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Additional Critical Experiments
for Computer Code Validation Base

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ADDITIONAL CRITICAL EXPERIMENTS FOR CRITICALITY ANALYSIS COMPUTER CODE VALIDATION BASE

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ABSTRACT

This paper describes the validation, in accordance with ANSI/ANS-8.1-1983(R1988), of KENO V.a using the 27-group ENDF/B-IV cross section library for some neutronic systems containing highly-enriched uranium, carbon, and hydrogen. This constituent combination is present in many packaging applications for the safe transportation of fissile and fissionable materials. The validation has been performed for two separate computational platforms: an IBM 3090 mainframe and an HP 9000 Series 700 workstation, both using the Oak Ridge Y-12 Plant Nuclear Criticality Safety Software (NCSS) code package. Critical experiments performed at the Oak Ridge Critical Experiments Facility in support of the Rover reactor program were identified as having the constituents desired for this validation as well as sufficient experimental detail to allow accurate construction of KENO V.a calculational models. Calculated values of k_{eff} for the Rover experiments, which contain uranium, carbon, and hydrogen, are between 1.0012 +/- 0.0026

and 1.0245 +/- 0.0023. These experiments can now be added to KENO V.a and other computer code critical experiment data bases which are used for validation and to establish upper limits on calculated values of k_{eff} for specific applications.

INTRODUCTION

Safe transportation of fissile and fissionable material depends on the prevention or mitigation of undesirable consequences resulting from plausible accidents. Containers, or packages, are used as a means of achieving this end. 10CFR71¹ requires a demonstration of package suitability for specific applications by prescribing various analysis parameters to be considered in analysis of both normal and hypothetical accident conditions. For the subcriticality evaluation, this includes calculation of the neutron multiplication factor (k_{eff}) of finite and infinite arrays of packages under a spectrum of interspersed moderator densities and other conditions which maximize array reactivity.

Specifically, packages used for transportation of highly-enriched uranium often incorporate urethane foam (or other hydrogenous material) and cellulose for cushioning and thermal

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insulation, respectively.² These materials can be broadly classified as organic and consist of mainly hydrogen, carbon, and oxygen such that package arrays can be neutronicly categorized as highly-enriched uranium systems with carbon and hydrogen moderation. In some instances, the presence of materials such as cellulose in the package array is necessary for maintenance of subcriticality since they reduce reactivity by providing neutron moderation. Moderation in these cases increases the probability of parasitic absorption in the packaging materials, thus decreasing the neutronic interaction of the fissile material within the package arrays. It has been shown that the mass of the organic material has the greatest influence on array reactivity, with configuration effects (i.e., close fitting or offset from the fissile material) being secondary at best.³ Thus, it is necessary to have confidence that the criticality code is accurately representing the effects of these materials when performing the calculations. Validation (or benchmarking) of codes using experimental data is a method used to provide this confidence and to identify any biases that may exist in a calculational methodology (computer code, computational platform, and cross section library/nuclear data). Critical experiments are used to validate criticality codes such as KENO V.a (part of the SCALE⁴ system) and to establish upper bounds for k_{eff} in accordance with national standards⁵ such that a sufficient safety margin is maintained for particular applications.

Standard reference documents contain many critical experiments whose k_{eff} values can be calculated using computer codes to provide confidence in code accuracy and to establish k_{eff} limits. However, these documents do not contain experiments containing both hydrogen and carbon as moderators. The purpose of this work is to validate KENO V.a and the 27-group ENDF/B-IV cross section library in accordance with the appropriate national standard⁵ using critical experiments from the Rover program, which contain the materials discussed above. These experiments can then be incorporated into the validation data base for KENO V.a and

other criticality codes to provide additional data in establishing upper bound k_{eff} values for packaging and other applications.

CRITICAL EXPERIMENTS

Critical experiments containing the constituents of interest together with sufficient detail to construct accurate KENO V.a models were identified through a literature search. A set of twenty-five experiments conducted at the Y-12 Plant during the mid-1960s in support of the Rover reactor program contained highly-enriched uranium, carbon, and hydrogen.⁶ These experiments are summarized in the paragraphs below.

The Rover program was conceived during the late 1950s as a means of propulsion for space missions. From this project came a design for a spacecraft engine called the Nuclear Engine for Rocket Vehicle Application (NERVA). The NERVA fuel elements were hexagonal graphite rods extruded to create 19 holes which ran throughout the length of the element and through which hydrogen gas was passed during reactor operation. Uranium dicarbide beads, enriched to 93.15% in U^{235} , were mixed with the graphite before extrusion and as a result were uniformly distributed throughout the element. Two variations of this element, designated NRX-A3 and NRX-A4, were used in the Oak Ridge critical experiments. These variants were similar to each other, the only differences being the diameter of the holes in the element (0.244 cm for the NRX-A3 elements versus 0.252 cm for the NRX-A4), overall length (132.58 cm and 131.83 cm for the NRX-A3 and NRX-A4 elements, respectively), and average U^{235} loading (118 grams per NRX-A3 element; 123 grams per NRX-A4 element). Some of the elements were cut into 7.62 cm segments which were used to simulate a partial length element.

