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Rapid 1-D and 3-D Radiation Transport and Detector Response

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INTRODUCTION

Computed gamma-ray spectra are used for a variety of predictive modeling and analysis applications. Simulations have become an integral aspect of sensor evaluations because of limited access to the types of radiation sources they are intended to detect. Improved accuracy is an open-ended objective because it is difficult to predict how much computational error is acceptable without biasing performance evaluations. In addition to being accurate, calculations must execute quickly because thousands of simulations may be required to complete the evaluation. This document describes how fast and accurate radiation transport and detector response calculations are performed using the Gamma Detector Response and Analysis Software (GADRAS). Examples presented in this paper focus on special nuclear materials because gamma-ray continua associated with fission and Bremsstrahlung radiation, and the physical extent of the materials, make these sources computationally challenging.

DETECTOR RESPONSE FUNCITON

The detector response function (DRF) applies a combination of analytic models and interpolation of a pre-computed scatter library to compute the response of gamma-ray detectors to incident gamma rays. The detector efficiency is determined by a simple application of cross sections to detectors with known dimensions and elemental compositions. Computation of the Compton continuum and escape peaks are more complex, but it can be performed rapidly by applying analytic approximations. The method for performing these calculations has not changed greatly since initial development in the 1980s. [1] However, requirements for three-dimensional (3-D) simulations dictated substantial changes in the representation of gamma rays that scatter into detectors, so directionality is preserved and near and far-field effects are described independently.

ONE-DIMENSIONAL CALCULATIONS

Representing a radiation source as a series of concentric spherical shells would appear to be unacceptably restrictive, but 1-D models are sufficient for many purposes. For example, computed spectra are reasonably accurate if surface areas and masses can be preserved when models are rendered, [2] and inverse modeling often yields non-unique solutions even in this simple case. Although numerous changes have contributed to improved accuracy, the method for 1-D modeling, which combines discrete ordinates [3] and ray-trace calculations, is essentially unchanged since the initial development in the 1980s. In addition to tallying the gamma-ray leakage, the ray-trace calculations also tally the leakage-weighted atomic numbers (Z) and areal densities ($\rho\ell$) of intervening materials, which vary for each energy depending on the mean depth from which the gamma-rays interact in the materials. These parameters are used to interpolate a pre-computed database of scatter spectra. Computed spectra derived from ray-trace calculations are stripped from the discrete spectrum to obtain residuals, with a coarse group structure that is smoothed by linear interpolation. Using the DRF to combine the two photon tallies yields a good representation of the total spectrum. Figure 1 presents an example for a 1-kg depleted uranium (DU) sphere.

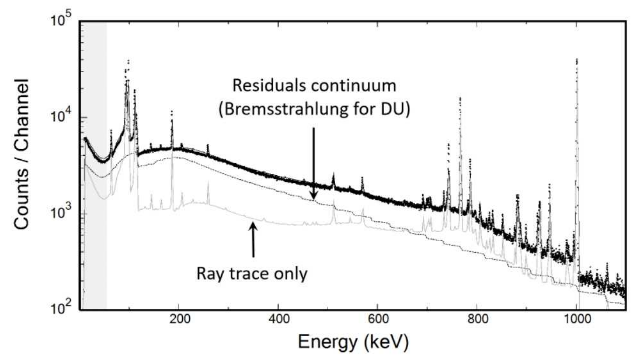

Fig. 1. The ray-trace spectrum for discrete gamma rays is displayed in gray, and the dashed continuum is the difference between discrete ordinates and ray-trace. The total computed spectrum (black) is virtually indistinguishable from the measured spectrum (dots).

THREE-DIMENSIONAL CALCULATIONS

The discrete ordinates calculations that are performed on spherical models are saved to produce volumetric gamma-ray source terms. These volumetric source terms are discarded for 1-D calculations, which only utilize computed leakages. In our initial foray into 3-D calculations, we began utilizing this information to compute the acceptance of photons incident on asymmetric and collimated detectors, which are 3-D effects even for 1-D sources. Discrete ordinates calculations can be computed in higher dimensionality, but the computational time increases from seconds to hours or longer. Rapid 3-D calculations are achieved by retaining the volumetric source terms for spherical equivalents of the primitive objects (i.e., spheres,

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cylinders, slabs, etc.) that collectively describe 3-D models. The computational challenges are that the ray-trace calculations must accommodate arbitrary geometric configurations, and residual spectra cannot be applied to compensate for discrepancies in the interpolation of the scatter spectra, as they were for 1-D calculations. These challenges are addressed as described below.

