LA-UR 93-757

CONF-930907--1

TITLE: MCNP/KENO CRITICALITY BENCHMARKS

AUTHOR(S): Gregg W. McKinney
John C. Wagner
James E. Sisolak

DISCLAIMER

RECEIVED

APR 05 1993

OSTI

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

FORM NO 836 R4
ST NO 2629 5/81

MASTER

MCNP/KENO CRITICALITY BENCHMARKS

by

Gregg W. McKinney
Los Alamos National Laboratory
Los Alamos, NM 87545

by

John C. Wagner
Pennsylvania State University
University Park, PA 16802

by

James E. Sisolak
University of Wisconsin
Madison, WI 53706

I. INTRODUCTION

In the past, criticality safety analyses related to the handling and storage of fissile materials were obtained from critical experiments, nuclear safety guides, and handbooks. As a result of rising costs and time delays associated with critical experiments, most experimental facilities have been closed, triggering an increased reliance on computational methods. With this reliance comes the need and requirement for redundant validation by independent criticality codes. Currently, the KENO[1] Monte Carlo transport code is the most widely used tool for criticality safety calculations. For other transport codes, such as MCNP,[2] to be accepted by the criticality safety community as a redundant validation tool, they must be able to reproduce experimental results at least as well as KENO.

1

The Monte Carlo neutron, photon, and electron transport code MCNP, developed by Los Alamos National Laboratory (LANL), X-6 Group, has an extensive list of attractive features, including continuous energy cross sections, generalized 3-D geometry, time dependent transport, criticality k_{eff} calculations, and comprehensive source and tally capabilities. It is widely used for nuclear criticality analysis, nuclear reactor shielding, oil well logging, and medical dosimetry calculations (to mention a few) in many research laboratories within the United States, Canada, Europe, and Japan, in addition to over 100 universities and private companies throughout the world.

This benchmark study is third in a series of LANL MCNP benchmark reports. The two prior reports[3,4] demonstrate that MCNP can accurately model several analytic problems as well as a diverse set of neutron and photon experiments. This report specifically addresses criticality and benchmarks the KENO 25 problem test set. These sample problems constitute the KENO standard benchmark set and represent a relatively wide variety of criticality problems.[1] The KENO Monte Carlo code was chosen because of its extensive benchmarking against analytical and experimental criticality results. Whereas the uncertainty in experimental parameters generally prohibits code validation to better than about 1% in k_{eff}, the value of k_{eff} for criticality is considered unacceptable if it deviates more than a few percent from measurements.[5]

II. BENCHMARK OVERVIEW

Table I presents an overview of the computer systems and code input associated with this benchmark effort. Upon converting the KENO 25 problem test set to an equivalent MCNP test set, every effort was made to duplicate features employed in the KENO input files (the MCNP inputs are given in Appendix A of Ref. 6). Whenever possible, a description of the actual experiment was used to verify the geometry specifications and results. In addition,

all volumes and material densities calculated by KENO and MCNP were compared to ensure consistency.

With one exception (natural boron), the MCNP calculations were performed using the LANL "recommended" cross-sections (i.e., atomic identifiers ending with .50c at 300 K, based on ENDF/B-V as processed by the NJOY code - see Ref. 2). Where applicable, the $S(\alpha,\beta)$ treatment for hydrogen (in water and paraffin) was included to account for molecular scattering of thermal neutrons (the hydrogen $S(\alpha,\beta)$ data for polyethylene was substituted for paraffin). KENO was run in stand-alone mode, separate from the SCALE package which provides cross-section processing, thus the Hansen-Roach 16 group library was employed.

Key features of the KENO 25 problem test set are summarized in Table II, and additional details can be found in Ref. 6. Note that over half of the configurations include the uranium metal 2C unit shown in Fig. 1(a). The remaining figures (b-d) are indicative of the geometric diversity included in the test set. Although several of these problems model the same geometry, they were included to test various features of the KENO/MCNP transport codes.

III. BENCHMARK RESULTS

The MCNP values for k_{eff} are those of the covariance-weighted combined estimator (a combination of the collision, absorption, and track-length estimators). MCNP provides seven estimators of k_{eff}, and although the optimal estimator is problem dependent and should be determined from calculated correlation coefficients, a single estimator is reported here to eliminate ambiguity. The KENO output, on the other hand, includes a single estimator for k_{eff} (which appears to be a collision-based estimator).

