

Computational Physics and Engineering Division (10)

**EMSP Project Summary**

**Project ID: 60077**

**Project Title:**

**Development of Nuclear Analysis Capabilities for DOE Waste Management Activities**

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## **Development of Nuclear Analysis Capabilities for DOE Waste Management Activities**

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### **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. 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 DOE spent fuel.

To address these problems, this project has been investigating the implementation of sensitivity and uncertainty methods within existing Monte Carlo codes used for criticality safety analyses. It is also investigating the use of 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**

This report summarizes work after 2-1/2 years of a 3-year project. 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 three-dimensional (3-D) Sensitivity Analysis Module for SCALE (SAMS)<sup>1</sup> and enhancements to the KENO V.a Monte Carlo code to calculate the angular neutron fluxes and flux moments necessary for sensitivity analyses. With these codes, which are now in limited internal use as beta versions, it is possible to calculate sensitivity parameters for several reaction types for any system that can be modeled using the Criticality Safety Analysis Sequence (CSAS) of SCALE which applies the KENO V.a Monte Carlo code.

Through this project, new techniques have been developed for the calculation of angular neutron fluxes and flux moments in Monte Carlo calculations. With these first-of-their-kind capabilities, it is now possible to calculate sensitivity parameters for numerous important reactions in criticality safety calculations. These reaction types include the total reaction rate, multiple types of scattering, numerous absorption reactions, and fission as well as  $\bar{\nu}$ , the average number of neutrons produced per fission, and  $\chi$ , the energy spectrum for neutrons emerging from fission. Many of the limitations that were placed on this methodology early in the research process have been resolved, and the solution techniques have been demonstrated to produce accurate solutions for many different types of systems. The systems investigated included those with thermal, intermediate and fast neutron spectra, mixed-oxide and uranium-fueled systems, and various geometrical configurations ranging from simple spheres to large arrays of fuel rods. These systems have also included various moderating materials. Although the calculation time and

computed uncertainties in the results varied widely for the various systems, the validity of the methodology has been demonstrated.

This new technology is currently being used in conjunction with sensitivity and uncertainty (S/U) techniques recently developed at ORNL to assess the applicability and completeness of certain sets of critical experiment benchmarks for code validation for desired DOE Office of Environmental Management (EM) applications.<sup>2,3</sup> The use of sensitivity coefficients generated from the SAMS module has enabled researchers to greatly expand the number of experiments that can be considered using these new S/U techniques. Prior to this work, only 1-D and 2-D models of systems could be considered.

The generalized geometry deterministic neutron transport code NEWT has also evolved significantly since the inception of this project. The method for obtaining adjoint solutions was improved and debugged. Binary interface files were created to allow forward and adjoint flux data to be read by sensitivity/uncertainty analysis modules. The use of a hybrid differencing scheme and improved grid generation method have significantly improved the speed and accuracy of the calculations.

Much work has been directed toward improvements in the code's user interface. 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. More recent work has focused on an input scheme that includes array capabilities, which allow one to build a sequence of repeating structures. Efforts are being made to create an input format similar to 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 is being 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 and EM-managed spent fuel inventory. An operational prototype of this sequence has been completed and is undergoing testing and debugging.

## **PLANNED ACTIVITIES**

During the remaining 6 months of this project, work will be performed to further refine the capabilities of these new computational tools. An automated SCALE sequence SEN3 will be developed to simplify the input for the 3-D sensitivity calculations. Further refinements will be made to NEWT to improve the code performance and user interface. Collaborative funding has been provided by the Idaho National Engineering and Environmental Laboratory (INEEL) to apply these prototypic sensitivity analysis tools to DOE/EM fuel storage applications. These applications will help demonstrate benefits and to understand limitations of the tools and techniques developed under this project. Where possible, enhancements will be made as identified via applications.

## INFORMATION ACCESS (REFERENCES)

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