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FINAL REPORT

U.S. Department of Energy

DEVELOPMENT OF NUCLEAR ANALYSIS CAPABILITIES FOR DOE WASTE MANAGEMENT ACTIVITIES

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1 EXECUTIVE SUMMARY

The objective of this three-year Environmental Management (EM) Science Program (EMSP) project has been to develop and demonstrate prototypical analysis capabilities that can be used by nuclear safety analysis practitioners to:

1. demonstrate a more thorough understanding of the underlying physics phenomena that can lead to improved reliability and defensibility of safety evaluations; and

2. optimize operations related to the handling, storage, transportation, and disposal of fissile material and spent nuclear fuel of interest to the U.S. Department of Energy (DOE).

Domestic standards for criticality safety computations call for validation through comparisons with critical experiments with characteristics similar to the desired application. The use of computer programs or “codes” for assessments of fissile material under DOE EM authority often involves novel configurations and/or material mixtures for which few, if any, critical experiments exist. Uses of sensitivity and uncertainty (S/U) methods have been demonstrated to provide a ready means for qualifying the similarity between experiments and the application of interest. However, prior to this research, the capabilities to perform the required S/U analyses were restricted to one- (1-D) and two-dimensional (2-D) system models. Many systems of interest to DOE EM activities, for both critical experiments and practical applications, can only be adequately modeled using three-dimensional (3-D) Monte Carlo techniques. To meet this need, SEN3, a prototypic computational sequence for obtaining S/U information for criticality safety applications has been developed. The use of this analysis sequence provides data, which enables the further development and implementation of S/U analysis techniques in concurrent projects. This sequence works in conjunction with the Standardized Computer Analyses for Licensing Evaluation (SCALE),[1] which is widely used throughout the nuclear safety community. The SEN3 computational sequence calculates S/U parameters from neutron flux information derived from an enhanced version of the industry standard KENO V.a Monte Carlo code. Thus, the same application model used by criticality practitioners for safety analyses can be used in the S/U analysis with only minor modifications. The ready use of a Monte Carlo S/U technology can enable criticality safety specialists to select a broad set of relevant critical experiments and improve the understanding of the safety margin related to fissile operations. With experience, this capability will help prevent the use of unnecessary conservatism in establishing the subcritical margin resulting in improved efficiency and reduced costs in EM activities.

The techniques used in the development of the SEN3 sequence were the subject of a Ph.D. dissertation in nuclear engineering from Texas A&M University. This dissertation can be obtained from the Texas A&M University library.

Demonstration applications of this new technology have been performed for highly enriched spent nuclear fuel applications at the request of Idaho National Engineering and Environmental Laboratory (INEEL). Criticality safety analysts at both the Yucca Mountain Project and the Savannah River Site have expressed interest in this technology.

With the new computational techniques demonstrated through the prototypic version of SEN3, it is anticipated that continued development through subsequent projects will yield a version of this code suitable for external distribution and use throughout the nuclear safety community.

Under a separate task of this project, work has been conducted to improve the 2-D generalized geometry deterministic neutron transport code, NEWT. This code is capable of solving the neutron transport equation using an arbitrary grid, which permits geometrical inputs not previously allowed in deterministic neutron transport. One of the most significant advantages of the use of NEWT over other deterministic neutron transport codes is its automated mesh generation capability. This feature allows the user to input the geometrical specification of a system in terms of elemental components. The code then automatically subdivides the geometry into the appropriate polygon-based mesh necessary for accurate calculation using deterministic transport methods. The code allows for irregular and curved surface input typically allowed only in Monte Carlo codes. Many systems, which could previously be analyzed only with Monte Carlo techniques, can now also be analyzed with NEWT. NEWT can produce more precise solutions for problems that are difficult to solve with Monte Carlo methods. The NEWT code is a valuable tool for performing detailed physics analyses of nuclear systems as it can calculate the effect of miniscule changes in system parameters on the overall system performance. It can also be used to produce detailed flux solutions in regions that are difficult to solve using Monte Carlo techniques. Interface files have been developed under this project that will allow the use of NEWT generated neutron flux data for the calculation of sensitivity coefficients.

2 RESEARCH OBJECTIVES

Nuclear criticality safety engineers across the DOE complex are required to perform safety analyses for the transport and storage of fissile nuclear materials. The Nuclear Regulatory Commission (NRC) Regulatory Guide 3.4 and ANSI Standard 8.1[2] require that analytical methods and nuclear data used to predict the subcritical margin of a system under normal and upset conditions be validated against critical experiments in order to establish the bias and uncertainty of the calculation. Because of the unique nature of the materials and configurations used by DOE, critical experiments similar to the intended application are not always available. Since it is not possible to perform critical experiments for every system for which the subcritical margin must be determined, it is necessary to establish a range of applicability for existing experiments. For systems that fall outside of the applicable range of the data, estimates of the subcritical margin must be made based on the existing data. Although the ANSI Standard allows for extrapolation beyond the range of applicability, there is no guidance to establish valid trends in the bias or uncertainty.

Currently, quantitative approaches for extending the range of applicability are being established at Oak Ridge National Laboratory (ORNL). These approaches utilize several implementations of S/U analysis methodologies for data validation tasks associated with criticality safety computational studies.[3,4] With the proper application of these techniques, the similarity of two systems can be quantitatively evaluated on a number of criteria through the use of sensitivity coefficients. Physically, sensitivity coefficients are defined such that they represent the percentage effect on some system response due to a one-percent change in an input parameter. For systems containing fissionable material, one response of interest is the system multiplication factor (k_{eff}), and the appropriate input parameters are the nuclear reaction probabilities or cross sections.