The elements were arranged in a large tank using Plexiglas^(R) strips or Plexiglas^(R) templates to achieve the desired spacing and then flooded with water. At least 15.2 cm of water reflection was present on all sides (including top and

bottom) of the assembly. The number of elements present in a given critical assembly varied based on lattice pitch. The twenty-five experiments fall into four general categories:

1. Square pitch lattices, elements in aluminum tubes
2. Triangular pitch lattices, elements in aluminum tubes
3. Triangular pitch lattices, bare elements
4. Triangular pitch lattices, 38.1 cm long bare elements

KENO V.a MODELS

KENO V.a models of the Rover critical experiments are very explicit to minimize assumptions and approximations. The Rover experiments are well described either in reports or in logbooks kept by the experimenters. Utilization of this information greatly reduced the number of modeling assumptions. However, some assumptions as listed below were necessary to build the KENO V.a models. For each case, the KENO V.a model reflected the actual experimental configuration as indicated in the logbooks.

The following assumptions, resulting mainly from limitations of the computer code, were necessary to model the Rover critical experiments:

1. Due to KENO V.a geometry limitations, the hexagonal fuel elements had to be approximated as equivalent volume cylinders. The compromise thus introduced is small since the maximum dimensional discrepancy is .127 cm.
2. In some of the experiments, Plexiglas^(R) spacers were placed at 30 and 60 degree angles which cannot be modeled in KENO V.a. Therefore, the Plexiglas^(R) and water were homogenized into a

single mixture at axial levels where Plexiglas^(R) was present.

3. The uranium is assumed to be homogeneously distributed throughout the graphite fuel elements.

RESULTS

The results, segregated by computational platform, are presented in Tables 1 and 2 and Figures 1 and 2.

Calculations of the Rover experiments are slightly high for both the IBM and HP platforms, with k_{eff} values ranging between 1.0012 +/- 0.0026 and 1.0245 +/- 0.0023 (Tables 1 and 2). A linear least squares fit of the data seems to indicate an upward trend with increasing Average Energy Group (AEG) of the neutrons causing fission (decreasing neutron energy), but the difference in the end points of this line (around 0.006) is within approximately two standard deviations for a typical calculation and is therefore not considered to be statistically significant.

To determine if the Rover critical assemblies could be considered homogeneous in nature, three cases were selected and the overall critical assembly homogenized to represent a fictitious homogeneous system: 2.794 cm pitch square lattice (in tubes), 5.563 cm pitch triangular lattice (in tubes), and the 4.140 cm pitch triangular lattice (bare). These cases were run using two different methods of cross section treatment, as discussed below:

1. The first method employed BONAMI, NITAWL, and KENO V.a with the infinite homogeneous medium approximation for cross section processing. Spatial variation of the neutron flux was thus ignored. These calculations yielded k_{eff} values of 1.0522 +/- 0.0030, 1.2902 +/- 0.0021, and 1.1749 +/- 0.0029, respectively, for the three cases. These results are different than those of the explicitly modeled

heterogeneous assemblies, but are in agreement with the calculated k_{eff} of solutions with the same fissile material concentration.

2. The second method used BONAMI, NITAWL, XSDRNPM, and KENO V.a. The cross sections are flux weighted by XSDRNPM to reflect spatial variations in neutron flux due the fuel/moderator unit cell arrangement. This approach would reveal whether the increase in k_{eff} observed using the first method was due to something other than heterogeneous effects from the lattice arrangement of fuel elements. The k_{eff} values from these calculations are 1.0288 +/- 0.0040, 1.019 +/- 0.0024, and 1.0182 +/- 0.0033, respectively, which compare well with the heterogeneous cases.

The Rover assemblies cannot be considered homogeneous systems since there is a pronounced spatial neutron flux variation due to the fuel/moderator unit cell arrangement. The heterogeneous cases yield calculated k_{eff} values in good agreement with the experiments over the entire range of H/U²³⁵ ratios. The heterogeneous models should be used in the validation data base since they are based on the actual experimental configuration.

