MONTE CARLO CALCULATIONS OF LOW
BACKGROUND DETECTOR RESPONSE

H. S. Miley

November 1993

Presented at the
IEEE 1993 Nuclear Science Symposium
November 2-6, 1993
San Francisco, California

Work supported by
the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
Richland, Washington 99352

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

VED

DEC 30 1993

OSTI

Monte Carlo Calculations of Low Background Detector Response

Harry S. Miley, Pacific Northwest Laboratory¹
Battelle Blvd., Richland, WA 99352

Abstract

An implementation of the Electron Gamma Shower 4 code (EGS4)[1] has been developed to allow convenient simulation of typical gamma ray measurement systems. Coincidence gamma rays, beta spectra, and angular correlations have been added to adequately simulate a complete nuclear decay and provide corrections to experimentally determined detector efficiencies. This code has been used to strip certain low-background spectra for the purpose of extremely low-level assay. Monte Carlo calculations of this sort can be extremely successful since low background detectors are usually free of significant contributions from poorly localized radiation sources, such as cosmic muons, secondary cosmic neutrons, and radioactive construction or shielding materials.

Validation of this code has been obtained from a series of comparisons between measurements and blind calculations. The singles counting efficiency of a particular counting experiment was reproduced within the accuracy of the known dimensions of the detector components. This allowed the complete simulation of a nuclear decay, including two coincident gamma rays with a non-isotropic angular correlation. In addition, text-book efficiency curves have been reproduced for several sizes of sodium iodide detectors.

Examples of the use and several spectral results will be presented.

I. INTRODUCTION

In the Nuclear Chemistry Section at Pacific Northwest Laboratory (PNL), Monte Carlo radiation transport calculations have long been successfully applied to specialized double-beta decay needs. In most cases, Monte Carlo methods have been the sole solution. However, most modeling efforts needs have required a new geometry code. Due to the time-consuming nature of writing, debugging, and testing codes, most laboratory projects have been conducted with simplified geometry codes, material selections, and source specifications. As a result, these generic calculations have suffered in accuracy.

To solve a detector optimization problem involving many geometrical regions, yet requiring good accuracy, a geometry code allowing coaxial cylinder combinations was written. With coaxial geometry, many typical germanium and sodium iodide detectors may be completely simulated, including most

major components of the cryostat or capsule. As a result, much greater accuracy is obtainable.

This code has been used to predict detector efficiency for unusual sodium iodide configurations, to calculate *in situ* signal strength in environmental applications, to predict effects of angular correlation on detector response, and to perform research into the effects of inhomogeneously produced calibration sources.

Key features of this code are designed to facilitate ordinary laboratory uses. The code records spectra for up to four detectors in a single simulation. Point and extended sources are supported, as well as coincident beta or positron emission. Multiple coincident gamma rays may be generated, either a pair with angular correlation or a succession of six, isotropically emitted. Most nuclear decays can be simulated. In fact, the entire decay schemes of many complex nuclei have been simulated in a single run of the code.

II. SOFTWARE DESIGN

The EGS4 code system forms the basis of the software reported here. The EGS4 system basically consists of a set of subroutines which actually transport the photons or electrons and keep track of all physical parameters. The user must write a main routine, a geometry routine, and a routine to keep track of, or score, the energy deposition.

The succession of EGS4 codes written within the PNL Nuclear Chemistry group have gradually incorporated more sophisticated simulation of a nuclear decay. The original application was simulation of radioactive contaminants within an ultra-low background germanium crystal. This application focused as heavily on the continuum as on the photopeaks in the simulated spectrum and required summing of gamma rays and coincidentally emitted betas. In this particular case, only after the simulation included the final x-ray associated with the nuclear decay did the experimental and simulated spectra agree. More ordinary applications might only require the estimation of photopeak efficiency, which is easily accomplished.

To simulate a complete nuclear decay, the user must evaluate each possible path from the ground state of the parent nucleus to the ground state of the daughter. This usually produces, for each path, a short list of gamma rays, a beta or positron, an x-ray, and a relative probability for that decay path. To save preparation time, very weak branches can be ignored at the cost of accuracy in the final result. Each

¹Pacific Northwest Laboratory is operated by Battelle Memorial Institute for the US Department of Energy under Contract DE-AC06-76RLO 1830.

simulated decay path requires a record in the input file to instruct the main routine to originate a group of radiations at a certain location.