Recently, deterministic neutron transport codes were adapted to produce the desired sensitivity coefficients based on 1-D and 2-D models of the systems of interest.[5] However, these codes were insufficient for accurately modeling geometrical configurations often encountered in DOE storage and transport applications. After demonstration of the usefulness of the S/U analysis techniques with the 1-D and 2-D codes, it became clear that a 3-D sensitivity analysis code was necessary for full implementation of these techniques. Furthermore, because of the nature of the systems to be analyzed, the 3-D sensitivity analysis code needed to be based on Monte Carlo neutron transport. At the inception of this project, some Monte Carlo codes could produce sensitivity coefficients on a limited basis, but none could produce the number of coefficients (usually thousand per system) efficiently enough to be of practical use. Through the design and implementation of novel computational techniques, an efficient tool for the calculation of the necessary sensitivity data has been developed.

A significant number of issues of concern to EM involve the application of computational methods for a diverse range of applied nuclear fields. In general, issues such as criticality safety, isotopic depletion, radiation shielding, and radiation damage are areas of concern in the stewardship of DOE-owned spent nuclear fuel. Specific applications include, for example, resolution of technical issues related to application of burnup credit for DOE-owned spent fuel and accurate prediction of activation fluxes needed for characterization of DOE-owned reactors scheduled for decommissioning.

Each of the above issues requires an accurate characterization of radiation transport phenomena based on the solution of the Boltzmann equation for neutral-particle transport. Although much work has been performed in these fields, it is often the case that existing computer codes and calculational methods are poorly suited for certain applications. Modeling simplifications and approximations are usually required in order to solve complex problems due to geometry-modeling limitations inherent in more accurate neutral-particle-kinematics computational techniques. One such case is the application of discrete-ordinates methods in complicated or irregular geometries; the discrete-ordinates approximation to the transport equation is applied in problems where the angular distribution of neutron flow is important. Discrete-ordinates methods are considered to be the most rigorous deterministic approximations to the Boltzmann equation, yet this approach is often limited in applicability due to the geometric constraints of the orthogonal grid system associated with the finite-difference numerical approximation.[6] Currently, the only general means for treating the angular aspects of radiation transport in irregular domains is through the use of Monte Carlo simulations. Monte Carlo methods have their own limitations, however, and have traditionally proven inappropriate for sensitivity, uncertainty, depletion, and deep-penetration analyses, and therefore may have limited application in many EM problems.

An Extended Step Characteristic (ESC) method[7] was developed in 1992 to apply the discrete-ordinates approximation to complicated geometries for which traditional methods provide fewer satisfactory solutions. This is accomplished through the implementation of the calculational techniques into an arbitrary geometrical grid. The objectives for this subtask of the project were to further the development of this code through improvements of the computational efficiency, input capabilities, and user interface. It was also desired to configure this code to produce the data necessary for use in sensitivity analysis.

Each of these capabilities can facilitate improved estimates of the required subcritical margin and potentially enable the use of a broader range of experiments in the validation process. The new arbitrary-grid radiation transport code will also enable detailed geometric modeling valuable for improved accuracy in application to a myriad of other problems related to waste characterization.

3 METHODS AND RESULTS

Since the work on the project began, significant advances in the state-of-the-art in nuclear criticality safety analyses have been achieved. One substantial accomplishment is the completion of a working version of the SEN3 3-D sensitivity analysis sequence consistent with the SCALE code system. This analysis sequence is capable of producing sensitivity coefficients, which predict the percentage change in the system multiplication factor that would be expected due to a percentage perturbation in a constituent cross section data component. A flow diagram detailing the functional modules and interface files of this sequence is shown in Figure 1. The SEN3 sequence performs automated problem-dependent cross section processing, then executes an enhanced version of the KENO V.a Monte Carlo code to produce both the forward and adjoint neutron transport solutions for the system under investigation. The adjoint neutron flux solution is an importance function for the forward flux solution and is necessary for this type of sensitivity analysis. After producing the necessary flux solutions, the SEN3 sequence executes the new Sensitivity Analysis Module for SCALE (SAMS), which produces sensitivity parameters using perturbation theory. For the convenience of the end user, this sequence uses input very similar to the widely-used, industry-standard Criticality Safety Analysis Sequence (CSAS25) of SCALE.

The enhanced version of KENO V.a developed for this project uses first-of-the-kind techniques to calculate the angular neutron fluxes and flux moments necessary for sensitivity analysis. No other known Monte Carlo code used for criticality safety can calculate these flux components. A novel approach to the calculation of these flux components has been taken, where a coordinate transformation is used to obtain the desired data. Also, previous to this work, adjoint solutions for certain classes of system models were difficult to obtain using Monte Carlo techniques. Through this project, methods for routinely producing adjoint solutions for a broad range of systems have been developed. Furthermore, under this project volume calculation routines have been added to the generalized geometry Monte Carlo code KENO-VI. Volumes of the individual material regions comprising a problem are required for sensitivity calculations. A new statistical technique was developed so that sensitivity parameters can eventually be calculated using KENO-VI.

The new SAMS code, developed for this project, produces sensitivity coefficients using a first-order linear perturbation theory approach similar to that used in FORSS code.[8] SAMS uses flux data from the forward and adjoint KENO V.a solutions with the problem-dependent cross section data libraries to automatically produce region- and energy-dependent sensitivity coefficients for each possible reaction type for each nuclide in the system. The sensitivity data is also output in summary formats showing the sensitivity values integrated over energy and region. SAMS reports the uncertainties in the sensitivity data due to uncertainties in the Monte Carlo solution and writes the sensitivity data in a variety of sensitivity data file formats for post-processing with other codes. The development and validation of the SEN3 sequence and its components has been well documented in literature attached to this report and will not be repeated here.