Adaptive Mesh

Acceptable results can be obtained by performing ray-trace calculations for 3-D models that are subdivided into numerous mesh points, but there is a computational penalty for applying an excessively fine mesh. This problem is approached by applying an adaptive mesh, which starts with a crude mesh, then reduces the size for regions over which rapid changes occur. Meshes are computed for several energy groups to retain accuracy while eliminating unnecessary calculations. Figure 2 shows the mesh for the energy group encompassing 60-keV that is derived for a plutonium cylinder beneath a shadowing sphere.

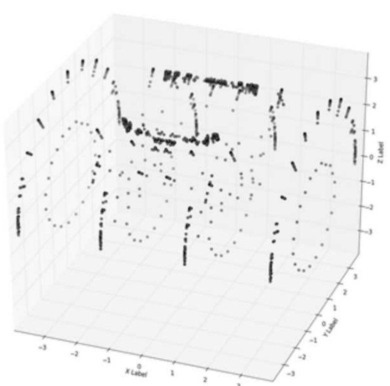

Fig. 2. Adaptive mesh points for a plutonium cylinder beneath a shadowing sphere (60-keV energy group).

RESULTS

Computed gamma-ray spectra have been compared with numerous benchmark measurements to validate the computational approach. Figure 3 shows the configuration for the measurement a solid 4.5-kg plutonium ball inside a 7.6-cm-thick polyethylene sphere. [4] Figure 4 shows that the computed spectrum is in good agreement with the measurement over the energy range 0 to 11 MeV (the inset shows the range 50 to 800 keV). The steel tables that support the test object and the HPGe detector emit high-energy gamma rays following the neutron capture by iron, which is an effect that cannot be replicated by a 1-D model. The continuum in the range 3-8 MeV is dominated by fission gamma rays, and the continuum above 8 MeV derives primarily from neutron absorption in the HPGe crystal. Inelastic neutron scatter on germanium is also notable near 600 and 700 keV.

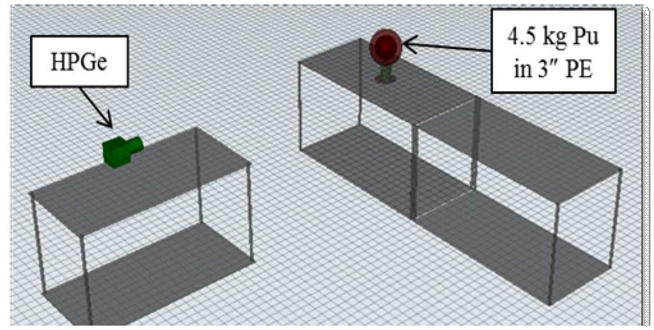

Fig. 3. Configuration used to measure emission from 4.5-kg of plutonium inside a 7.6-cm-polyethylene sphere with an HPGe detector.

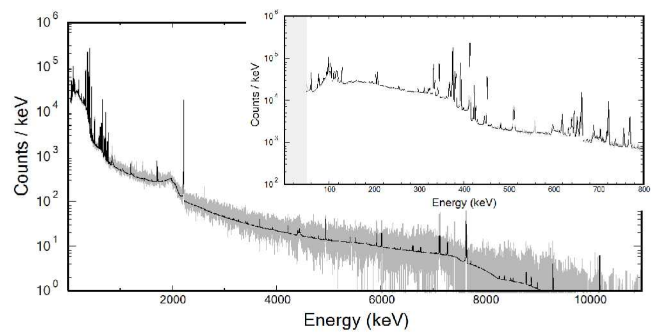

Fig. 4. The computed spectrum (black) for a solid 4.5-kg plutonium inside a 7.6-cm-polyethylene sphere is compared with a measurement (gray).

FUTURE DEVELOPMENT

Ray-trace calculations associate leakage-weighted values of Z and $\rho\ell$ to each gamma ray. These values do not reflect the sequence of materials, so the interpolated scatter continuum may not be accurate if heterogeneous shields are present. The residuals spectrum compensates for these errors for 1-D calculations, but the discrete ordinates leakages are not always applicable for 3-D models, which may nest objects within other objects. We are currently evaluating more sophisticated methods for deriving Z and $\rho\ell$ to account for the greater influence of external materials on the scatter spectra. The objective is to achieve this and several other refinements without increasing computation time appreciably.

CONCLUSIONS

The methodology described in this report enables computation of spectra for complex 3-D objects in about one minute with a typical office computer whereas other methods generally require orders of magnitude more computational time. This capability is achieved in part by using the output of ray-trace calculations to interpolate pre-computed continuum templates.

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