FINAL REPORT:
Subcontract 9-X60-D1200, Task 6
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FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994
Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

Dr. Robert Busch of the Department of Chemical and Nuclear Engineering was the principal investigator on this project with technical direction provided by the staff in the Nuclear Criticality Safety Group at Los Alamos. During the period of the contract, he had a number of graduate and undergraduate students working on subtasks. The objective of this work was to develop information on Uranium systems to enhance benchmarks for use in the verification of criticality safety computer models.

During the first year of this project, most of the work was focussed on setting up the SUN SPARC-1 Workstation and acquiring the literature which described the critical experiments. By August 1990, the Workstation was operational with the current version of TWODANT loaded on the system. MCNP, version 4 tape was made available from Los Alamos late in 1990. There were some problems noted with the Hansen-Roach cross section library which was sent for implementation on the SUN workstation. It appears that there are only 87 isotopes in the library instead of the usual 118. This created some problems in the analysis of the benchmarks, but did not affect the initial checkout of the TWODANT implementation.

Various documents were acquired which provide the initial descriptions of the critical experiments under consideration as benchmarks. The major document is UCRL-53369, Nuclear Criticality Safety Experiments, Calculations, and Analyses - 1958 to 1982, Volumes 1 and 2, by Brian Koponen and Viktor Hampel. This provides a compilation of papers which appeared in the Transactions of the American Nuclear Society in the area of critical experiments. Through the reference and bibliography listings at the end of each paper, additional literature citations have been identified and acquisition of documents pertinent to Uranium systems and possible benchmark experiments continued throughout the duration of the project.

The next four years were spent working on various benchmark projects. A number of publications and presentations were made on this material. The first area of work and concentration was on the understanding of moderating properties of a system. Brent Bredehoft, a Master's student, did his thesis research on a parameter to characterize the thermalness of a system. This work was presented at ANS meetings, published in Nuclear Technology, and documented in his thesis. The abstract of the Nuclear Technology article follows.

CHARACTERIZATION OF THE THERMALNESS OF A FISSILE SYSTEM
WITH A TWO-GROUP DIFFUSION THEORY PARAMETER

Brent B. Bredehoft and Robert D. Busch, UNM
Nuclear Technology, Vol. 102, May 1993

In tabulating critical data, the hydrogen-to-fissile atom ratio (H/X) is commonly used to characterize the amount of moderation in a system. Though adequate in many cases, H/X

FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994

Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

does not account for the moderating contribution of other light nuclei contained in common uranium-moderator mixtures. This ratio also does not account for enrichment of the system, which affects the resonance absorption characteristics and, therefore, the moderating behavior of that system.

To alleviate these problems, a two-energy-group diffusion theory analogy to the six-factor formula was applied to define a new parameter $p/(\eta_2 \cdot f_2)$, which describes the moderation characteristics or the "thermalness" of a fissioning system and includes the effects of enrichment and the presence of moderators other than hydrogen.

From an analysis of several low-enriched uranium systems with different moderators, it was found that the values of $p/(\eta_2 \cdot f_2)$ corresponding to minimum critical mass and volume tend to center in a narrower range than do the values of H/X for the same systems. Also, the thermalness parameter does not vary with the addition of a reflector and is applicable to systems with other than hydrogenous moderators. Based on these results, the thermalness parameter $p/(\eta_2 \cdot f_2)$ provides an effective means of characterizing moderated systems relative to optimum conditions.

At the same time, Bob Busch and Doug O'Dell worked on a paper clarifying the use of the potential scattering cross sections in the LANL Hansen-Roach library. This paper was presented at the International Conference on Nuclear Criticality Safety '91 in Oxford, UK. The abstract of this paper follows:

VALIDITY OF HANSEN-ROACH CROSS SECTIONS WITH LOW ENRICHED URANIUM SYSTEMS

Robert D. Busch, UNM and R. Douglas O'Dell, LANL

Within the nuclear criticality safety industry, the Hansen-Roach 16 group cross section set has been the "standard" for use in k-effective calculations over the past 30 years. Yet even with its widespread acceptance, there are still questions about its validity and about the proper procedure for calculating sigma-p for uranium and plutonium. This paper addresses both issues: it compares the different prescriptions for the calculation of the potential scattering; and it uses Monte Carlo codes and discrete ordinates codes with and without the H-R cross sections to determine the validity of the H-R set when applied to low enriched Uranium systems.