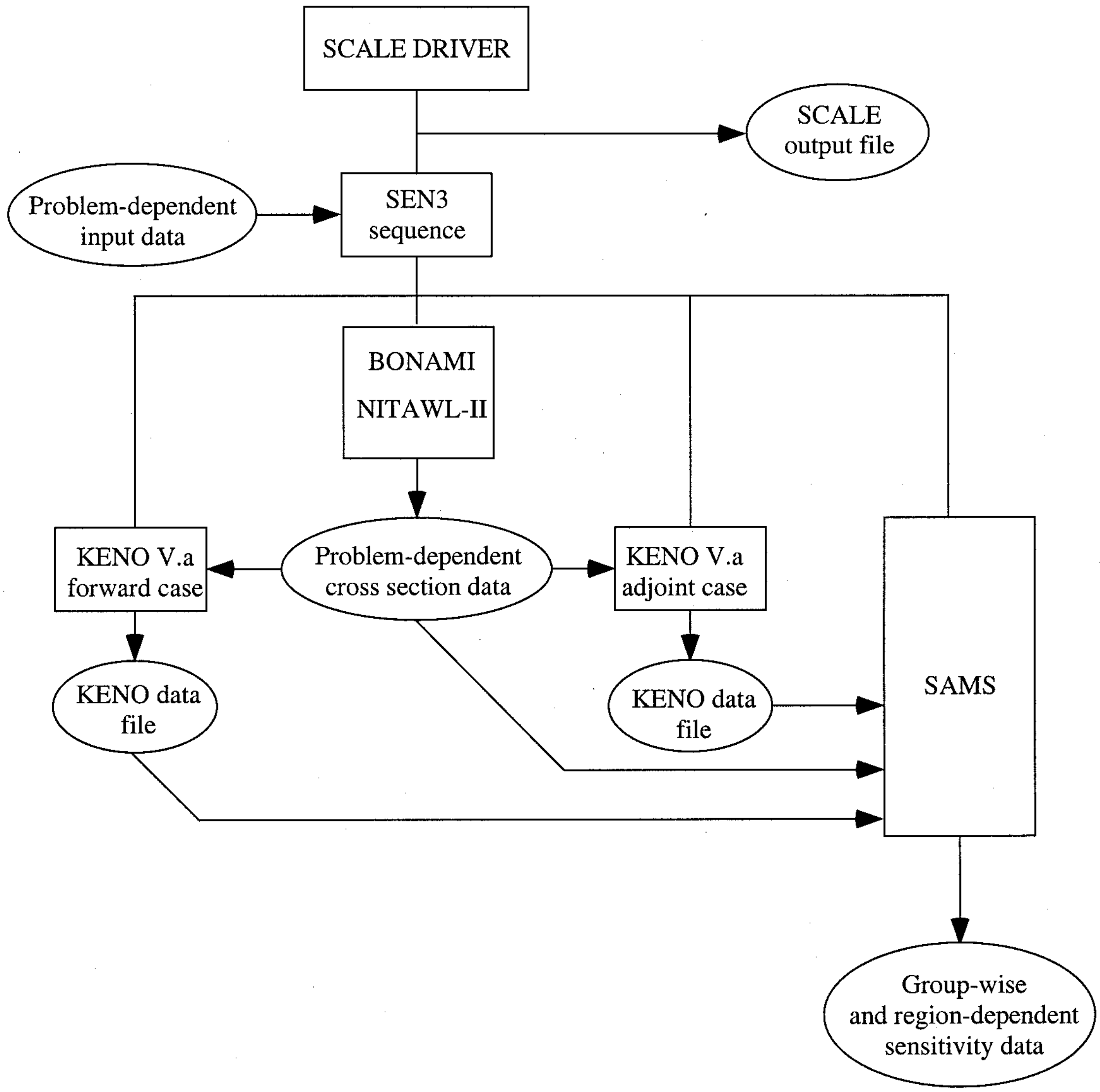

Figure 1. Flow diagram for the prototypic SEN3 sensitivity analysis sequence.

A prototypic version of the SEN3 sequence is currently in use to complement and supplement the use of S/U techniques for applications to criticality safety. These S/U techniques, initially developed under a NRC project, are currently being further investigated for broad application to criticality safety by the DOE Nuclear Criticality Safety Program (NCSP). [9] These S/U techniques can be used to determine if data available from critical experiments are adequate to validate the computational methodologies used in the design of nuclear systems.[10] They can also be used to determine if gaps exist in the experimental data and help design new experiments to fill these gaps. Work on this and related projects has involved the application of SEN3 to hundreds of critical benchmark experiments. The use of sensitivity coefficients generated from the SEN3 sequence has enabled researchers to greatly expand the number of experiments that can be considered using these new S/U techniques. Many experiments have features that require 3-D modeling. Prior to this work, only 1-D and 2-D models of systems could be considered.[11]

The calculation of the sensitivity of the multi-group neutron cross-section data to the model input data was also explored in this project.[12] As currently implemented, the SEN3 sequence calculates the sensitivity of k_{eff} to perturbations in the multi-group cross-section data. However, it has been demonstrated that the cross-section data is also sensitive to the same perturbations for which the k_{eff} sensitivities are calculated. Thus, the sensitivity of the cross-section data must be propagated to the sensitivity of k_{eff} to ensure the most accurate calculation of the response.

The usefulness of the sensitivity methodology extends beyond its application in the S/U techniques. The sensitivity coefficients produced by SEN3 predict the percent change in the k_{eff} of a system that would occur if a given component of the cross-section data were changed by 1%. SEN3 produces tens of thousands of sensitivity coefficients in a single execution. Each of these can aid the criticality safety practitioner in rapidly determining the effect on the overall system performance of the various components within a system. For example, if one finds that a calculated value does not match a measured value in an experiment, the sensitivity data can be used to help identify the source of the discrepancy. The current DOE NCSP project is using this new sensitivity data from SEN3 to expand upon the knowledge base developed under the NRC project (mentioned above) to develop guidance for the use of sensitivity data in safety evaluations. The purpose of this EMSP project has been to provide the means of generating the sensitivity data. Prototypic applications related to Hanford tank issues and disposal of DOE spent nuclear fuel have been part of the applications studied to develop guidance on the use of sensitivity data. To aid in the analysis of sensitivity data, the SenPlot plotting package has been developed. This package allows the user to generate plots of the energy dependent sensitivity profiles generated with SEN3. A great deal of insight relative to system behavior can be quickly gained by viewing these sensitivity profiles.