The MCNP/KENO estimates of k_{eff} for each of the 25 sample problems is presented in Table III, with percent differences between the transport codes as well as from experiment.

Note that experimental results are not provided for several of the inputs (6,8,9,16,17,18). Of these, 6 and 8 are clearly subcritical, whereas experimental results for 9 and 16, being geometrically infinite, most likely do not exist. Problem 17 is likely a critical experiment, and the KENO input for problem 18 appears to deviate significantly from its related experiment.

While the MCNP average deviation from experiment (.2%) is notably smaller than that of KENO (.4%), both codes provide excellent agreement with experimental results. The impact of the MCNP $S(\alpha,\beta)$ thermal scattering treatment is evident in Table IV. Any reduction in the MCNP/KENO discrepancies as a result of including this treatment can be debated; however, its inclusion clearly improves MCNP's agreement with experimental data.

IV. CONCLUSIONS

The criticality capability of MCNP and its related continuous energy cross-section data have been benchmarked to the KENO criticality transport code as well as to experimental data. The KENO 25 problem test set was chosen for use in this analysis since it represents a relatively wide variety of criticality problems and is used to validate KENO. Results from this benchmark study indicate that MCNP can successfully predict experimental measurements, in some cases better than KENO, and thus can accurately model a variety of criticality problems within expected data and statistical uncertainties.

REFERENCES

1. L.M. Petrie and N. F. Landers, "KENO V.a An Improved Monte Carlo Criticality Program with Supergrouping," NUREG/CR-0200, Vol. 2 Section F11, 1984.

4

2. J. F. Briesmeister, Editor, "MCNP - A General Monte Carlo Code for Neutron and Photon Transport, Version 3A," LA-7396-M, Rev. 2, 1986.

3. D. J. Whalen et al., "MCNP: Neutron Benchmark Problems," LA-12212, 1991.

4. D. J. Whalen et al., "MCNP: Photon Benchmark Problems," LA-12196, 1991.

5. W. C. Jordon et al., "Validation of KENO V.a Comparison with Critical Experiments," ORNL/CSD/TM-238, 1986.

6. J. C. Wagner et al., "MCNP: Criticality Safety Benchmark Problems," LA-12415, 1992.

TABLE I

OVERVIEW OF COMPUTER SYSTEMS AND CODE INPUT

	MCNP	KENO
COMPUTER		
Hardware	Cray Y-MP	Cray X-MP
Operating System	UNICOS	CTSS
CODE		
Version	4.2	V.a
Parameters		
Initial Source	Uniform Volume	Uniform Volume
Particles/Cycle	3000	3000
Settle Cycles	20	20
Total Cycles	200	200
Data	Continuous Energy ENDF/B-V with $S(\alpha,\beta)$	Hansen-Roach 16 Group

TABLE II

FEATURES OF THE KENO 25 PROBLEM TEST SET

Problem No.	Enrichment	Array	Description
URANIUM METAL			
1,2,10,11, 22,23,24,25	93.2	2x2x2	2C8 (uranium metal cylinders)
3,4	93.2	2x2x2	2C8 with 15.24cm paraffin ref.
5	93.2	2x2x2	2C8 with 30.48cm paraffin ref.
6	93.2	–	2C single unit
7	93.2	2x2x2	2C with specular ref. on 3 sides
8	93.2	–	2C with specular ref. on ends
9	93.2	Infinite	2C with specular ref. on all sides
13	93.2	–	2 cuboids in a cylindrical annulus
14	93.2	–	1 cylinder in a cylindrical annulus
15	92.6	–	Sphere 6.5cm radius with water ref.
URANIUM METAL/URANYL NITRATE SOLUTION			
12,19	93.2/92.6	2x2x2	4 metal 2C units + 4 aqueous units
URANYL NITRATE SOLUTION			
18	92.6	3x3x3	1F27 with 15.24cm paraffin ref.
URANYL FLUORIDE SOLUTION			
16	93.2	Infinite	5 slabs specular ref. on all sides
17	93.0	–	Sphere 16.0cm radius
20	93.2	7	Triangular pitched cylinders
21	4.89	–	Sphere 34.6cm radius, 98% filled

