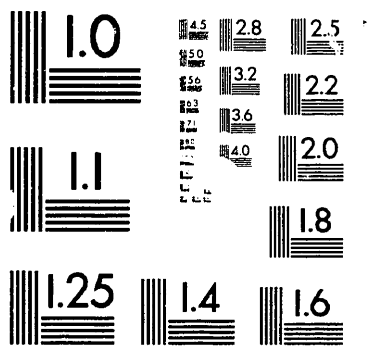
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OAK RIDGE Y-12 PLANT

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Validation of KENO V.a for Highly Enriched Uranium Systems with Hydrogen and/or Carbon Moderation

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VALIDATION OF KENO V.a FOR HIGHLY-ENRICHED URANIUM SYSTEMS WITH HYDROGEN AND/OR CARBON MODERATION

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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 systems containing highly-enriched uranium, carbon, and hydrogen and for systems containing highly-enriched uranium and carbon with high carbon to uranium (C/U) atomic ratios. The validation has been performed for two separate computational platforms: an IBM 3090 mainframe and an HP 9000 Model 730 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, and at the Pajarito site at Los Alamos National Laboratory 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. Calculation of the Los Alamos experiments, which contain uranium and carbon at high C/U ratios, yields values of k_{eff} between 0.9746 +/- 0.0028 and 0.9983 +/- 0.0027. Safety criteria can be established using this data for both types of systems.

INTRODUCTION

The Oak Ridge Y-12 Plant generates several types of recycle and waste materials contaminated with highly-enriched uranium. Examples include hydrocarbons, cellulose-based materials, and graphite casting molds. These materials can be categorically divided into two general types of systems: highly-enriched uranium, carbon, and hydrogen systems and highly-enriched uranium and carbon systems at high C/U atomic ratios. The Y-12 Plant version of KENO V.a could be used without further validation efforts to analyze these materials by modeling them as more reactive materials for which KENO V.a has been validated. However, this overly conservative approach would result in underutilization of storage containers and undersizing of process equipment which, in turn, would lead to inefficiency and increased costs. Validation of KENO V.a for systems containing highly-enriched uranium, hydrogen, and/or carbon would be beneficial by allowing more efficient use of processing and waste storage capabilities. The purpose of this work is to validate KENO V.a and the 27-group ENDF/B-IV cross section library for these two categories of systems in accordance with the appropriate national standard.[1] Many of the previously mentioned materials are indigenous to any facility that processes fissile material; therefore, the usefulness of this effort extends beyond the Y-12 Plant.

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 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.[2] Results from the Rover critical experiments have not previously been available to the general public. Also, Los Alamos National Laboratory (LANL) performed a series of experiments during 1957 which contained highly-enriched uranium and carbon at high C/U ratios.[3] These two sets of critical experiments are summarized below.

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[a] Managed for the U.S. Department of Energy by Martin Marietta Energy Systems, Inc., under contract number DE-AC05-84OR21400.

Rover Experiments

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 hexagonally-shaped graphite rods extruded to create 19 holes which ran throughout the length of the element. Uranium dicarbide beads, enriched to 93.15% in U^{235}, were uniformly distributed throughout the graphite matrix of each element. Two variations of this element, designated NRX-A3 and NRX-A4, were used in the critical experiments. These variants were very 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 for the NRX-A3; 123 grams for NRX-A4). 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 each side of the assembly. The number of elements present in a given critical assembly varied based on lattice pitch. The twenty-four 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

LANL Experiments

These experiments utilized the Honeycomb split-table machine.[3] This machine is comprised of a 24 x 24 array of 7.62 cm square aluminum tubes into which materials are inserted. The materials used in these critical experiments were CS-312 grade graphite blocks of various thicknesses and 1-mil (.0025 cm) uranium metal foils, enriched to 93.2% in U^{235}. The uranium foils were interleaved with graphite blocks to form fuel regions. Moderator regions containing only graphite were placed between the fuel regions to form a checkerboard pattern. The fuel regions contained from one to four uranium foils depending on the experiment. All of the critical assemblies were surrounded by a 30.48 cm thick graphite reflector and were slightly supercritical once assembled.