Recently, under a separate project, INEEL requested that ORNL perform an analysis using the S/U techniques with SEN3 generated sensitivity data to assess the adequacy of experimental benchmarks for validation of codes and data used in the design of a shipping cask and storage rack for the disposition of DOE owned spent fuel.[13] Energy-dependent sensitivity profiles for ^{235}U fission generated with SEN3 for this project are shown in Figure 2. The S/U analysis techniques make use hundreds of these profiles to determine the similarity of the shipping cask application to the critical experiments. It is expected that the results of this analysis will help determine the if new experimental measurements are necessary before the existing safety analysis codes can be validated for the transport and storage of DOE waste.

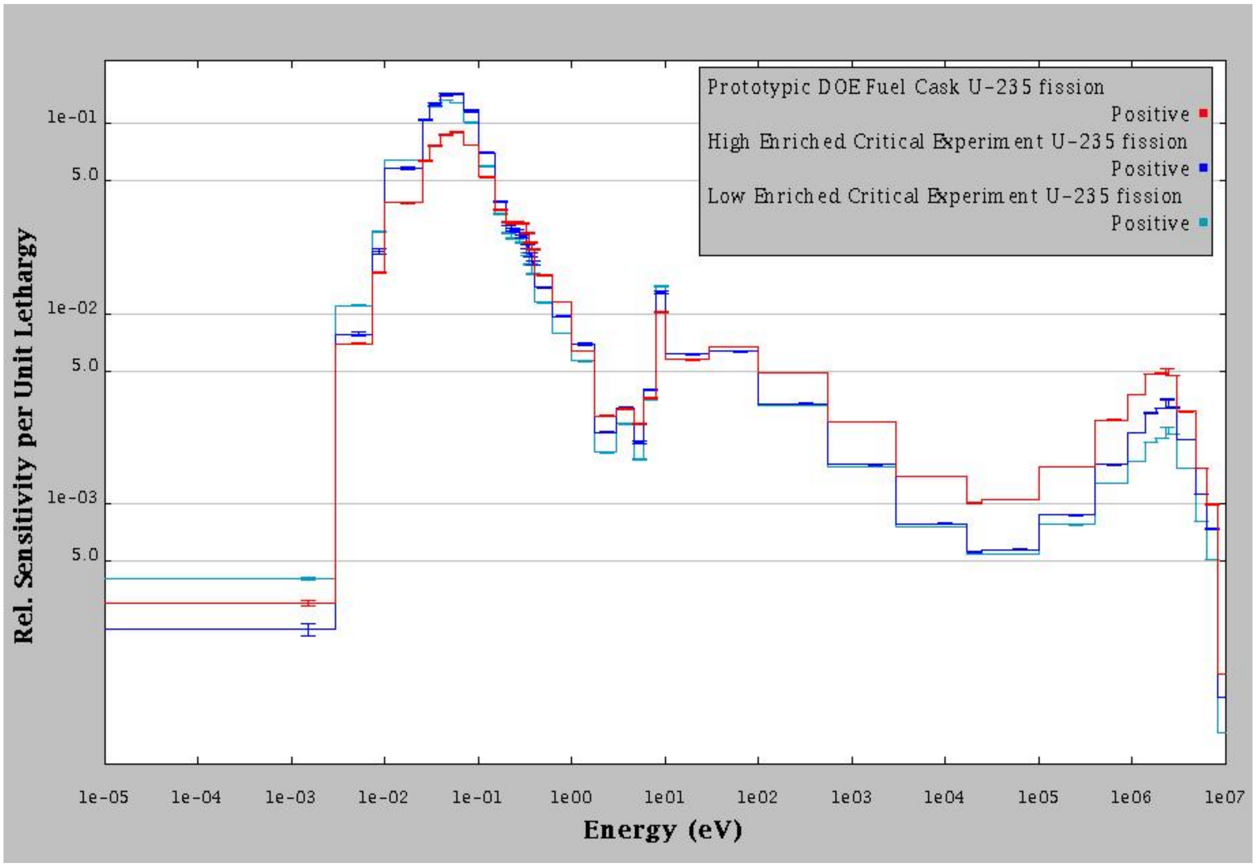

Figure 2. Energy-dependent sensitivity profiles for prototypic DOE nuclear fuel shipping cask and two critical experiments.

Another task under this project was the development of enhancements for the NEWT generalized-geometry deterministic neutron transport code. NEWT is capable of solving the neutron transport equation using an arbitrary 2-D grid, which permits geometrical inputs not previously available in deterministic neutron transport. One of the most significant advantages to the use of NEWT over other deterministic neutron transport codes is its automated mesh generation. This capability allows the user to input the geometrical specification of a system in terms of simple bodies (e.g., cylinder, cuboid, etc.). The code then automatically subdivides the geometry into the appropriate polygon-based mesh necessary for accurate calculation using deterministic transport methods. The code allows for irregular and curved surface input typically allowed only in Monte Carlo codes. Many systems, which could previously be analyzed only with Monte Carlo techniques, can now also be analyzed with NEWT. NEWT can also produce more precise solutions for problems that are difficult to solve with Monte Carlo techniques. The

NEWT code is a valuable tool for performing detailed physics analyses of nuclear systems as it can calculate the effect of miniscule changes in system parameters on the overall system performance. It can also be used to produce detailed flux solutions in regions that are difficult to solve using Monte Carlo techniques.

The NEWT code has evolved significantly since the inception of this project. The method used to perform adjoint solutions, necessary for performing sensitivity analysis, was completed and tested. Binary interface files were created to allow forward and adjoint flux solutions to be read by S/U analysis modules. Methods for precalculating and saving relational coefficients for transport between cell boundaries have been improved, such that the computational cost per cell side is competitive with that seen in traditional diamond-differencing (DD) schemes during the iteration process. A two-pass acceleration approach developed prior to EMSP support became obsolete with improved extended step characteristic (ESC) solution efficiency, and was removed from the code. However, a hybrid approach was implemented that can use the DD approach in rectangular cells while simultaneously solving non-rectangular polygons using ESC. This concept is believed to be an unprecedented solution strategy for numerical transport methods. Although this tactic offers little advantage in terms of computational efficiency, the hybrid approach can provide a higher-order accuracy solution, which can be important for problems where the flux varies rapidly in space, such as near a vacuum boundary condition or a strong absorber.