Eventually, support for non-allowed beta shapes was added, as was support for angular correlations among two gamma rays. Various PNL EGS4 codes have also simulated simplified scintillation light transport, phototube response and statistical effects at the photocathode. Certain nuclear electronics have also been simulated. For instance, energy discriminators and multi-detector coincidence logic have been included in some codes to predict the signals obtained from complex, multi-detector arrays.

Previous EGS4 implementations have had 'fixed' geometry codes. That is, any significant geometry change would require additional coding, compilation, and testing. As an example, a code was written that simulated a small disk-shaped radiation source at the end of a coaxial germanium detector, with no cryostat. Making a simple change like adding a thin absorber required some additional coding and compilation. Enlarging the source beyond the radius of the detector required more subtle changes to the geometry, and therefore required considerably more effort. On a MicroVAX II, a complete compile and link takes about 6 minutes. This hampers rapid changes to codes and makes the software maintenance more difficult.

A code that allows geometry variation without software changes was developed and tested. The new geometry code requires a geometry data file containing the dimensions of cylinders and planes normal to the z axis. This geometry data is then used to partition the volume to be simulated into rings of rectangular cross section. Additional data in the geometry data file supplies information concerning the media in each region, determining if the region is one of the four allowed detectors, or a source of radiation.

The main routine randomly chooses decay locations from the source-designated regions. After each decay, the energy deposited in each detector region is recorded into the histogram corresponding to the detector number.

Besides the executable code, a decay information file, a geometry file, and materials data file are required. By replacing the few platform dependent subroutines, the FORTRAN level code has been easily transported from a VAX to a 486/66 MHz PC and a Sun Sparcstation II.

In addition, a simple geometry visualizer has been written for the PC to check the validity of the geometry data. This program displays three cross sectional views of the regions with colors designated first according to medium number (0-10), according to detector number (0-4), and finally according to source number (0-1). This was originally written to test the geometry data input code, but became indispensable to test complex geometry files. Since most of the effort in using the code system described by this communication is involved with the creation of the geometry input file, one could infer that a better geometry input system is needed that would require less user sophistication.

III. TESTING

Besides a number of simplistic evaluations of compiled photopeak efficiencies for sodium iodide detectors, the code was tested by high accuracy simulation of photopeak efficiencies in a complex geometry. The simulation was compared to an actual experiment performed in a low-background detector placed in an underground location beneath about 1000 meters-water-equivalent (mwe) of overburden in the Soudan mine in Soudan, Minn. The geometry consisted of a germanium detector assembly, complete with a germanium dead layer and a copper vacuum jacket, as shown in Fig. 1. The detector was surrounded by a plastic container filled with molybdenum oxide powder well mixed with a trace level of natural radioactivities (Radium-226 and daughters). An extended counting period assured that statistical errors were insignificant, and the resultant efficiency curve was of exceptional quality (approximately 1% total error in the 500-600 keV region).

Fig. 1 Test Geometry

The analysis of the molybdenum experiment required the precise knowledge of the detection efficiency for a pair of gamma rays (539 keV and 590 keV in molybdenum-100 double-beta decay). These gamma rays are in coincidence and have a non-trivial angular correlation. As a confidence building exercise, the Monte Carlo simulation was first used to estimate the measured singles efficiency, then to estimate the angle correlated efficiency.

Precise dimensional accuracy is required to begin any simulation. Germanium detectors are frequently delivered with only a single nearest-millimeter measurement of the crystal length and diameter. Fortunately, the detector in question had been carefully measured at the time of manufacture by technicians at Princeton Gamma Tech of Princeton, NJ.

However, to produce a scientifically honest atmosphere, the first simulation effort was run blind. The experimental efficiency of the detector was too well known to be a secret, so the length and width dimensions of the crystal were transposed without the knowledge of the person simulating the efficiency. The first efficiency results were 15% too low.

The accuracy of the test geometry was extensively checked and values for material densities, absorber thicknesses, and relative spacing were slightly improved. The new results were then 19% too low.

At this point, the correct detector dimensions were revealed. Transposing the length and diameter of the crystal changed the detector volume by 19%. The final efficiency simulations, obtained only by this transposition, were an average of about 1.5% high. Additional variation of parameters could have essentially nullified this difference, but the critical dimensions were not known beyond this precision, and the measured efficiency values were no better.

An additional test was performed by simulating several backgrounds in an ultra-low background copper shield operated beneath 4000 mwc in the Homestake mine in Lead, SD. In essence, the decay products of thorium-232 and cosmogenic cobalt-58 in a 11 kg marinelli electroformed copper shield were simulated for the purpose of assay and spectrum stripping. The simulated spectra of thorium-228 (and daughters in equilibrium), cobalt-58, and actinium-228 are shown in fig. 2. These represent simulations of 11e5, 3e6, and 32e5 decays, respectively.

