CONF-950910--24

LA-UR- 95-1932

Title: TRANSX/DANT BENCHMARK STUDIES USING AN ENDF/B-V BASED MATXS LIBRARY

Author(s): R. C. Johns, R. D. Mosteller, R. T. Perry

Submitted to: ICNC '95, Albuquerque, NM, September 17-22, 1995

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Los Alamos
NATIONAL LABORATORY

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. The Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy.

Form No. 836 R5
ST 2629 10/91

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

TRANSX / DANT Benchmark Studies Using an ENDF/B-V Based MATXS Library

Russell C. Johns, Russell D. Mosteller, and R. T. Perry
Reactor Design and Analysis Group
Technology and Safety Assessment Division
Los Alamos National Laboratory
Los Alamos, NM 87545
505 665.3521
505 665.3167 - FAX
rtperry@lanl.gov

Final Paper to be Submitted to ICNC '95
at Albuquerque, NM
Sept. 1995

TRANSX/DANT BENCHMARK STUDIES USING AN ENDF/B-V BASED MATXS LIBRARY

Russell C. Johns, Russell D. Mosteller, and R. T. Perry
Reactor Design and Analysis Group
Technology and Safety Assessment Division
Los Alamos National Laboratory
Los Alamos, NM 87545
505 665.3521
505 665.3167 - FAX
rtperry@lanl.gov

SUMMARY

A series of 20 benchmark critical experiments were studied using the DANT code with cross section libraries prepared by TRANSX from ENDF/B-V based MATXS libraries. The benchmarks were selected to cover both fast and thermal systems utilizing either uranium or plutonium as the primary fissile isotope. An effort was made to cover the range of isotopes prevalent in nuclear systems, though no heterogeneous thermal plutonium cases were included. The results indicate that the code package and library give satisfactory results for the majority of cases, though the results are somewhat poorer for thermal plutonium cases.

METHODOLOGY

The analysis was performed using DANT[1,2] with ISOTXS formatted cross sections prepared in TRANSX[3] from a standard 69 group MATXS-12 library[3]. These benchmarks were derived from specifications given by either the Cross Section Evaluation Working Group (CSEWG)[4] or by the International Criticality Safety Benchmark Evaluation Project (ICSBEP)[5]. The majority of these cases are spheres modeled one-dimensionally, but there are a few cylindrical cases as well. All cases were prepared using transport-corrected, truncated Legendre expansions, and appropriate self shielding. Additional runs were made with varying mesh, quadrature order, and Legendre expansion order to assure that the results were within 0.001 Δk of the best possible setting for that parameter. The results should be within 0.002 Δk of the best possible settings for all parameters. A summary of the actual cases studied is presented in Table I. Brief descriptions of the case types are given below. The results of these case studies have been compared with both the actual benchmark values or in cases where there were significant idealizations, a corrected value was used. The details of these corrections and the full model specifications can be found in either the CSEWG benchmarks or in a forthcoming publication known as the ICSBEP Handbook. The results have also been compared with previous MCNP runs[6].

CASE DESCRIPTIONS

The benchmarks fit into five groups: metallic ^{235}U systems with fast spectra, highly enriched solutions of uranyl nitrate, metallic plutonium spheres, plutonium nitrate spheres, and a bare sphere of ^{233}U.

Metallic ^{235}U Systems With Fast Spectra

There are three cases of metallic ^{235}U with fast spectra: the bare Godiva sphere, the reflected Topsy sphere, and a generic water-