Much development has been directed toward improvements in the code's user interface to facilitate use by the nuclear safety community. An automated grid-generation scheme has been implemented, to provide the user with an easy-to-use input process that will rapidly and flexibly generate complex geometric models. Grid schemes are generated based on the specification of elementary bodies in a problem domain, with user-defined grid refinement parameters. Within this scheme, localized grid refinement is possible to improve geometric detail and accuracy. More advanced grid generation schemes for additional body types and general polynomial surfaces have been conceptualized and studied for potential inclusion in the grid generation logic of NEWT. More recent efforts focused on an input scheme that includes array capabilities that allow one to build a sequence of repeating structures. This both simplifies input specifications and reduces internal storage and processing requirements. The code changes have resulted in an input format similar in many ways to that of the KENO V.a Monte Carlo code commonly used in criticality analysis, so that input will be familiar to KENO users.

An input interface consistent with the specifications typically used by control modules of the SCALE code system has been developed for the application of NEWT. In addition, NEWT has been implemented within a 2-D depletion sequence that is under development as part of SCALE. Using the arbitrary-grid capabilities of NEWT, it is possible to obtain accurate 2-D flux distributions which, when used within the depletion sequence, will allow improved characterization of the complicated, heterogeneous fuel assemblies typical of the DOE-owned spent fuel inventory. An operational prototype of this sequence has been completed and is undergoing testing and enhancement.

In cooperation with the DOE NCSP, efforts have begun to identify applications where these new methodologies would have potential benefits. Applications related to the disposal of

DOE spent fuel and activities at Rocky Flats seem the most likely candidates for study. These application areas are DOE Office of Environmental Management responsibilities.

4 RELEVANCE, IMPACT AND TECHNOLOGY TRANSFER

4.1 How does this new scientific knowledge focus on critical DOE environmental management problems?

The computational techniques developed in this project are specifically designed for the analysis of storage and transport applications of fissile nuclear materials. The 3-D sensitivity analysis techniques were required by the complex geometrical configurations of DOE fissile material and spent nuclear fuel, which could not be accurately modeled with existing 1-D or 2-D capabilities.

The improved 2-D deterministic methods allow both improved sensitivity analysis capabilities where Monte Carlo method is inadequate, and more robust depletion analysis methods.

4.2 How will the new scientific knowledge that is generated by this project improve technologies and cleanup approaches to significantly reduce future costs, schedules, and risks and meet DOE compliance requirements?

Safety assessments for fissile material under EM authority often involve novel configurations and/or material mixtures for which few, if any, critical experiments exist. Use of S/U methods have been demonstrated to provide a ready means for qualifying the similarity between experiments and the application of interest. Thus, ready use of a Monte Carlo S/U technology can enable criticality safety specialists to select a broad set of relevant critical experiments and improve the understanding of the safety margin related to fissile operations. With experience, this capability will help prevent the use of unnecessary conservatism in establishing the subcritical margin. For applications for which applicable critical experiments do not exist, these techniques can be used to design experiments that are optimized to meet the design requirements of the application. Furthermore, these techniques can be used to establish any computation bias that is required as part of the margin of subcriticality for regulatory compliance. S/U methods are enhanced by the addition of a deterministic 2-D transport method. Additionally, improved capabilities have been developed for the assessment of depletion, source term, and radiotoxicity of irradiated materials.

4.3 To what extent does the new scientific knowledge bridge the gap between broad fundamental research that has wide ranging applications and the timeliness to meet needs-driven applied technology development?

The computational techniques allow the application of the S/U techniques to realistic 3-D models of actual systems. Because the input requirements for SEN3 are very similar to those of the established criticality safety analysis sequences of SCALE, existing criticality input models could be used for sensitivity analysis with very little modification. Thus, obtaining the valuable sensitivity data requires very little user intervention and saves considerable time. Similarly, enhancements to the NEWT code have provided a simple and easy to use interface for transport analysis.

4.4 What is the project's impact on individuals, laboratories, departments, and institutions? Will results be used? If so, how will they be used, by whom, and when?

Several nuclear safety organizations have expressed interest in using these new analysis tools and techniques for their applications. Some work has already been performed by ORNL for INEEL for the storage and transport of DOE-owned highly-enriched uranium fuels, and INEEL has expressed interested in obtaining this software for in-house use involving classified systems when a release version is available. Interest in the use of these methods has been specifically expressed by those associated with the Yucca Mountain Project and the Savannah River Site.

4.5 Are larger scale trials warranted? What difference has the project made? Now that the project is complete, what new capacity, equipment, or expertise has been developed?

Through this project, the techniques for the 3-D sensitivity analysis have been developed and applied to a wide range of systems. This has enabled the application of the S/U techniques developed in concurrent projects to realistic models of actual systems. Additionally, fundamental techniques that have been developed or enhanced are now ready for incorporation into a production level nuclear safety analysis code package.

4.6 How have the scientific capabilities of collaborating scientists been improved?

Although not a formal collaborative effort, the techniques developed through this project have enabled those developing the S/U analysis methods under the NRC and NCSP projects to have better data with which they can improve upon their analysis techniques.

4.7 How has this research advanced our understanding in this area?

These tools have provided unique insight into the sensitivity of fissile systems to various materials and components. The SEN3 sequence provides unique data regarding the impact of individual components on the overall criticality condition of a system.

4.8 What additional scientific or other hurdles must be overcome before the results of this project can be successfully applied to DOE Environmental Management problems?

At this point, the 3-D sensitivity analysis tool operates as a prototypic analysis sequence. Although the techniques are accurate, their practical implementation can lead a novice user to inaccurate conclusions. This is also true to some extent for the NEWT code and the SCALE sequence developed to automate NEWT. Further work is required in the areas of cross-section data and geometric input processing. Since these computational tools were developed as part of the SCALE code system, it is important to update the techniques for compatibility with the latest version of SCALE, which has advanced since the inception of this EMSP project. These issues are addressed in more detail in the Future Work section of this report.