TABLE III

k_{eff} Values for KENO and MCNP

case	MCNP k_{eff}	MCNP relative error(%)	KENO k_{eff}	KENO relative error(%)	%DIFFERENCE mcnp from keno	%DIFFERENCE mcnp from exp	%DIFFERENCE keno from exp
1	0.9999	.09	0.9996	.11	0.0	-0.0	-0.0
2	0.9999	.09	0.9996	.11	0.0	-0.0	-0.0
3	0.9990	.11	1.0009	.13	-0.2	-0.1	0.1
4	0.9945	.28	1.0016	.15	-0.7	-0.5	0.2
5	0.9995	.27	1.0210	.09	-2.1	-0.0	2.1
6	0.7461	.10	0.7487	.13	-0.3	*	*
7	0.9993	.09	0.9984	.11	0.1	-0.1	-0.2
8	0.9401	.09	0.9430	.12	-0.3	*	*
9	2.2905	.05	2.2617	.04	1.3	*	*
10	0.9979	.14	0.9996	.11	-0.2	-0.2	-0.0
11	0.9979	.14	0.9982	.12	-0.0	-0.2	-0.2
12	0.9997	.12	1.0055	.13	-0.6	-0.0	0.6
13	0.9942	.09	1.0026	.12	-0.8	-0.6	0.3
14	0.9991	.09	1.0011	.10	-0.2	-0.1	0.1
15	1.0016	.11	1.0012	.20	0.0	0.2	0.1
16	0.9902	.09	0.9936	.07	-0.3	*	*
17	1.0029	.14	0.9783	.23	2.5	*	*
18	1.0302	.13	1.0088	.15	2.1	*	*
19	0.9997	.12	1.0044	.13	-0.5	-0.0	0.4
20	0.9960	.12	0.9791	.14	1.7	-0.4	-2.1
21	0.9962	.08	1.0012	.09	-0.5	-0.4	0.1
22	0.9992	.09	0.9996	.11	-0.0	-0.1	-0.0
23	0.9999	.09	0.9996	.11	0.0	-0.0	-0.0
24	0.9994	.08	0.9999	.11	-0.1	-0.1	-0.0
25	1.0004	.08	0.9987	.11	0.2	0.0	-0.1

* Experimental values of k_{eff} could not be located for these problems.

TABLE IV

k_{eff} Values for MCNP with and without the S(α, β) Treatment

	MCNP with S(α,β)		MCNP no S(α,β)		%DIFFERENCE			
case	k_{eff}	relative error(%)	k_{eff}	relative error(%)	with S(α,β) from keno	no S(α,β) from keno	with S(α,β) from exp	no S(α,β) from exp
3	0.9990	.11	1.0168	.11	-0.2	1.6	-0.1	1.7
4	0.9945	.28	1.0181	.25	-0.7	1.6	-0.5	1.8
5	0.9995	.27	1.0156	.28	-2.1	-0.5	-0.0	1.6
12	0.9997	.12	1.0010	.13	-0.6	-0.4	-0.0	0.1
15	1.0016	.11	1.0189	.12	0.0	1.8	0.2	1.9
16	0.9902	.09	0.9953	.09	-0.3	0.2	*	*
17	1.0029	.14	0.9830	.15	2.5	0.5	*	*
18	1.0302	.13	1.0479	.12	2.1	3.9	*	*
19	0.9997	.12	1.0010	.13	-0.5	-0.3	-0.0	0.1
20	0.9960	.12	0.9932	.16	1.7	1.4	-0.4	-0.7
21	0.9962	.08	0.9811	.10	-0.5	-2.0	-0.4	-1.9

* Experimental values of k_{eff} could not be located for these problems.