Results indicate that very little difference occurs among k-effective calculations using the different sigma-p prescriptions. However, if no prescription is used or the uranium/plutonium cross section is selected at random, differences of 25% in k-effective may occur. Also it appears that with the proper use of sigma-p, the H-R set is valid when used with low enriched uranium systems, both powders and solutions. There also seems to be good agreement between the discrete ordinates codes and the Monte Carlo codes.

FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994

Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

This paper has received widespread dissemination through the NCS short courses given by UNM and through requests received at the Nuclear Criticality Technology Safety Project meetings.

The Nuclear Criticality Technology Safety Project meetings were the primary focus of communications for many of the project's results. Starting with the meeting in Knoxville in 1990, then Albuquerque in 1991, Gaithersburg in 1992, Monterey in 1993, and Williamsburg in 1994, presentations were made at each meeting on the ongoing work performed by UNM in the area of nuclear criticality safety and code benchmarks/validation.

Some of the work presented at the NCTSP meetings was that done during the second year of the project. This was work done by an undergraduate student, Deborah Bearden, in analyzing the variation of buckling with geometry. This involved the analysis of the buckling conversion process and its validity among the different geometries encountered in critical experiments. As TWODANT is only a two-dimensional code, some geometry conversion is usually required to handle the parallelepiped/cuboid experiments as well as some array experiments. It appears from previous work that buckling conversion from a geometry with curved leakage surfaces to one with flat leakage surfaces and vice versa doesn't seem to work as well as when conversion is done between geometries with similar leakage surface curvature. Debbie presented her results at an ANS student conference. The basic conclusion of the research was that the extrapolation distance did vary with geometry, but she was unable to find any correlation in the variations which would allow the creation of either an empirical formula or a graph. For most of the cuboid experiments, the size of the cuboid is usually much larger than the extrapolation distances so variations of a few percent in extrapolation distance led to variations of less than one percent in critical size.

In the Spring of 1992 (beginning of project's third year), another undergraduate, Leland Maez, worked on the project compiling information on uranium solutions. This involved creating a library of articles and papers which discussed the various physical, chemical, and thermodynamic properties of uranyl fluoride, uranyl sulfate, and uranyl nitrate. Since this involved more the acquisition of materials than any lengthy analysis, the results of this task are two binders full of the solution property data.

During the third and fourth years, Tracy Wenz was the primary graduate student on the project. She started by thoroughly analyzing GODIVA using TWODANT and KENO. This entailed an reasonable analysis of the impact of experimental parameters on the model efficacy. In addition, she also examined the data requirements for accurate translation between the experimental record and the computer input. This task was then extended to include the evaluation of the ability of TWODANT to accurately model flux and reactivity in GODIVA. The end result of this work was Tracy's thesis, A Transport Based One-Dimensional Perturbation Code for Reactivity Calculations in Metal Systems and a paper in Nuclear Technology on GODIVA reactivity worth calculations. The abstract for the Nuclear Technology article follows.

FINAL REPORT
for the Period of February 16, 1990 to December 31, 1994
Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

MODELING OF CENTRAL REACTIVITY WORTH MEASUREMENTS IN LADY GODIVA

Tracy R. Wenz and Robert D. Busch, UNM
Nuclear Technology, Vol. 105, January 1994

The central reactivity worth measurements performed in Lady Godiva were duplicated using TWODANT, a deterministic neutron transport code, and the 16-group Hansen-Roach cross-section library. The purpose of this work was to determine how well the Hansen-Roach library predicts the reactivity worths for a fast neutron system. Lady Godiva is a spherical uranium metal (93.7 wt% ^{235}U) critical assembly with a neutron flux distribution dominant in the first five groups of the Hansen-Roach energy structure (0.1 MeV and up). Provided that the cross sections of the replacement material do not undergo large variations (less than an order of magnitude) in any of the aforementioned groups, the calculated reactivities were within 10% of the experimental values. For cases where the reactivities were outside this range, a large variation in the cross section was found to exist in one of the groups, which was not fully accounted for in the Hansen-Roach group structure. However, even in the cases where the agreement between calculation and experiment was not good, the calculated reactivity appeared to be an extremum in that the effect was found to be either more negative or more positive than the experimental value.