4.9 Have any other government agencies or private enterprises expressed interest in the project? Please provide contact information.

Several end users have expressed interest in this project and the analysis tools that have been developed. The NRC staff within the Office of Nuclear Materials Safety and Safeguards (NMSS) is interested in using the SEN3 technology to help in their independent evaluation of subcritical margins. Harry Felsher at 301-415-5521 is the NRC/NMSS contact. Similarly, ORNL has used the technology to support efforts of the NRC Office of Regulatory Research (RES) to develop guidance on selection of experiments for use in burnup credit applications. The contact in NRC/RES is Richard Lee at 301-415-6795. NRC/RES has also initiated efforts to fund the inclusion of the NEWT code into the SCALE code system as a means to produce physics constants for reactor analyses. In the private sector, Duke/Cogema/Stone and Webster (DCS) has indicated interest in using the methods to help evaluate their subcritical margins associated with certain processes within their fabrication plant for mixed-oxide fuel. The contact at DCS is Keyes Niemer at 704-382-9525. Framatome ANP has also collaborated with ORNL on a proposal sent to DOE to use the SEN3 system and the S/U methodology to help define critical experiments that may be needed to move fuel fabrication beyond 5 wt %.

5 PROJECT PRODUCTIVITY

This project completed all of its goals. A no-cost extension was requested at the end of the project so that the most recent results could be included in this report.

6 PERSONNEL SUPPORTED

All supported personnel are currently staff members at ORNL.

Dr. Cecil V. Parks, P.I.

Dr. Bradley T. Rearden, Co-P.I.

Dr. Mark D. DeHart, Co-P.I.

Dr. Bryan L. Broadhead, Co-P.I.

Dr. Lester M. Petrie, Co-P.I.

7 PUBLICATIONS

The following publications have resulted from this research project:

1. B. T. Rearden, "Perturbation Theory Eigenvalue Sensitivity Analysis with Monte Carlo Techniques," Submitted to *Nucl. Sci. Eng.* Feb, 2001.

2. M. L. Williams, B. L. Broadhead, and C. V. Parks, "Eigenvalue Sensitivity Theory for Resonance-Shielded Cross Sections," Submitted to *Nucl. Sci. Eng.* June, 2000.

3. B. T. Rearden, "Development of SAMS: A Sensitivity Analysis Module for the SCALE Code System Using KENO V.a in the CSAS25 Sequence," Ph.D. Dissertation, Texas A&M University (1999).

4. B. T. Rearden, "SAMS: A Sensitivity Analysis Module for Criticality Safety Analysis Using Monte Carlo Techniques," *Proc. of PHYSOR 2000, ANS Int. Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium*, CD-ROM, Pittsburgh, Pennsylvania, May 7–12, 2000, ANS.

5. B. T. Rearden, L. M. Petrie, and D. F. Hollenbach, "Sensitivity and Uncertainty Analysis for Nuclear Criticality Safety Using Keno in the Scale Code System," *MC2000, International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications*, 23–26 October, 2000 Lisbon, Portugal.

6. B. T. Rearden and R. L. Childs, "Prototyic Sensitivity and Uncertainty Analysis Codes for Criticality Safety with the SCALE Code System," *ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings*, November 12–16, 2000, Washington, D.C. *Trans. Am. Nucl. Soc.*, **83,** 98–99 (November 2000).

7. B. T. Rearden, C. M. Hopper, K. R. Elam, B. L. Broadhead, and P. B. Fox, "Prototypic Applications of Sensitivity and Uncertainty Analysis for Experiment Needs," ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings, November 12–16, 2000, Washington, D.C. *Trans. Am. Nucl. Soc.*, **83,** 103–106 (November 2000).

8. C. V. Parks, M. D. DeHart B. L. Broadhead, C. M. Hopper, and L. M. Petrie, *Annual EMSP Summary Progress Report. Project Title: Development of Nuclear Analysis Capabilities for DOE Waste Management Activities*, ORNL/M-6549, June 1998.

9. C. V. Parks, B. T. Rearden, M. D. DeHart, B. L. Broadhead, C. M. Hopper, and L. M. Petrie, *Annual Environmental Management Science Program (EMSP) Summary Progress Report. Project Title Development of Nuclear Analysis Capabilities for DOE Waste Management Activities*, ORNL/TM-1999/101, June 1999.

10. B. L. Broadhead, R. L. Childs, and B. T. Rearden, "Computational Methods for Sensitivity and Uncertainty Analysis in Criticality Safety," *Proceedings of ICNC'99, Sixth International Conference on Nuclear Criticality Safety*, Vol. I, 57–65 Palais des Congrès, Versailles, FRANCE, September 20–24, 1999.

11. C. V. Parks, B. T. Rearden, M. D. DeHart B. L. Broadhead, C. M. Hopper, and L. M. Petrie, *Annual Environmental Management Science Program (EMSP) Project Summary. Project Title: Development of Nuclear Analysis Capabilities for DOE Waste Management Activities*, ORNL/TM-2000/65, February 2000.

12. M. D. DeHart, "A Deterministic Study of the Deficiency of the Wigner-Seitz Approximation for Pu/MOX Fuel Pins," *Proceedings of M&C'99-Madrid, Mathematics and Computations Meeting*, 689-699, in September 27–30, 1999, Madrid, Spain.

13. M. D. DeHart, "A Deterministic Study of Deficiencies in the Wigner-Seitz Cell Approximation," *Trans. Am. Nucl. Soc.*, **80**, 149–151 (1999).

14. M. D. DeHart, "An Advanced Deterministic Method for Spent-Fuel Criticality Safety Analysis," *Trans. Am. Nucl. Soc*. **78**, 170–172 (June 1998).

8 INTERACTIONS

8.1 Participation/presentations at meetings, workshops, conferences, seminars, etc.

1. Presented posters at EMSP workshops in 1998 and 2000. Oral presentation given at 2000 EMSP workshop.

2. Presented paper at PHYSOR 2000, ANS International Topical Meeting on Advances in Reactor Physics and Mathematics and Computation into the Next Millennium in Pittsburgh, Pennsylvania in May of 2000.