TABLE I
Summary of Benchmark Critical Experiments

Case Title	Description	Source	Ref.	Spectrum
Godiva	Bare HEU Sphere	ICSBEP	7,8	Fast
Topsy	HEU Sphere in natural-U sphere	ICSBEP	9	Fast
HEU Sphere in H_20	HEU sphere reflected by water	ICSBEP	10,11	F w/ Tail
ORNL - 1	Bare sphere of uranyl nitrate	CSEWG	12,13	Thermal
ORNL - 2	Bare sphere of uranyl nitrate	CSEWG	12,13	Thermal
ORNL - 3	Bare sphere of uranyl nitrate	CSEWG	12,13	Thermal
ORNL - 4	Bare sphere of uranyl nitrate	CSEWG	12,13	Thermal
ORNL -10	Bare sphere of uranyl nitrate	CSEWG	12,13	Thermal
Jezebel -233	Bare sphere of ^{233}U	ICSBEP	14	Fast
Jezebel	Bare plutonium sphere	ICSBEP	14,15	Fast
Jezebel - 240	Bare plutonium sphere (20 a/o ^{240}Pu)	ICSBEP	14	Fast
Pu Sphere in H_20	Plutonium sphere reflected by water	ICSBEP	16	F w/ Tail
PNL - 1	Bare sphere of plutonium nitrate	CSEWG	17,18	Thermal
PNL - 2	Bare sphere of plutonium nitrate	CSEWG	17,18	Thermal
PNL - 3	Bare sphere of plutonium nitrate	CSEWG	17,18	Thermal
PNL - 4	Bare sphere of plutonium nitrate	CSEWG	17,18	Thermal
PNL - 5	Bare sphere of plutonium nitrate	CSEWG	17,18	Thermal
Pu Nitrate Sphere -1	Sphere of plutonium nitrate reflected by water	ICSBEP	17,18	Thermal
Pu Nitrate Sphere -2	$PuNO_3$ sphere, (low ^{240}Pu) reflected by water	ICSBEP	17,18	Thermal
Pu Nitrate Sphere -3	Dilute $PuNO_3$ sphere reflected by water	ICSBEP	17,18	Thermal

reflected sphere. All of the cases used highly enriched uranium (HEU).

The Godiva Sphere[7,8] is a bare, Homogenous sphere of uranium enriched to 93.71 wt. % ^{235}U. Godiva is modeled here one-dimensionally using six shells of slightly varying enrichment and is based on the ICSBEP specifications.

The reflected Topsy sphere[9] consists of a central sphere of HEU with an 8-in. thick reflector of natural uranium. The enrichment in the central sphere is 93.5 wt. % ^{235}U. The principal isotopes in this case are ^{235}U in the central sphere and ^{238}U in the outer reflector. Again the specifications come from the ICSBEP handbook.

The water-reflected sphere of HEU[10,11] differs from the other cases in that it has a significant fraction of fissions occurring at thermal and epithermal energies, almost 30% of the fissions occur at energies below 0.1 MeV. It is a sphere of HEU enriched to 97.67 wt. % ^{235}U, supported by a Plexiglas stand in a tank of water. It has been idealized in the ICSBEP handbook as a homogenous sphere surrounded by an effectively infinite spherical shell of water, and those are the specifications employed in this study. The principal isotopes are the ^{235}U in the sphere and the ^{1}H in the water.

Highly Enriched Solutions of Uranyl Nitrate

This series of experiments consists of the five CSEWG benchmarks. The benchmarks are designated as ORNL-1, ORNL-2, ORNL-3, ORNL-4, and ORNL-10, because they are based on experiments performed at Oak Ridge National Laboratory[12,13]. In these experiments, varying concentrations of uranyl nitrate solutions, with the uranium enriched to approximately 94 wt. %, are contained in homogenous spheres of light water. ORNL-2, ORNL-3, and ORNL-4 also contain small amounts of boron. The isotopes of principal interest in these experiments are ^{235}U and ^{1}H, as well as ^{10}B in the cases that contain boron.

Jezebel 233

The so-called Jezebel-233 experiment was a bare, homogenous uranium sphere comprised primarily of ^{233}U (98.13 a/o) [14]. It produced a very fast neutron spectrum, and it appears as a benchmark for both the CSEWG and the ICSBEP. The calculations in this study use the specifications given in the ICSBEP handbook.