KENO MODELS

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

Rover Models

The following assumptions, resulting mainly from limitations of the 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 error this 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.

LANL Models

No modeling approximations were needed to set up the KENO V.a models for these experiments since the components consisted of rectangular blocks which can be exactly modeled. However, other approximations had to be made:

1. Some of the dimensions for spacing of the uranium foils were incorrect or missing. Using dimensions from the other experiments, reasonable values were chosen for these inadequately described cases.
2. The uranium foils were coated with a small amount of Teflon™ to retard oxidation. This coating was smeared uniformly into the uranium foils in the KENO V.a model.
3. Since the arrangement of the fuel and moderator is significantly different than the standard unit cell arrangements found in SCALE,[4] several different

cases were run to determine the effect of cross section processing on the calculated k_{eff}. Two different slab unit cell arrangements were input to BONAMI and NITAWL to obtain minimum and maximum Dancoff factors for the problem which are then used in KENO V.a. Another approximation was to homogenize fuel and moderator regions at C/U ratios of the overall core to obtain a cross section library for use in KENO V.a. The last option employed the infinite homogeneous medium approximation for each isotope or mixture.

RESULTS

The results, segregated by computational platform, are presented in Tables 1, 2, and 3, and in Figures 1 through 4. Safety criteria can be derived from this data in accordance with facility-specific procedures.

Rover Calculations

Calculations of the Rover experiments are generally high for both the IBM and HP platforms, ranging from k_{eff} values of 1.0012 +/- 0.0026 to 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, 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 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 significantly 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/U^{235} ratios. Thus, safety criteria should be set based on the heterogeneous cases.

LANL Calculations

Calculation of the LANL experiments yields results that are below 1.00 for both the IBM and HP platforms ranging between 0.9746 +/- 0.0028 and 0.9983 +/- 0.0027 as shown in Table 3. A least squares fit of the data shows an upward trend with increasing AEG. The difference between the end points of this line (around .010) is approximately four standard deviations which is considered significant and indicative of a trend in the data. The actual k_{eff} values for each of the experiments calculated based on figures for excess reactivity given in the logbooks are shown in Table 3. As stated earlier, several cross section processing options were used to investigate the effect on the calculated values of k_{eff}. Regardless of the method chosen, no statistically significant difference was noted in the calculated values of k_{eff}. The effective absorption cross section of U^{238} varied from a minimum of 8.0 to a maximum of 267.0 barns, but since only a small amount of this isotope is present, no effect due to resonance absorption is discernable. Homogenized models for this set of experiments were constructed and run using the BONAMI, NITAWL, and KENO V.a. The infinite homogeneous medium approximation was used to process the KENO V.a cross section library. The results of these cases, which are slightly higher than the heterogeneous cases, are shown in Table 3. The increase in k_{eff} is in good agreement with previously reported values.[3] However, safety criteria should be set based on the heterogeneous cases since the calculated results of these cases compare favorably with the actual experiments.

CONCLUSIONS

The Y-12 Plant version of KENO V.a has been validated for two categories of systems: those containing highly-enriched uranium, carbon, and hydrogen, and those which contain highly-enriched uranium and carbon at high C/U ratios. 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 and also with results from several LANL Honeycomb split-table critical experiments. These experiments are neutronically representative of contaminated waste and recycle materials found in a typical fissile material processing plant. Safety criteria can be established using results from the heterogeneous cases of both experimental series since the calculated values of these cases are in good agreement with experimental results.

REFERENCES

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3. H. L. REYNOLDS, "Critical Measurements and Calculations for Enriched-Uranium Graphite-Moderated Systems," UCRL-5175, March, 1958.