3. Presented paper at MC2000, International Conference on Advanced Monte Carlo for Radiation Physics, Particle Transport Simulation and Applications in Lisbon, Portugal in October of 2000.

4. Presented two papers at ANS/ENS 2000 International Winter Meeting and Embedded Topical Meetings, November 2000 in Washington, D.C.

5. Presented paper at ANS Annual Meeting, June 1998 in Nashville, TN.

6. Presented paper at ANS Annual Meeting, June 1999 in Boston, MA.

7. Presented paper at Mathematics and Computations Meeting in September 1999 in Madrid, Spain.

8.2 Consultative and advisory functions to other laboratories and agencies, especially DOE and other government laboratories. Provide factual information about the subject matter, institutions, locations, dates and name(s) of principal individuals involved.

Consulting/Advisory Activity #1

DOE Nuclear Criticality Safety Program

Objective: Study application of sensitivity and S/U methodology to relevant EM problems of current interest.

Activity Description: Via Michaele Brady Raap at Hanford and Todd Taylor at INEEL, ORNL researchers reviewed applications related to the tank farms and disposal of spent nuclear fuel to assess the potential changes in safety margin that might be achieved using the S/U methodology. The SEN3 sequence developed under this project was used sparingly to assess its capabilities.

Result: Calculations and assessments have been completed.

Timeframe of Activity: April 1999 – March 2000

Consulting/Advisory Activity #2

R. Y. Lee, U.S. NRC

Objective: Study the relevance of current critical experiments to validation issues related to implementation of burnup credit in spent fuel safety analyses.

Activity Description: Plans call for investigating the use of SEN3 to evaluate adequacy of existing critical experiments and reactor critical configurations to validate codes for use in burnup credit in transport casks. SEN3 will be used to model the configurations and casks and the results used to evaluate similarity.

Result: Initial analysis of reactor critical configurations and proposed critical experiments have been completed and initial results used to provide NRC with guidance on top priority experiments for use in burnup credit.

Timeframe of Activity: FY2000 – FY2001

Consulting/Advisory Activity #3

Blair Briggs, INEEL

Objective: Investigate the applicability of a suite of critical experiments planned to support the storage and transport of high-enriched, DOE/EM fuel.

Activity Description: INEEL has significant quantities of highly enriched fresh and spent nuclear fuel in storage. INEEL has proposed to add to the data base of critical experiments relative to this application by having critical experiments performed in Russia. Prior to funding such experiments, INEEL has requested that ORNL use the S/U methodology and the SEN3 sequence to evaluate the neutronic similarity of the proposed experiments to the proposed application in transport and storage systems.

Result: Evaluations of these experiments have been completed and a draft report has been submitted to INEEL.

Timeframe of Activity: March 2000–September 2000

8.3 Collaborations

Louisiana State University participated in the derivation of the sensitivity of the multigroup cross sections to the resonance processing data.

9 TRANSITIONS

9.1 Describe cases where knowledge resulting from your effort is used, or will be used, in a technology, technique, or process improvement application. Transitions can be to entities in DOE, other federal agencies, or industry.

It is desired to fully implement the computational techniques developed in this project for global distribution through the SCALE code system. Several nuclear criticality safety organizations (mentioned in Consulting/Advisory Activities above) have expressed interest in using the SEN3 analysis tool in conjunction with the S/U methodology developed under NRC and NCSP projects. Both the NRC and DOE OCRWM/YMP are very interested in the application of the SAS2D depletion sequence developed based on NEWT for spent nuclear fuel analysis.

9.2 Briefly list the enabling research, the laboratory or company, and an individual in that organization who made use of your research.

To date, the actual methods have not been used outside of ORNL. ORNL personnel have conducted all consulting and advisory activities. A pre-release version of NEWT has been tested and used by Anthony Ulses of the NRC for fuel lattice analysis. He also established the feasibility of a parallel version of NEWT.

10 PATENTS

No new discoveries, inventions, or patent disclosures were made as a result of this research project.

11 FUTURE WORK

Even in its prototypic state, the SEN3 sequence has already proven to be a valuable tool in expanding the types of systems that can be analyzed with the S/U techniques. However, there are several shortcomings, which limit its practical use in the EM community. First, the sensitivity methodology employed in the analysis sequence does not account for the resonance shielding effects in processing the problem-dependent multigroup cross sections. Second, limitations due to the use of Monte Carlo techniques to produce the necessary neutron flux solutions have been revealed by the prototypic version of this sequence. Last, the geometric restrictions of the KENO V.a Monte Carlo code, on which this sequence relies, limit the number of systems that can be analyzed. Several enhancements to the SEN3 sequence could alleviate these concerns. New research and development in these areas would result in a production level suite of sensitivity software that would enable the S/U methodologies to be used by the general criticality safety community. Each of the shortcomings and proposed remedies of the prototypic SEN3 sequence are detailed below.

In confirming the accuracy of perturbation theory based sensitivity coefficients generated with the 1-D sensitivity analysis sequence SEN1 through comparison with direct recalculations, it was discovered that the sensitivity of the system to the total hydrogen cross section could not be predicted as accurately as desired. For example, when investigating a homogeneous-fueled sphere with a thermal energy spectrum, by directly calculating the sensitivity coefficient, through repeated calculations, for the total reaction of ^{1}H a sensitivity coefficient of 0.2228 is found. However, the SEN1 sequence predicted a sensitivity coefficient of 0.2892. This difference of nearly 30% is clearly unacceptable for safety applications. A similar investigation of the total reaction for ^{235}U for the same system reveals a direct perturbation value of 0.2530 versus a SEN1 computed value of 0.2529, which is clearly much more acceptable. When this same test case was investigated with SEN3, nearly identical results were produced. The inconsistency in the ^{1}H sensitivity coefficient can be attributed to variations in the resonance absorption parameters of certain nuclides, especially ^{238}U, which occur when the cross sections of highly scattering materials are perturbed. It should be noted that the perturbation theory methodology used in all of the new ORNL sensitivity sequences, including SEN1 and SEN3, is adapted from that developed for fast reactor applications using the FORSS code. In its original application, the resonance shielding calculations were not significant concerns, and no methods were developed to account for their effect. Preliminary investigations have revealed that implementing perturbation theory in the resonance processing codes can produce perturbation theory results that are consistent with those generated by direct recalculation. It is desirable to fully investigate this methodology and implement it into SCALE to provide a robust computational sequence beginning with the problem-dependent processing of the nuclear data and ending with generation of system specific sensitivities of k_{eff} to this data. This would also allow sensitivity coefficients to be generated for geometrical parameters such as fuel rod diameter and pitch in addition to the current sensitivity parameters for material cross-section data.