(a)

(b)
Top view

Uranium metal

13.97 cm

19.05 cm

12.7 cm

Side view

Uranium metal

16.18 cm

0.2566 cm

11.176 cm

7.62 cm

0.2566 cm

Uranium metal

Uranium

11.496 cm

10.765 cm

(c)

200.0 cm

200.0 cm

Borated UO₂F₂ solution

UO₂F₂ solution

Pyrex

Borated UO₂F₂ solution

Borated UO₂F₂ solution

1.27 cm

4.958 cm

13.73 cm

34.958 cm

(d)

Paraffin

Plexiglas

Void

Uranyl nitrate solution

19.05 cm
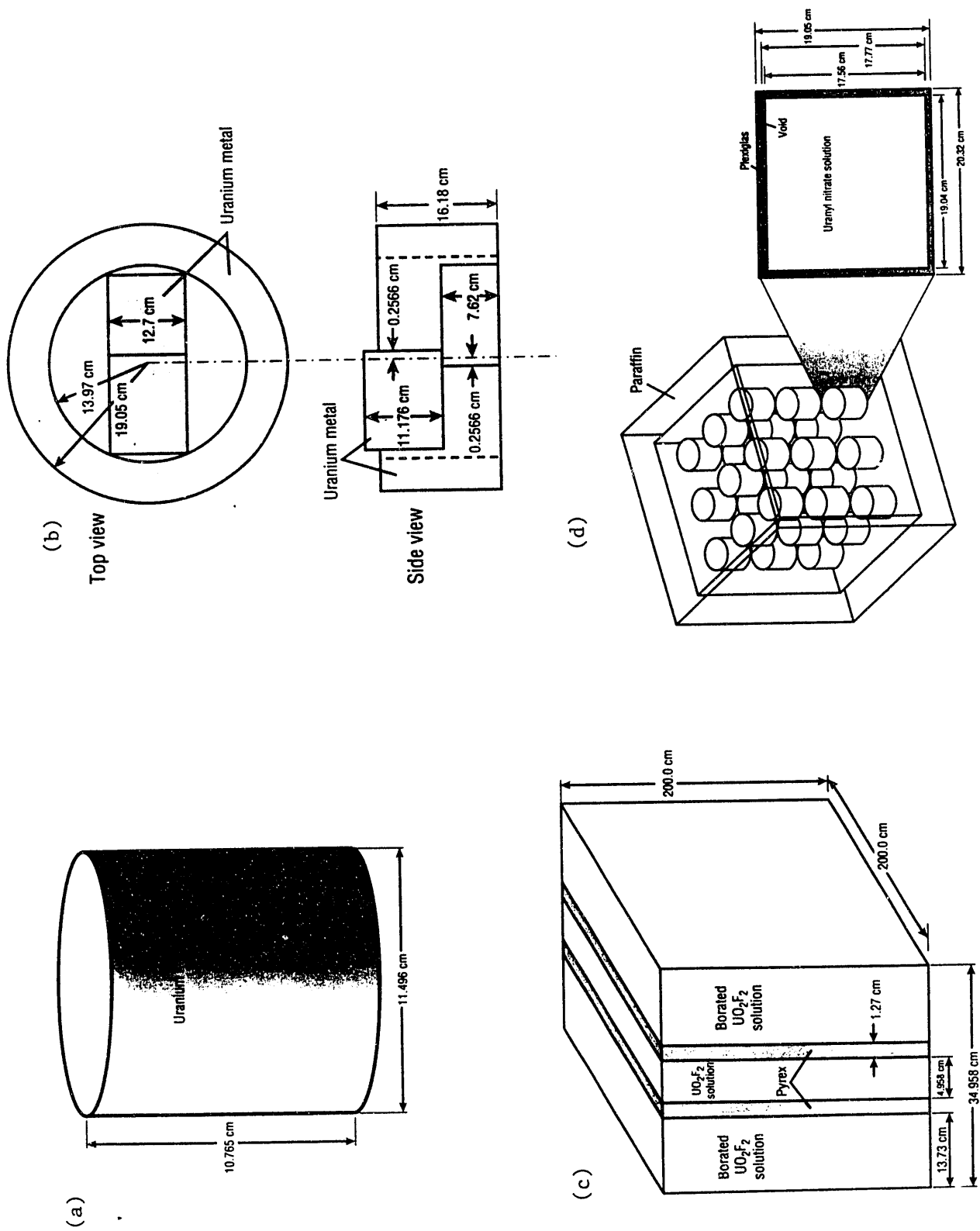
17.56 cm

17.77 cm

20.32 cm

19.04 cm

Fig. 1. Sample geometries of the KENO test set (problems 6,13,16, & 18).

END

DATE FILMED

8/17/93