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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}	AEG*	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

Lattice	Pitch (cm)	H/U^{235}	C/U^{235}	k_{EFF}	AEG*	Histories
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

TABLE 3

SUMMARY OF LANL RESULTS

Heterogeneous Models

Case	C/U			k_{EFF}		AEG*		Histories
	Reported	Calculated	Actual**	IBM	HP	IBM	HP	
LA1	6650	6810	1.00038	0.9895 +/- .00284	0.9901 +/- .00279	23.46	23.44	100000
LA2	4937	4992	1.00028	0.9812 +/- .00283	0.9888 +/- .00267	23.10	23.09	100000
LA3	3140	3198	1.00035	0.9746 +/- .00277	0.9760 +/- .00281	22.43	22.40	100000
LA4	2365	2420	1.00155	0.9816 +/- .00275	0.9779 +/- .00265	21.93	21.92	100000
LA5	4366	4506	1.00069	0.9930 +/- .00290	0.9983 +/- .00267	23.00	23.00	100000
LA6	2770	2885	1.00079	0.9915 +/- .00283	0.9918 +/- .00267	22.23	22.26	100000

Homogeneous Models

Case	Reported	Calculated	Actual**	IBM	HP	IBM	HP	Histories
LA1	-	6810	-	1.0303 +/- .00282	--	23.54	-	75000
LA2	-	4992	-	1.0156 +/- .00301	--	23.16	-	75000
LA3	-	3198	-	1.0084 +/- .00289	--	22.48	-	75000
LA4	-	2420	-	1.0082 +/- .00323	--	21.97	-	75000
LA5	-	4506	-	1.0164 +/- .00314	--	23.01	-	75000
LA6	-	2885	-	1.0214 +/- .00355	--	22.29	-	75000

*Average Energy Group of Neutrons Causing Fission
**Values of k_{EFF} Were Calculated Based on Figures for Excess Reactivity From Logbooks