CONCLUSIONS

The Oak Ridge Y-12 Plant version of KENO V.a and the 27-group ENDF/B-IV cross section library has been validated for certain systems containing highly-enriched uranium, carbon, and hydrogen. This validation is based on comparison of KENO V.a results using the 27-group ENDF/B-IV cross-section library with experimental results from the Rover program. These constituents are representative of those found in many packaging applications involving highly-enriched uranium and the experiments can be included in validation data bases since the results are in good agreement with those of the experiments. However, this work does not

validate all highly-enriched uranium systems with hydrogen and carbon moderation. It is incumbent on the user of this data to ensure that utilization and extension of it to specific applications be performed in accordance with appropriate standards⁵ and facility practices. Until critical experiments are performed with large arrays of small fissile masses, containing organic material(s) as interstitial moderation, the Rover results can be used to provide additional confidence that the uranium, hydrogen, and carbon cross section data and results from computer codes using that data are accurate and reliable.

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TABLE 1

SUMMARY OF ROVER RESULTS (IBM 3090)
Explicit, Heterogeneous Models

Lattice	Pitch (cm)	H/U ²³⁵	C/U ²³⁵	k _{eff}	AEΓ*	Histories	
Square, in Tubes	2.79	79	88.8	1.0083 +/- .00303	22.83	78000	
	3.05	121	88.3	1.0108 +/- .00338	23.35	84500	
	3.30	164	88.0	1.0111 +/- .00310	23.67	90500	
	3.56	215	87.8	1.0124 +/- .00287	23.87	93500	
	3.81	267	87.5	1.0117 +/- .00273	24.01	95000	
	4.06	324	87.5	1.0150 +/- .00247	24.11	97000	
	4.32	384	87.6	1.0160 +/- .00252	24.20	99000	
	4.57	450	87.7	1.0150 +/- .00214	24.26	100000	
	4.83	520	88.1	1.0166 +/- .00246	24.31	100000	
	5.08	594	88.3	1.0058 +/- .00251	24.36	100000	
Triang., in Tubes	3.23	112	88.4	1.0112 +/- .00274	23.29	82500	
	3.81	215	88.0	1.0125 +/- .00290	23.86	91500	
	4.11	271	87.9	1.0202 +/- .00292	24.04	95000	
	4.39	332	87.8	1.0155 +/- .00274	24.14	96500	
	4.70	399	87.9	1.0136 +/- .00240	24.21	97500	
	5.28	544	88.1	1.0162 +/- .00260	24.34	100000	
	5.56	627	88.5	1.0155 +/- .00233	24.38	100000	
	Triang., Bare	2.51	93	88.0	1.0136 +/- .00347	23.05	85000
		3.12	176	87.1	1.0051 +/- .00307	23.75	93500
		3.73	277	87.0	1.0072 +/- .00297	24.05	98500
4.14		354	87.0	1.0104 +/- .00268	24.18	100000	
4.78		497	87.6	1.0080 +/- .00233	24.31	100000	
Triang., Bare (38.1 cm)	3.12	166	87.0	1.0037 +/- .00346	23.66	90500	
	3.73	262	87.0	1.0070 +/- .00308	24.01	95000	
	4.14	336	87.0	1.0089 +/- .00275	24.13	96500	

*Average Energy Group of Neutrons Causing Fission

TABLE 2

SUMMARY OF ROVER RESULTS (HP 9000)

Explicit, Heterogeneous Models

<u>Lattice</u>	<u>Pitch (cm)</u>	<u>H/U²³⁵</u>	<u>C/U²³⁵</u>	<u>k_{eff}</u>	<u>AEG*</u>	<u>Histories</u>	
Square, in Tubes	2.79	79	88.8	1.0088 +/- .00321	22.81	83500	
	3.05	121	88.3	1.0072 +/- .00294	23.36	89000	
	3.30	164	88.0	1.0090 +/- .00289	23.66	90000	
	3.56	215	87.8	1.0062 +/- .00276	23.87	96000	
	3.81	267	87.5	1.0086 +/- .00273	24.00	98000	
	4.06	324	87.5	1.0160 +/- .00258	24.12	100000	
	4.32	384	87.6	1.0129 +/- .00251	24.20	100000	
	4.57	450	87.7	1.0112 +/- .00250	24.26	100000	
	4.83	520	88.1	1.0124 +/- .00234	24.32	100000	
	5.08	594	88.3	1.0099 +/- .00239	24.36	100000	
	Triang., in Tubes	3.23	112	88.4	1.0089 +/- .00338	23.30	83000
		3.81	215	88.0	1.0093 +/- .00282	23.88	90500
		4.11	271	87.9	1.0172 +/- .00275	24.03	97500
		4.39	332	87.8	1.0188 +/- .00259	24.13	99000
4.70		399	87.9	1.0168 +/- .00263	24.21	100000	
5.28		544	88.1	1.0178 +/- .00245	24.34	100000	
5.56		627	88.5	1.0245 +/- .00227	24.39	100000	
Triang., Bare	2.51	93	88.0	1.0125 +/- .00321	23.04	88000	
	3.12	176	87.1	1.0042 +/- .00302	23.76	94000	
	3.73	277	87.0	1.0012 +/- .00255	24.05	98500	
	4.14	354	87.0	1.0071 +/- .00262	24.19	100000	
4.78	497	87.6	1.0054 +/- .00251	24.32	100000		
Triang., Bare (38.1 cm)	3.12	166	87.0	1.0082 +/- .00291	23.66	92500	
	3.73	262	87.0	1.0073 +/- .00291	23.99	96500	
	4.14	336	87.0	1.0122 +/- .00273	24.13	98500	

