

Computational Physics and Engineering Division

Annual EMSP Summary Progress Report

Project Title:

Development of Nuclear Analysis Capabilities for DOE Waste Management Activities

C. V. Parks, B. T. Rearden, M. D. DeHart, B. L. Broadhead, C. M. Hopper, and L. M. Petrie

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Lead Principal Investigator: Cecil V. Parks
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-574-5280
E-mail: cvp@ornl.gov

Co-Principal Investigator: Bradley T. Rearden
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-574-6085
E-mail: reardenb@ornl.gov

Co-Principal Investigator: Mark D. DeHart
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-576-3468
E-mail: dehartmd@ornl.gov

Co-Principal Investigator: Bryan L. Broadhead
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-576-4476
E-mail: broadheadbl@ornl.gov

Co-Principal Investigator: Calvin M. Hopper
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-576-8617
E-mail: hoppercm@ornl.gov

Co-Principal Investigator: Lester M. Petrie
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 37831-6370
Telephone: 423-574-5259
E-mail: petrielm@ornl.gov

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Oak Ridge National Laboratory

RESEARCH OBJECTIVE

The objective of this project is to develop and demonstrate prototypical analysis capabilities that can be used by nuclear safety analysis practitioners to:

1. provide 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 DOE spent fuel.

To address these problems, this project will investigate the implementation of sensitivity and uncertainty methods within existing Monte Carlo codes used for criticality safety analyses, as well as within a new deterministic code that allows for specification of arbitrary grids to accurately model geometric details required in a criticality safety analysis. This capability can facilitate improved estimations 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. Application to these problems will also be explored.

RESEARCH PROGRESS AND IMPLICATIONS

In the last 12 months, the focus of work for this project has been the continued development of the SAMS module of the SCALE¹ code system for performing sensitivity analysis using three-dimensional (3-D) Monte Carlo methods. SAMS generates sensitivity information for a system model via a perturbation theory approach, in which changes in the system multiplication factor, k_{eff} , are related to changes in the constituent nuclear data parameters by relationships consisting of the forward and adjoint neutron fluxes. A similar technique has been applied to one-dimensional (1-D) and two-dimensional (2-D) deterministic codes in the SEN1 and SEN2² sensitivity analysis routines developed at ORNL under a separate project.

With SAMS, sensitivity analyses are performed on 3-D criticality calculations conducted with the KENO V.a Monte Carlo code. Techniques have been developed to obtain adjoint flux solutions for any system that can be modeled with KENO V.a. This capability has greatly expanded the range of problems that can be analyzed. Since perturbation analyses require angular fluxes and flux moments that are not calculated in the standard version of KENO V.a, an enhanced version of the code is under development. Techniques have been implemented to calculate the angular fluxes, and development continues for the calculation of the flux moments. With the angular flux

capability completed, it is now possible to calculate the sensitivity of k_{eff} to a number of nonscattering reactions types, such as fission and capture. Sensitivities to scattering reactions are not possible without implementing the calculation of flux moments into KENO V.a.

Over the past year, improvements have also been made to the user interface of SAMS. SAMS now calculates all possible sensitivities automatically. An early version of SAMS required the user to input the isotope and reaction of each desired sensitivity. The output of SAMS has also been enhanced to provide sensitivity information for each region defined in the KENO V.a geometry input. A new plotting package allows for sensitivity profiles to be displayed visually from SAMS generated data. These profiles are similar to those generated with the SEN1 plotting package, but they also include the Monte Carlo uncertainties and information about the calculational region to ease analysis by the user. Interface files are now written by SAMS, which are compatible for uncertainty analysis using current techniques.³

Further comparisons of SAMS results with those generated by both the SEN1 and SEN2 codes have been quite favorable. The test cases documented in the verification of SEN1 and SEN2 both show excellent agreement with SAMS analysis for fission, capture, $\bar{\nu}$, and χ reactions.

Further improvements have been made to the 2-D arbitrary geometry discrete-ordinates transport code NEWT. The ability to calculate adjoint fluxes has been added and validated. The code has also been modified to create binary data files in the form required by SEN2 for use in sensitivity analyses. Code logic for automated grid generation has been improved for greater stability and error checking during the grid-generation process. Capabilities to allow direct input of any type of polygon have been added. Finally, a theory for the implementation of a hybrid differencing scheme to combine the improved accuracy of diamond differencing with the geometric flexibility of the extended-step characteristic differencing approach has been developed.

In cooperation with the DOE Nuclear Criticality Safety Program, efforts have begun to identify applications where this new methodology 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.

PLANNED ACTIVITIES

During the remainder of FY 1999, work will be performed to further enhance the capabilities of SAMS. With the implementation of the flux moment calculations into KENO V.a, it should be possible to calculate in 3-D all sensitivities that can currently be calculated with the SEN1 and SEN2 codes. Additional improvements for automatic grid generation are planned for NEWT for FY 1999. Coupling and testing of NEWT with SEN2 for 2-D sensitivity analysis is also planned. Implementation and testing of the hybrid-differencing scheme is also anticipated. In FY 2000, these prototypic tools will be used on actual DOE/EM applications to help demonstrate benefits and to understand limitations of the tools and techniques developed under this project. When possible, enhancements will be made where the need has been identified via applications.

INFORMATION ACCESS (REFERENCES)

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