The thorium chain, measured to be at or near equilibrium, was assayed at $7e-2$ μ Bq/g, and the observable peaks from 238 keV to 2615 keV all agreed well with the relative intensities in the simulation. The cobalt, formed by fast cosmic secondary neutrons spallating the copper while on the Earth's surface, assayed at 98 μ Bq/g. The spectrum resulting

confirming that a single detector component containing about 300 μ Bq/g lead-210 dominated the background.

Since the stripped spectrum had the same spectral shape as that of the original shield, one can infer that the continuum part of the simulated spectrum was within statistical uncertainty of being correct.

Finally, multiple identical runs were made of a simple simulation of a germanium detector response to cobalt-60. The predicted photopeak intensities were histogrammed to explore the randomness of the results. The histogrammed results fit well within a poisson distribution whose only free parameters were the center and the integral of the distribution.

IV. CURRENT APPLICATIONS

The code has been used to correct experimentally determined singles photopeak efficiencies for angular correlations. The code has been used to estimate the efficiency of non-existent detectors for procurement evaluation. The code has been used to determine the efficiency factor for measuring trace isotopes distributed in a 1 meter diameter, 1 meter thick environmental sample. The code is being used to simulate photopeak efficiency in a complex source.

Several of these applications are simply designed to eliminate calibration by radiochemical means and thereby reduce radioactive waste and human exposure. Some

Fig. 2 Simulated spectra of thorium-228, cobalt-58, and actinium-228 at 2 keV per channel

from the stripping of these backgrounds was within error bars of that obtained without the copper marinelli shield.

applications, such as angular correlation corrections and internal contaminant simulations, simply are not practical to perform experimentally.

Most of the listed applications generally require a few hours to construct the geometry and decay information files, and then can be run in a few hours to obtain final results. As an example, the test geometry case described above simulated two medium energy gamma rays originating in a thick molybdenum powder source. A run of $1e5$ gamma ray pairs required about 2 hours on a 486/66MHz PC. Many runs were summed to produce the final result. The Sun machine ran this simulation in about half the time. The MicroVAX II required about eight times as much time.

The PC code required about 640K of RAM and has numerous VAX FORTRAN extensions. Therefore, it is not suited well by common PC FORTRAN compilers. The code was, however, easily compiled by a 32 bit FORTRAN compiler bundled with a special operating system extender. In addition, the code may be run in a background window without a significant penalty.

The most common failure mode of the code appears to be due to the straggling of electrons in thin regions. When the computed lateral straggling of the electron exceeds the distance to the nearest region boundary, an occasional fatal error may occur. For this region, it is much preferable to operate in a mode in which many short simulations are performed and summed later. In the test geometry, which contained a thin copper vacuum jacket (0.5 mm), a thin germanium dead layer (0.6 mm), and somewhat thin plastic walls (2 mm), about one fatal error occurred per 15 runs of $1e5$ decays.

Using PCs can be quite convenient, given the usual nature of the Monte Carlo effort and the most common failure mode of the code. Researchers usually run several versions of the simulation, varying one parameter to inspect the variability of the results. It becomes convenient to assign each PC a different parameter value. Because of the background nature of the computation, no loss of the PC capability is observed by the machine's owner, and five PCs can approach the computing power of much more expensive machines dedicated to this purpose. Overnight calculations on a single 66Mhz PC has easily provided the 1% statistical error reported in the test case.

V. CONCLUSIONS

The 4% variation seen in the blind test results when the entire set of dimensional parameters were heavily scrutinized substantiates the "5% error" rule of thumb frequently used by scientists who casually simulate radiation transport. However, Monte Carlo calculations can still give embarrassingly large errors, particularly when too many simplifications are assumed. Frequently, these assumptions are justified on the basis of the effort required to properly set up a geometry, or the difficulty in simulating the nuclear event of interest. Many of these concerns have been addressed in the code discussed here.

In conclusion, a very powerful implementation of the EGS transport code has been developed and verified for typical

laboratory experiments. Its operating mode favors distributed processing on very low cost machines, its geometrical flexibility allows accurate simulations, and its description of an entire nuclear decay enables users to produce more meaningful results in one class of simulations.

VII. REFERENCES

- [1] W.R. Nelson, H. Hirayama and D.W.O. Rogers, SLAC Report 265, Stanford Linear Accelerator Center, December 1985.

**DATE
FILMED**

2 / 4 / 94

END