It has been demonstrated through sample applications that the large geometrical regions commonly used in Monte Carlo modeling (typically each material is a region) do not provide adequate resolution of the flux solutions to accurately determine the sensitivity coefficients. At the present time, in order to obtain the necessary resolution of the flux solutions using SEN3 the problem geometry for many systems must be redefined by creating new, more complex, user input problem specifications. For example, in a simple homogeneous spherical test case, the SEN3 calculated sensitivity coefficients differed from the SEN1 coefficients by up to 7% when the sphere was modeled as a single Monte Carlo region.[14] The SEN3 results eventually converged to the SEN1 results when the SEN3 model was subdivided into 9 concentric spherical regions. In most analyses, the correct results are not known, and often several inputs must be tested to ensure that the geometrical regions are small enough (i.e., the sensitivity parameters converge to the most precise result). This technique is difficult for a novice or occasional user and time consuming for an experienced user. The investigation, development and implementation of an automated grid generation routine, similar to that used in NEWT, would alleviate this difficulty.

The statistical nature of the Monte Carlo technique in general presents difficulties in the generation of precise flux solutions necessary for sensitivity analyses. In regions where few particles interact, the standard deviation of the flux solution can be large, and the precision of the result is often poor. For typical criticality safety applications, this is not a concern because regions in which few particles interact do not significantly contribute to the overall system performance. However, in sensitivity analyses, these regions are important for system optimization, and new methodologies to improve the statistical variance of the flux solutions in these regions are desirable. This is somewhat contrary to traditional Monte Carlo development where it is desirable to concentrate more effort, via biasing techniques, to the solution in regions that provide a significant contribution to the system performance. For example, in systems with large non-fueled regions, such as thick reflectors, it is difficult to obtain an accurate calculation of the flux solution due to the limited number of particles that pass through the outer parts of these regions. Similarly, in very small regions where few interactions occur, it is difficult to obtain accurate flux solutions. These difficulties can be somewhat overcome by greatly increasing the number of neutron histories and the number of fission source generations in the problem. Obviously, this can greatly increase the computation time for the system and is undesirable. The most practical solution would be the implementation of new biasing techniques into the KENO V.a code, which would help to resolve these difficult issues.

Furthermore, the adjoint solution for systems with little moderation is difficult to obtain with Monte Carlo techniques. This is due to the adjoint form of the transport equation having a transposed scattering matrix and the cross-section data for the fission spectrum and fission cross section are interchanged. Also, the energy group structure is reversed in the adjoint solution. The combination of these conditions means that for fast systems, with little neutron moderation (i.e. the scattering matrix is sparse), adjunctons, or adjoint neutron particles, that are born with an energy distribution proportional to the fission cross section have little chance of scattering into the fission spectrum to tally the importance of the fission reaction. Methods to implement a source biasing technique whereby a larger proportion of the adjunctons are started in an energy range with a greater chance of causing an interaction have been investigated. Although, thus far, these techniques have met with limited success, further investigation and implementation is expected to produce significantly enhanced performance in the production of adjoint solutions. The current methodology used in SEN3 is to greatly increase the number of particles in the solution of the difficult problems. Even though the chance that any given particle will cause an interaction may be small, a huge number of particles will yield a statistically significant solution.

Because the sensitivity techniques were designed to work with the KENO V.a Monte Carlo code, the experimental configurations that can be analyzed are limited to those that can be modeled under its geometry input. KENO V.a was chosen for this project because it is an industry standard in the criticality-safety community. It is easier to modify than the newer generalized geometry KENO-VI code, thus an excellent test base for this research. Also, until recently developed under this project, the automated calculation of material region volumes was not available in KENO-VI. However, with the sensitivity methodology now proven with KENO V.a, it is desirable to implement these techniques into the KENO-VI code in order to analyze systems with more complex geometrical configurations. Both of the KENO codes are industry standards and are widely used by criticality safety practitioners throughout the world.

Unlike the 3-D capabilities of the KENO codes, NEWT at present is limited to 2-D calculations. Because of the nature of nuclear analyses, 2-D modeling is usually adequate and often preferred for efficiency. This will be true for some types of sensitivity analysis, but quantification of a system in terms of its relevance as a benchmark typically requires 3-D modeling to capture leakage effects or axial asymmetries. For criticality safety applications, bounding calculations or system investigations can be performed in 2-D, but safety calculations must be performed in 3-D. Therefore, it is desirable to further exploit the capabilities of arbitrary-grid deterministic methods with the extension of NEWT to 3-D. Some preliminary work has been done in this area and a conceptual approach for the extension has been conceived and discussed, but implementation and testing remain. Further, because of the computational constraints of 3-D modeling, simultaneous study of parallel implementation would be desirable. And although current input descriptions are based on 3-D KENO input, additional development will be necessary to accommodate the complexities of 3-D grid generation.

As each version of NEWT (2-D and 3-D) is completed, it could be combined into a sensitivity analysis sequence similar to SEN3. This will provide the criticality safety practitioner a choice of state-of-the-art tools to perform analyses. It is expected that the KENO based sensitivity sequences would be used for general criticality safety applications and the NEWT based sequences will be used for detailed physics analysis, perturbation studies, confirmatory analyses and investigation of anomalies.

12 LITERATURE CITED

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13 FEEDBACK

None.

14 APPENDICES

None.

15 QUANTITIES/PACKAGING

None.