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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 prototypic analysis capabilities that can be used by the 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, the 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 specification of arbitrary grids to accurately model the geometry 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 the progress achieved after only seven months of work on a three-year project. Earlier work[1] at ORNL has used one-dimensional (1-D) deterministic codes to provide a scientific basis for using sensitivity and uncertainty analyses techniques to estimate subcritical margins in safety analyses. This current project is investigating the reliability of sensitivity and uncertainty analysis techniques in the three-dimensional (3-D) Monte Carlo codes typically used for criticality safety analyses. Sensitivity information for a system model is generated via a perturbation theory approach where 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. However, in Monte Carlo codes, the angular fluxes needed to obtain sensitivities for certain important reaction types are quite difficult to obtain with the needed accuracy.

Initial studies with Monte Carlo codes have concentrated on using the KENO V.a code of the SCALE code system[2] to compute the sensitivity of k-eff to the $\bar{\nu}$ parameter. This parameter quantifies the number of neutrons generated per fission event and can be a very useful parameter in sensitivity studies; however, angular fluxes are not needed in determination of this parameter sensitivity. A new prototypic code called the <u>S</u>ensitivity <u>A</u>nalysis <u>M</u>odule for <u>S</u>CALE (SAMS) has been developed to read restart files from forward and adjoint KENO V.a calculations, along with the cross-section data associated with these cases, and then calculate sensitivity profiles (sensitivity as a function of neutron energy) requested by the user. This initial version of SAMS is very limited in the types of problems that can be handled and in the types of sensitivities that can be calculated.

Initial studies using KENO V.a and SAMS indicate that, without modifications, KENO V.a will not produce reliable adjoint solutions for cases that are not well moderated. Thus, as an initial reference point, low-enriched, well-moderated systems have been investigated. To verify the $\bar{\nu}$ sensitivity capability of SAMS for a thermal system, a test case was modeled using both the 1-D deterministic codes XSDRNPM and KENO V.a. The test case chosen was an unreflected parallelepiped of homogeneous $U(2)F_4$ and paraffin with an H/X ratio of 195.2 and external dimensions of 71.47 cm × 71.47 cm × 94.14 cm. This geometry was explicitly modeled in KENO V.a and was approximated in XSDRNPM as a sphere. The $\bar{\nu}$ sensitivities for ^{235}U and ^{238}U demonstrate excellent agreement between the two sensitivity analyses.

An automated grid-generation scheme has been implemented in the two-dimensional (2-D), arbitrary-grid code NEWT.[3] The goal is 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 (initially only cylinders and cuboids) 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.

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 the area of criticality safety. In addition, NEWT is being implemented within the depletion sequence 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 is expected to be complete by the end of FY 1998 and could be used within the DOE/EM program to investigate the adequacy of the spent fuel characterization methods currently obtained only through the application of several simplifying approximations.

PLANNED ACTIVITIES

During FY 1998 and 1999 work will be performed to identify and implement techniques and code improvements that will enable full utilization of the sensitivity/uncertainty methodology within 3-D Monte Carlo codes. Also, during this period, a general automated grid generation will be developed and implemented within a SCALE criticality sequence that uses the NEWT code and interfaces with the existing sensitivity/uncertainty analysis module. Extension of NEWT to 3-D will be explored. 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. Where possible, enhancements will be made as identified via applications.

INFORMATION ACCESS (REFERENCES)

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