*Average Energy Group of Neutrons Causing Fission

K-EFFECTIVE VS AVERAGE ENERGY GROUP
 ROVER EXPERIMENTS (HP 9000)

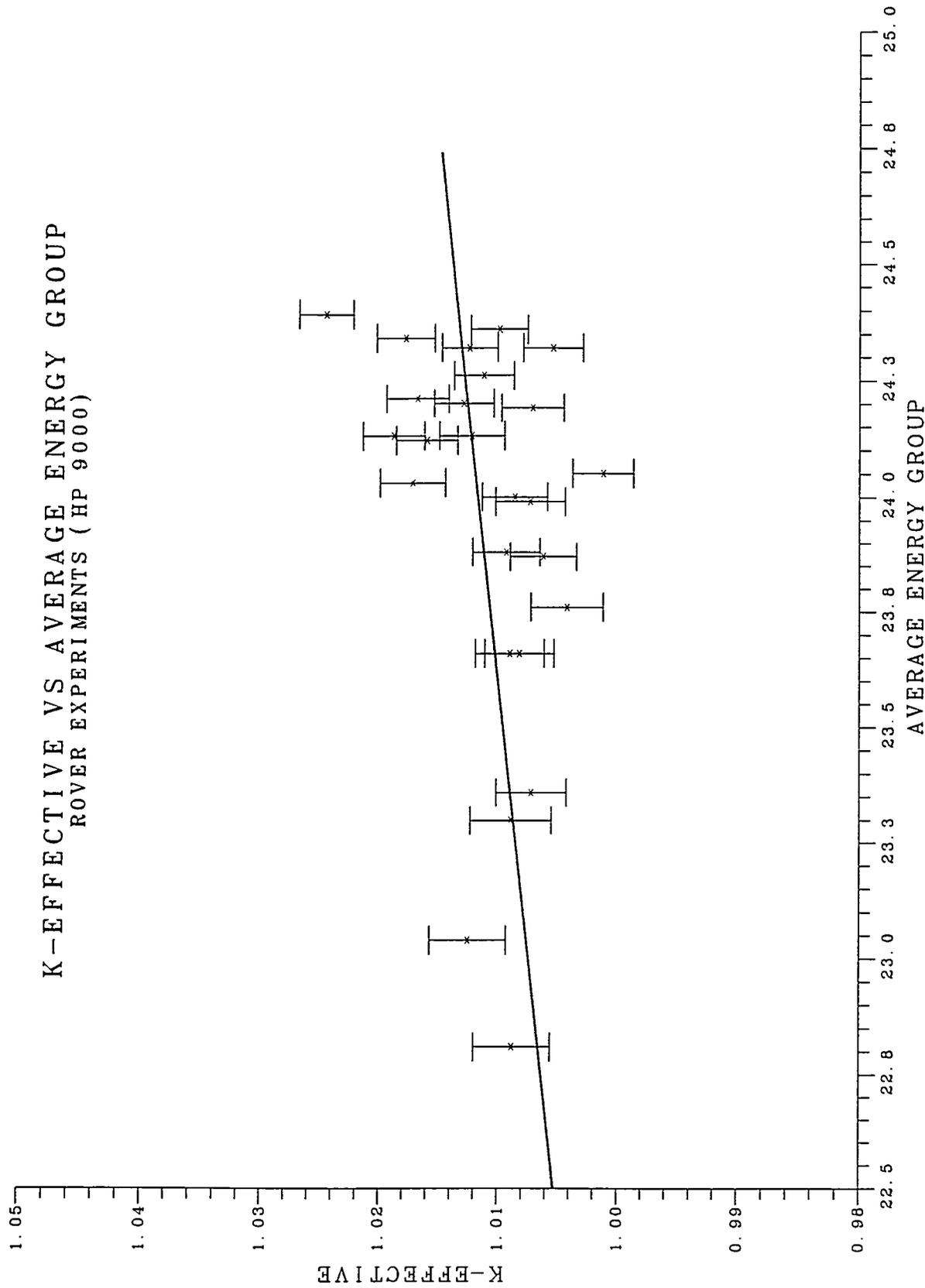


FIGURE 2 K-EFFECTIVE VS. AVERAGE ENERGY GROUP FOR ROVER EXPERIMENTS

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