Metal Spheres of Plutonium

These cases include the standard Jezebel experiment, the so-called Jezebel-240 experiment and a plutonium sphere reflected by water.

The configuration for both Jezebel experiments[14,15] was simply a bare sphere of plutonium. The most significant difference between the two experiments is that the standard Jezebel contained only 4.5 at. % of ^{240}Pu, while the Jezebel-240 contained almost 20 at. %. The isotopes of principal importance in the experiments are ^{239}Pu, and for the Jezebel-240 experiment, ^{240}Pu. Both of these experiments appear as benchmarks for both the CSEWG and ICSBEP. The specifications for the cases in this study are taken from the ICSBEP handbook.

The configuration for the water reflected plutonium sphere experiment[16] was very similar to that for the water-reflected HEU sphere discussed above. A sphere of plutonium was placed on a stand inside a tank of water, and the benchmark model like the HEU case, consists of the plutonium sphere surrounded by an effectively infinite spherical shell of water. The bulk of the fissions are produced by fast neutrons with energies above 0.1 MeV, but there is a significant thermal tail in the spectrum due to moderation by the water. The isotopes of principal interest are ^{239}Pu, ^{240}Pu, and ^{1}H.

Spheres of Plutonium Nitrate

This set of cases consists of two subsets, though all of them are based on experiments conducted by Batelle Pacific Northwest Laboratory(PNL) [17,18].

The first subset contains the CSEWG benchmarks designated as PNL-1 through PNL-5, all of which are bare spheres of plutonium nitrate. The plutonium concentration in PNL-2 is more than four times as concentrated as in PNL-1; the concentration in PNL-3 and PNL-4 is approximately one-half that of PNL-1, and the spheres are somewhat larger. The plutonium concentration in PNL-5 is approximately the same as in PNL-1, but the sphere is slightly larger. Results for these cases are affected primarily by ^{239}Pu, ^{240}Pu, ^{1}H, and to a lesser extent ^{14}N.

The second subset, taken from the ICSBEP handbook, consists of three cases in which a solution of plutonium nitrate and water is contained inside a stainless steel sphere that is surrounded by an effectively infinite spherical shell of water. The second case contains a much lower concentration of ^{240}Pu than the first (approximately 0.5 a/o, as opposed to 4.6 a/o), while the plutonium nitrate in the third case is considerably more dilute than the first case (about one-quarter the plutonium concentration). Results for these three cases are affected primarily by ^{239}Pu, ^{240}Pu, ^{1}H,^{14}N, and stainless steel.

RESULTS

The numerical results for the benchmark cases are given in Table II. As a whole, the uranium based cases agreed well with the benchmarks, generally within 0.002 Δk, for both fast and thermal spectrum cases, with the exceptions of the fast, water-reflected, HEU sphere and a sphere of ^{233}U.

The plutonium benchmarks did not agree as well as the uranium benchmarks. The fast spectrum cases yielded eigenvalues that were 0.002 to 0.005 Δk low of the benchmark value. The thermal plutonium nitrate solution cases were typically a percent or more in k higher than the benchmark values. A substantial part of the thermal behavior could be this particular MATXS library, as the agreement between MCNP and DANT for these cases degraded significantly. Previous DANT cases agreed with MCNP typically within a tolerance of a quarter percent in k, whereas these plutonium nitrate solution cases are typically nearing a half percent in k and are always higher.

Metallic ^{235}U Systems with Fast Spectra

The results are reasonably good and compare well in general with the benchmark for these cases. The worst case, the water reflected HEU sphere, which was 0.004 Δk low of the benchmark value, has a significant thermal and epithermal fission component. The epithermal range could be responsible for the discrepancy as most of the thermal cases came high of their benchmark values.

Highly Enriched Solutions of Uranyl Nitrate

Again, all of these cases agreed well with their benchmark values, though the cases with boron did not compare as well with MCNP. ORNL-3 appears to be an aberration as it is an intermediate step between ORNL-2 and ORNL-4. ORNL-2 has approximately half of the ^{10}B concentration of ORNL-3, and a more dilute concentration of uranyl nitrate. The increase in boron between ORNL-3 and ORNL-4 is only about 25% again with a further increase in the concentration of uranyl nitrate. The enrichment remains constant, and MCNP also shows this irregularity, so there appears to be no other explanation.

