99590	0.00033	-0.00410
7	3-A-2	0.99904	0.00020	-0.00096	0.99746	0.00041	-0.00254
	Arithmetic Mean	0.99218			0.99426		
	Variance Weighted			-0.00782			-0.00574
	Standard Deviation			± 0.00361			± 0.00509

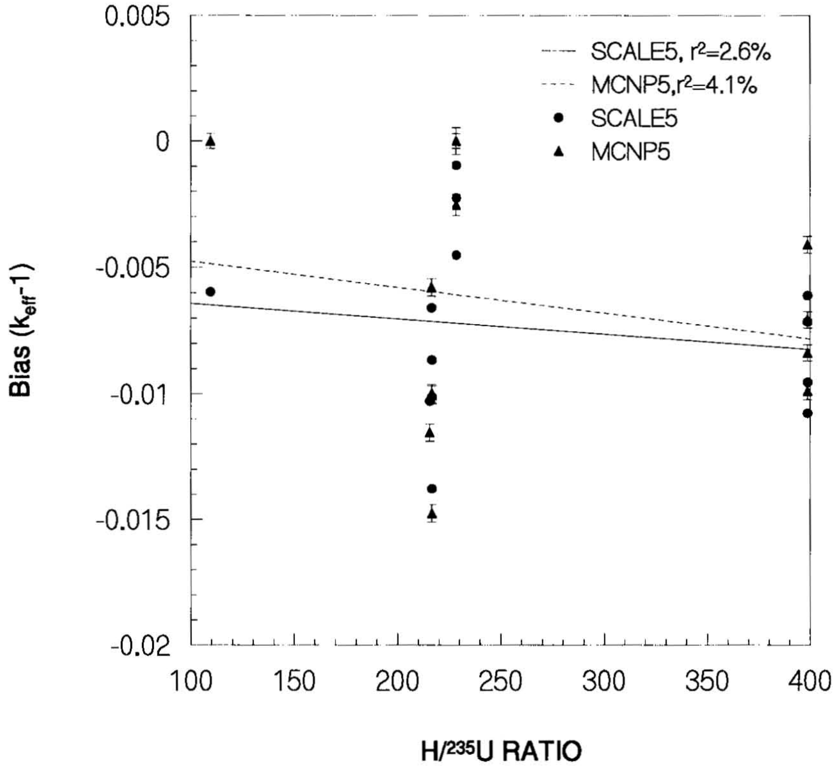

Figure 3-1: Variation of Bias (k_{eff} -1) with Moderator-to-Fuel Ratio

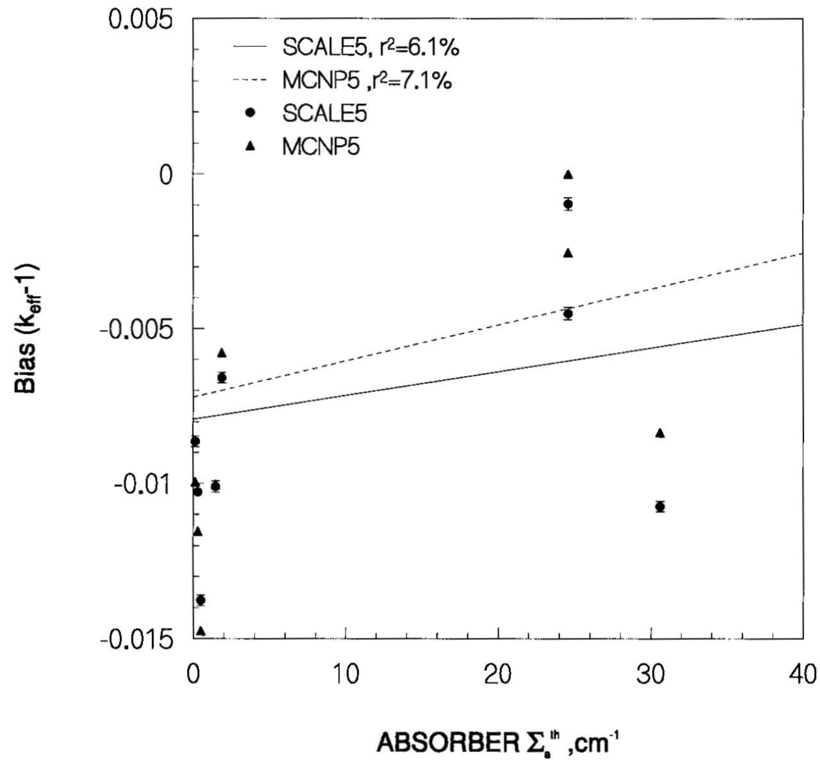

Figure 3-2: Variation of Bias (k_{eff} -1) with Absorber Strength

3.2 BENCHMARKING OF CASMO-4

This section compares SCALE-5[1] and CASMO-4[2] calculations for k_4 of the same five B&W critical experiments[6] discussed in Section 3.1. CASMO-4 is limited in its ability to render a geometric model and can only be used for infinite arrays of assemblies. Thus, for this benchmark analysis, the central assembly of the 3x3 array of assemblies in the B&W critical experiments was modeled and then assumed to be infinitely reflected. The assembly pitch was preserved in the model, but the effect of the finite water reflector around the 3x3 array was lost, making the model supercritical.

SCALE-5 was also used to model the B&W critical experiments with exactly the same geometry as they were rendered in CASMO-4. Because the bias of SCALE-5 is known (see Section 3.1), it can be applied to the SCALE-5 result to obtain a best-estimate of the supercritical state of the infinitely reflected assembly model. The CASMO-4 result can then be compared with this best estimate to obtain a CASMO-4 bias.

The results of the SCALE-5 and CASMO-4 analyses are compared in Table 3-3. The CASMO-4 bias is calculated as

$$bias_{CASMO\text{-}4} = k_{CASMO\text{-}4} - k_{SCALE\text{-}5,\ best\ estimate}$$

where

$$k_{SCALE\text{-}5,\ best\ estimate} = k_{SCALE\text{-}5} - bias_{SCALE\text{-}5}$$

For CASMO-4 the resulting mean bias and standard deviation for the 238 Group ENDF/B-V library are -0.01028 and 0.00198 respectively.

Table 3-3: B&W Critical Experiments as CASMO Infinite Arrays - Results

Experiment	CASMO-4	SCALE-5 (bias corrected)		
		238GROUPNDF5		
		Keff	sigma	bias
XIII	1.08816	1.10160	0.00050	-0.01423
XIV	1.08860	1.10175	0.00049	-0.01523
XV	1.09832	1.10961	0.00045	-0.01280
XVII	1.10740	1.11732	0.00045	-0.00945
XIX	1.11614	1.12330	0.00043	-0.00832
			bias	-0.01028
			Sigma	± 0.00198