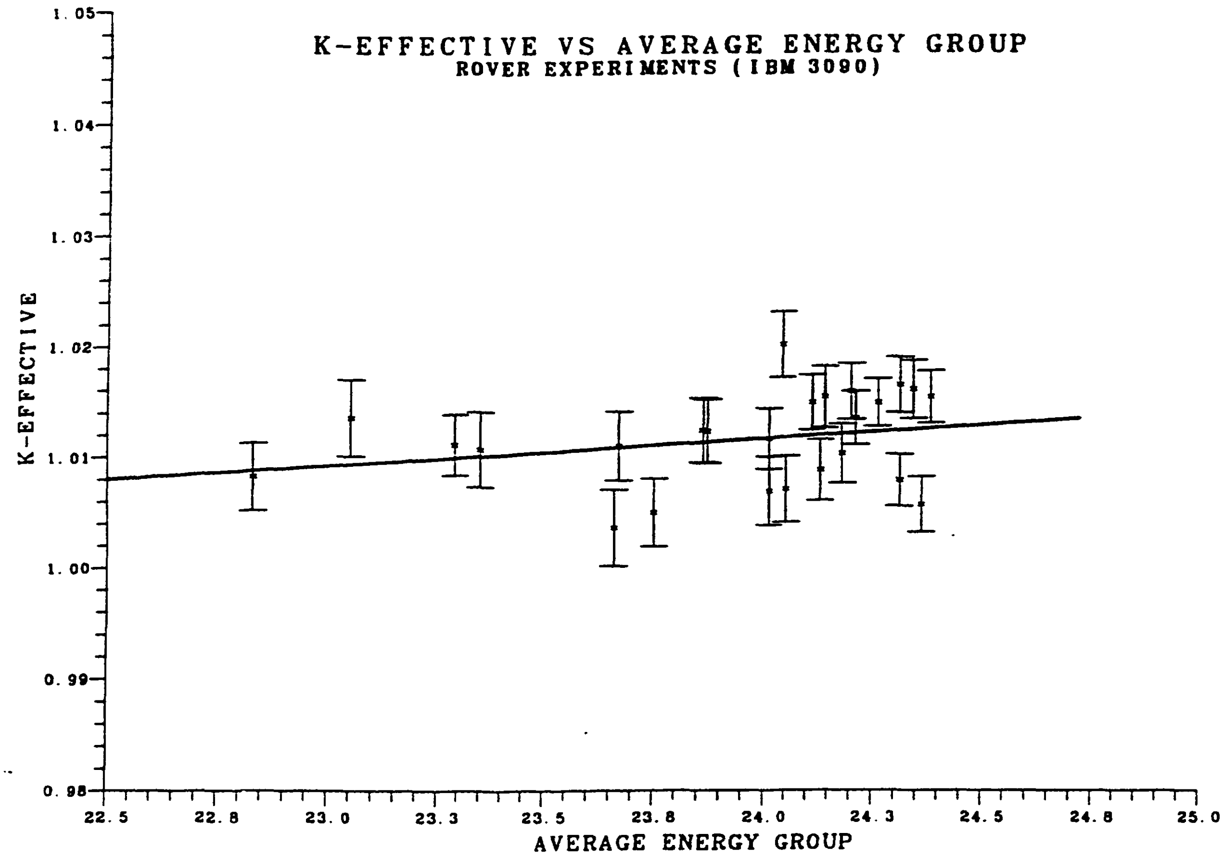

FIGURE 1 K-EFFECTIVE VS. AVERAGE ENERGY GROUP FOR ROVER EXPERIMENTS

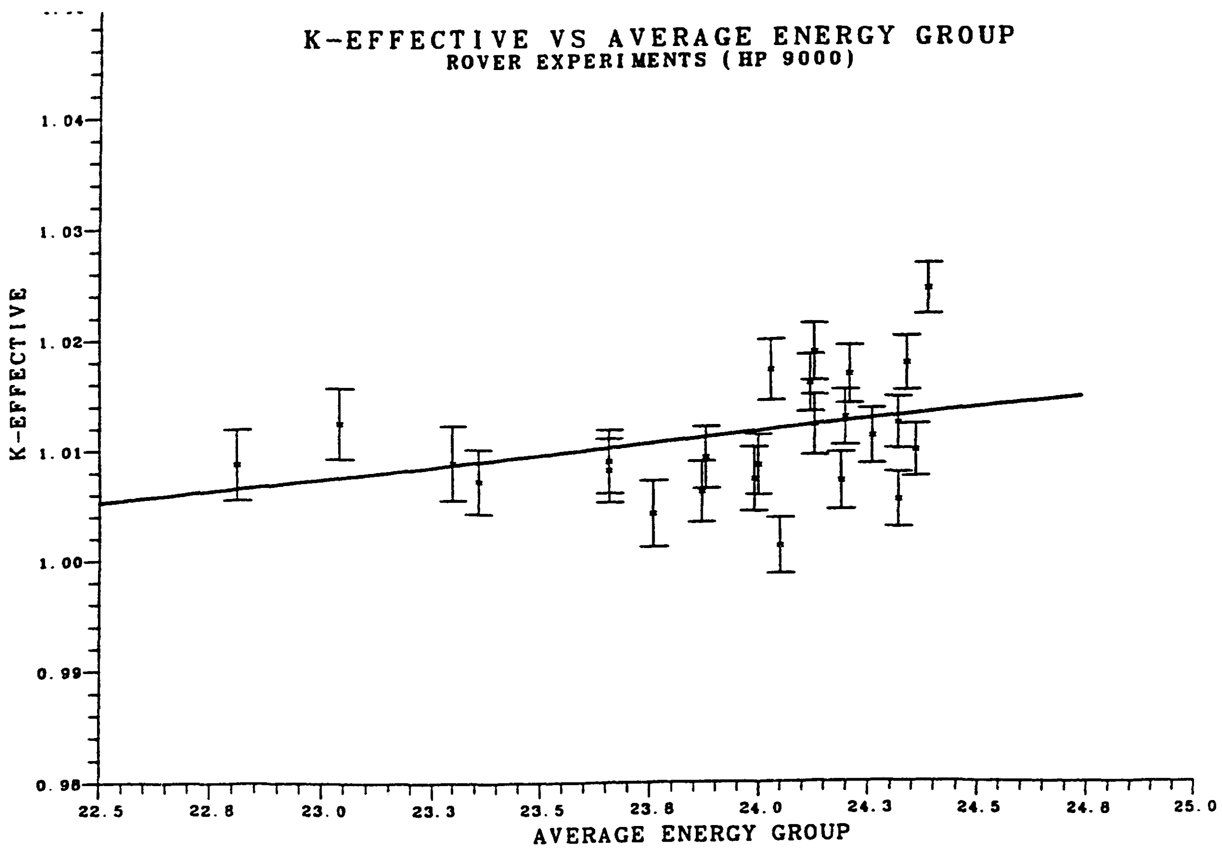