Jezebel 233

The ENDF/B-V result for k_{eff} of Jezebel-233 has the worst agreement with the benchmark values of any of the uranium cases. This is probably due to the ^{233}U cross sections as it is the only isotope present in abundance. Preliminary studies with ENDF/B-VI libraries show a small but significant improvement in the computed value due almost exclusively to changes in the worth of ^{233}U, though the new evaluation is merely a reprocessing of the ENDF data.

Metal spheres of Plutonium

As mentioned above, the plutonium cases were as a whole worse than the uranium cases, though the fast spectrum cases fared better than the thermal spectrum cases. In contrast to the fast uranium cases the best result with the plutonium cases was the water reflected sphere, which has a significant epithermal and thermal tail. This is explained easily as fast spectrum plutonium cases tended to compute low of the benchmark value, while thermal cases computed high of their respective benchmark values.

Spheres of Plutonium Nitrate.

The PNL spheres have been problems for several generations of ENDF/B (ENDF/B-IV produced even higher values for k_{eff} than ENDF/B-V). The only good result in both the PNL spheres and the ICSBEP

TABLE II
Results from Benchmark Experiments

Case Title	Benchmark k_{eff}	ENDF/ B-V	Δ K Benchmark	Δ K MCNP
Godiva	1.0000	0.9984	-0.0016	0.0001
Topsy	1.0000	1.0026	0.0026	-0.0001
HEU Sphere in water	0.9985	0.9947	-0.0038	-0.0018
ORNL - 1	1.0003	1.0017	0.0014	0.0012
ORNL - 2	0.9998	1.0017	0.0019	0.0036
ORNL - 3	0.9999	0.9985	-0.0014	0.0024
ORNL - 4	0.9992	1.0001	0.0009	0.0037
ORNL -10	1.0003	1.0009	0.0006	0.0013
Jezebel -233	1.0000	0.9909	-0.0091	-0.0023
Jezebel	1.0000	0.9948	-0.0052	-0.0027
Jezebel - 240	1.0000	0.9963	-0.0037	-0.0031
Pu Sphere in water	1.0000	0.9982	-0.0018	-0.0017
PNL - 1	1.0	1.0202	0.0202	0.0056
PNL - 2	1.0	1.0122	0.0122	0.0062
PNL - 3	1.0	1.0007	0.0007	0.0047
PNL - 4	1.0	1.0076	0.0076	0.0043
PNL - 5	1.0	1.0123	0.0123	0.0035
Pu Nitrate Sphere -1	1.0000	1.0146	0.0146	0.0020
Pu Nitrate Sphere -2	1.0000	1.0138	0.0138	0.0022
Pu Nitrate Sphere -3	1.0000	1.0150	0.0150	0.0046

benchmarks is PNL-3, which reportedly has revised specifications forthcoming that should increase the computed value for k_{eff} significantly[19]. Preliminary studies with ENDF/B-VI libraries indicate that notable improvement has been made with the thermal plutonium evaluations, although the results still aren't ideal. The source of the changes in worth between libraries is an almost even mix of ^{239}Pu and ^{16}O (typically 0.0035 Δk and 0.003 Δk, respectively), and a measurable contribution from ^{240}Pu.

CONCLUSIONS

DANT in combination with TRANSX and ENDF/B-V libraries give reasonable results that can be used to predict the criticality of simple systems. Uranium-235 based systems agree reliably within 0.003 Δk of the benchmarks. Care should be exercised, however, if the system has a substantial epithermal or intermediate fissioning, as these cases could exceed this margin. It may be advisable to implement a bias with ^{233}U and plutonium based systems. With an appropriate bias most plutonium cases agree within 0.005 Δk.