The basic conclusion of Tracy's work was that TWODANT could adequately characterize reactivity worths using the Hansen-Roach library, but that for very small samples with large thermal or resonance cross sections, the absolute worth values may be off by a factor of two.

While Tracy was finishing her research, Charles Harmon started working on the project as a graduate student. During the fourth year, Chuck did the primary work of the project which was focussing on two areas: characterization of experiments and comparison of data requirements and results among different computer codes. The first area dealt with how to categorize benchmarks so that they can be related to the area of applicability as defined in ANS Standard 8.1. The results of the analysis indicated both a physical and a neutronic categorization were required to accurately determine the area of applicability. This work was presented at the 1993 ANS meeting in San Diego. The conclusion of the paper follows.

FINAL REPORT
for the Period of February 16, 1990 to December 31, 1994
Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

UTILITY OF CATEGORIZATION IN DETERMINING APPLICABILITY
OF NUCLEAR CRITICALITY BENCHMARK PROBLEMS

Charles D. Harmon II and Robert D. Busch
University of New Mexico

Note that is only a few instances will all physical and neutronic parameters match between the system being evaluated and the set of available benchmarks. Even with categorization, professional judgement will still be required in evaluating which physical and neutronic parameters are important and therefore should match, and which are not important and are not applicable for that system. By combining a physical categorization scheme with one that identifies the neutronic characteristics of a system, we believe that categorization can be a very useful tool for the evaluation of the applicability of benchmarks. However, as will all techniques in the criticality safety discipline, good professional judgment is required to accurately assess the match between a benchmark and a system to be evaluated. Categorization will not completely solve the problem for the criticality safety specialist, but it certainly provides the specialist with a powerful tool for identification of the utility of benchmarks in the evaluation of nuclear systems.

Chuck then worked on the second subtask analyzing selected critical experiments with deterministic and statistical codes. The objective was to provide evidence of correlation between computer model and experimental results with indications of ranges of applicability for the codes, cross sections, and experiments. The results of this were presented at the 1993 NCS Topical Meeting in Nashville. The introduction and conclusion of that paper follow.

COMPARISON OF RESULTS FROM KENO, MCNP, MONK, AND
TWO-DANT ON 12 CRITICALITY BENCHMARK PROBLEMS

Charles D. Harmon II, Robert D. Busch, and Thomas H. Jones
University of New Mexico

INTRODUCTION

The Evaluation Working Group for the Nuclear Criticality Technology and Safety Project has proposed a group of twelve sample problems for comparison of evaluation techniques. Although some of these problems are derived from experiments, they are not to be construed as experimental benchmarks. They represent a set of common computational benchmark problems provided for user analysis and comparison of results. These problems involve both uranium and plutonium in metal and solution states as single units and as arrays. The Nuclear Criticality Group from the University of New Mexico has evaluated these

FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994
Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

problems using three different Monte Carlo codes (KENO-Va, MCNP4xd, MONK6B) and an S_n Transport code (TWO-DANT). For this analysis, the Hansen-Roach 16 group library was used with KENO and TWO-DANT, the continuous energy cross sections derived primarily from ENDF-V were used with MCNP, and an 8221 pointwise library derived from JEF was used with MONK. The objective of the analysis was to determine how each of the codes performed with the variety of problems and to identify advantages and disadvantages associated with using specific codes or types of codes in certain problems. Each of the twelve problems were analyzed with the four codes where appropriate (three of the twelve were lattice problems which were not analyzed with TWO-DANT).

CONCLUSION

The basic conclusion of this study is that each problem should be analyzed with two or more different and independent techniques. There is no apparent set of general guidelines derivable from our results which would indicate that one technique should be applied in a given situation. In some cases, a specific code may be better suited to handling a given geometry (e.g. a large hexagonal lattice), but for a different type of problem, that code may be more difficult to use. There was not sufficient agreement in our study among the codes to allow an analyst to confidently state a value of k_{eff} within one percent of the actual physical value. Comparison of results from KENO and TWO-DANT indicated a possible problem with the lack of Plutonium fission fractions in the TWO-DANT H-R library. This finding was only possible because multiple codes were used in the analyses.