FIGURE 2 K-EFFECTIVE VS. AVERAGE ENERGY GROUP FOR ROVER EXPERIMENTS

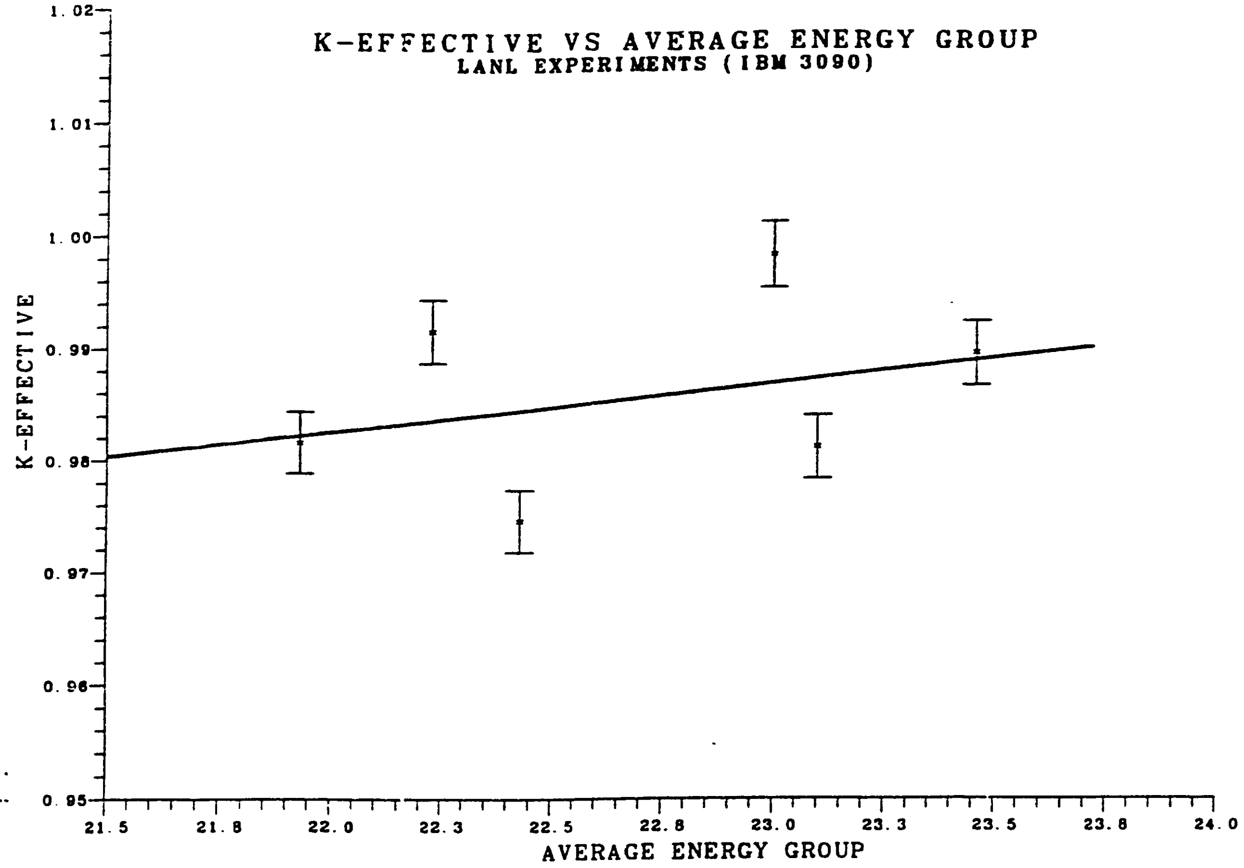

FIGURE 3 K-EFFECTIVE VS. AVERAGE ENERGY GROUP FOR LANL EXPERIMENTS