REFERENCES.

1. O'Dell, R., F. Brinkley Jr., D. Marr, and R. Alcouffe; "Revised Users Manual for ONEDANT: A code Package for One-Dimensional, Diffusion Accelerated, Neutral Particle Transport," Los Alamos National Laboratory report LA-9184M (Dec. 1989).

2. O'Dell, R., F. Brinkley Jr., D. Marr, and R. Alcouffe; "Users Guide for TWODANT: A code Package for Two-Dimensional, Diffusion Accelerated, Neutral Particle

Transport," Los Alamos National Laboratory report LA-10049M (1984).

3. MacFarlane, R., "TRANSX 2: A Code for Interfacing MATXS Cross-Section Libraries to Nuclear Transport Codes," Los Alamos National Laboratory report LA-12312-MS.

4. "Cross Section Evaluation Working Group Benchmark Specifications," Brookhaven National Laboratory report BNL-19302 (ENDF-202) (November 1974).

5. "International Handbook of Evaluated Criticality Safety Benchmark Experiments," OECD Nuclear Energy Agency report NEA/NSC/DOC(95)03 (April 1995).

6. Iverson, J., and R. Mosteller, ."MCNP Calculations for Criticality-Safety Benchmarks with ENDF/B-V and ENDF/B-VI Libraries," submitted for presentation at the 1995 Annual Meeting of the American Nuclear Society.

7. Hansen, G., and H. Paxton, "Reevaluated Critical Specifications of some Los Alamos Fast-Neutron Systems," Los Alamos Scientific Laboratory report LA-4208 (June 1969).

8. Peterson, R., "Lady Godiva: An Unreflected Uranium-235 Critical Assembly," Los Alamos Scientific Laboratory report LA-1614 (September 1953).

9. Josephson, V., "Critical-Mass Measurements on Oralloy in Tuballoy and WC Tampers," Los Alamos Scientific Laboratory report LA-1114 (May 1950).

10. Byers, C., J. Koelling, G. Hansen, D. Smith, and H. Dyer, "Critical Measurements of a Water-Reflected Enriched Uranium Sphere," *Trans. Am. Nucl. Soc.*, **27**,412 (November 1977).

11. Taylor, R., "Fabrication and Isotopic Data for the Water Reflected U(97.67) Metal Sphere Critical Experiment," Oak Ridge Y-12 Plant report Y/DD-622 (November 1993).

12. Gwin, R., and D. Magnuson, "Eta of ^{233}U and ^{235}U for Critical Experiments," *Nucl. Sci. Eng.*, **12**, p. 364-380 (March 1962).

13. Staub, A., D. R. Harris, and Mark Goldsmith, "Analysis of a Set of Critical Homogenous U-H_2O Spheres," *Nucl. Sci. Eng.*, **34**, p. 263-274 (December 1968).

14. Jarvis, G., G. Linenberger, D. Orndoff, and H. Paxton, "Two Plutonium-Metal Critical Assemblies," *Nucl. Sci. Eng.*, **8**, pp. 525-531 (December 1960).

15. Engle, L., G. Hansen, and H. Paxton, "Reactivity Contributions of Various Materials in Topsy, Godiva, and Jezebel," *Nucl. Sci. Eng.*, **8**, pp. 543-569 (December 1960).

16. Smith, D., and W. Geer, "Critical Mass of a Water-Reflected Plutonium Sphere," *Nucl. Appl. Technol.*, **7**, pp. 405-408 (November 1969).

17. Lloyd, R., C. R. Richey, E. D. Clayton, and D. R. Skeen, "Criticality Studies with Plutonium Solutions," *Nucl. Sci. Eng.*, **25**, pp. 165-173 (November 1966).

18. Richey, C., "Theoretical Analyses of Homogenous Plutonium Critical Experiments," *Nucl. Sci. Eng.*, **31**, p. 32-39 (January 1968).

19. Private communication with Mark L. Williams (LSU) August 1994.