As with most situations, the analyst is best advised to utilize the code that he or she is most familiar with, but the analysis should not stop at that point. A complete analysis must include the use of at least one more, independent code to verify applicability and identify anomalies.

We believe that this paper was the first documented presentation of the working group benchmarks and provided added indication that there were some cross section problems relating to plutonium solutions. Additional work has been done in the cross section evaluation area which has provided newer evaluations, specifically ENDF/B-VI, which seem to take care of some of the discrepancies.

After Chuck finished working on these tasks, he used the experience gained to work on a project with LANL X-6 in the development of a criticality primer for MCNP. Although not directly funded under this contract, the knowledge acquired while working with ESH-6 was quite useful in the creation of this publication.

FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994

Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task 6

While Chuck was working on the code comparisons, another graduate student, Thomas Jones, worked with Doug O'Dell on the evaluation of the ORNL Hansen-Roach library. Tom did comparisons between entries in the LANL library and entries in the ORNL library to identify differences. Based on these reviews, a new 167 isotope Hansen-Roach library was created which is now being used in the benchmark work.

In the fifth year, John Miller became the primary graduate student on the project. His work in the Fall of 1994 was in the area of independent review of some of the benchmarks documented as part of the NCS Benchmark Project. He reviewed TOPSY and found that his calculations agreed with those in the revised report. This review was documented in a report delivered to ESH-6 on August 29, 1994. As the project was winding down, John started looking at plutonium nitrate and the problems with accurately determining its chemical composition. It turns out that although plutonium nitrate is usually reported in the literature as $\text{Pu}(\text{NO}_3)_4$, the number of nitrate molecules for one plutonium atom varies from 2 to 5 depending on how the solution was made. John has searched the literature to find reports on the composition of plutonium nitrate and has identified some from the early fifties which provide a little insight into the variation of valence. John expects that future work in the area will focus on assessing the criticality safety (k-effective) impact of the variation in nitrate valence and in documenting the chemical composition of plutonium nitrate solutions used in benchmark experiments.

PUBLICATIONS

Directly Resulting from Project

Busch, R.D. and R.D. O'Dell, "Validity of Hansen-Roach Cross Sections in Low-Enriched Uranium Systems," Transactions of the Third International Conference on Nuclear Criticality Safety, Oxford, England. September 1991.

Bredehoft, B.B. and R.D. Busch, "A Study of Parameters for Describing the Moderating Capabilities of Uranium Systems," Transactions of the American Nuclear Society, Vol. 64, p.343-344, November 1991.

Bredehoft, B.B. and R.D. Busch, "Characterization of the Thermalness of a Fissile System with a α -Z-Group Diffusion Theory Parameter," Nuclear Technology, Vol. 102, Number 2, pp. 259-269. May 1993.

Hannon II, C.D. and R.D. Busch, "Utility of Categorization in Determining Applicability of Nuclear Criticality Benchmark Problems," Transactions of the American Nuclear Society, Vol. 68 - Part A, pp. 238-239, June 1993.

FINAL REPORT

for the Period of February 16, 1990 to December 31, 1994
Los Alamos National Laboratory, Subcontract 9-X60-D1200, Task G

Harmon II, C.D., R.D. Busch, and T.H. Jones, "Comparison of Results from KENO, MCNP, MONK, and TWODANT on Twelve Criticality Benchmark Problems," in Proceedings of the 1993 Topical Meeting on Physics and Methods of Criticality Safety, September 19-23, 1993, Nashville, Tn., pp. 210-213.

Wenz, T.R. and R.D. Busch, "Modeling of Central Reactivity Worth Measurements in Lady Godiva," Nuclear Technology, Vol. 105, Number 1, pp. 31-36, January 1994.

Associated Publication

Harmon II, C.D., R.D. Busch, J.F. Bricsmeister, and R.A. Forster, Criticality Calculations with MCNP: A Primer, Los Alamos National Laboratory Manual, LA-12827-M, August 1994.

EQUIPMENT

All of the computer analyses performed on this project were done using the two Sun SPARC-1 workstations or later the SPARC-10 workstation on loan to the UNM Chemical and Nuclear Engineering Department by Los Alamos National Laboratory, ESH-6. These machines are configured with the latest versions of the TWODANT code, the MCNP code and cross sections, the SCALE package, and the Hansen-Roach 167 isotope library.