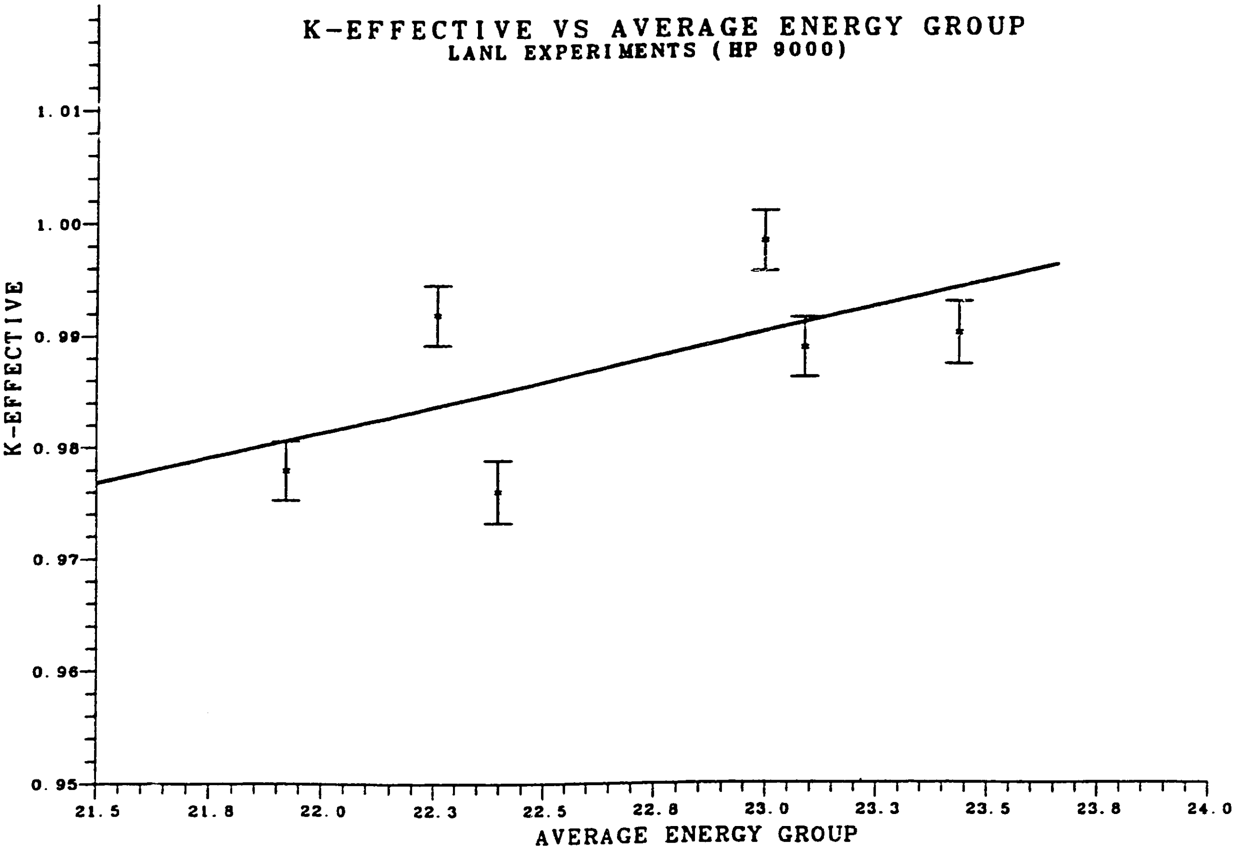

FIGURE 4 K-EFFECTIVE VS. AVERAGE ENERGY GROUP FOR LANL EXPERIMENTS

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