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Conf-9309296--1

PNL-SA-22707

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September 1993

Presented at the
Theory and Phenomenology in Astroparticle
and Underground Physics Conference
September 19-23, 1993
Gran Sasso Lab, Italy

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

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Simulated Progress in Double-Beta Decay

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A Monte Carlo code has been developed to accurately simulate double-beta decay measurements. Coincident gamma rays, beta spectra, and angular correlations have been added to adequately simulate a complete ¹⁰⁰Mo nuclear decay and provide corrections to experimentally determined detector efficiencies. This code has been used to strip certain low-background spectra obtained in the Homestake gold mine in Lead, SD, for the purpose of extremely sensitive materials assay for the construction of new, large, enriched germanium detectors. Assays as low as 9 μ Bq/g of ²¹⁰Pb in lead shielding were obtained.

1. 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 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, an implementation of the Electron Gamma Shower 4 code (EGS4)¹, has been used to compute detector efficiencies in a variety of situations. The work reported here consists of efficiency computations for a ¹⁰⁰Mo double-beta decay experiment and materials assays conducted in the Homestake mine in support of the International Germanium Experiment (IGEX).

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

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

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.

2. MOLYBDENUM-100 SIMULATIONS

Besides a number of simplistic evaluations of compiled photopeak efficiencies for sodium iodide detectors, a challenging confidence-building task was undertaken to validate the simulation for use in the ^{100}Mo double-beta decay data analysis. Simulated photopeak efficiencies were compared to an actual calibration 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 Figure 1. The detector was surrounded by a plastic container filled with molybdenum powder well mixed with a trace level of natural radionuclides (^{226}Ra and daughters). An extended counting period assured that statistical errors were insignificant, and the resultant efficiency curve was of exceptional quality (approximately 1% total uncertainty in the 500-600 keV region).

Figure 1 Molybdenum Geometry.

The analysis of the molybdenum experiment data required the precise knowledge of the detection

efficiency for a pair of gamma rays (539 keV and 590 keV in ^{100}Mo double-beta decay). These gamma rays are in coincidence and have a non-isotropic angular correlation. The variation of the efficiency due to coincidence and angular correlation cannot be conveniently experimentally determined. Thus it was required that the singles efficiency should be well simulated before the calculated coincidence correction factor would be accepted.

Precise dimensional accuracy is required to begin any simulation. Germanium detectors are frequently delivered with only a single measurement of the crystal length and diameter made to the nearest millimeter. 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 singles efficiency simulations, obtained only by this transposition, were an average of about 1.5% higher than the experimental values. 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.

3. MATERIALS ASSAY IN HOMESTAKE

Several backgrounds were simulated in an ultra-low background copper shield identical to one operated beneath 4000 mwe in the Homestake mine. The system geometry was similar to the molybdenum case above. In essence, the decay products of ^{232}Th and cosmic ^{58}Co in an 11 kg Marinelli

Figure 2 Simulated spectra of ^{228}Th and daughters (A), ^{58}Co (B), and ^{228}Ac (C) at 2 keV per channel.

electroformed copper shield were simulated for the purpose of assay and spectrum stripping. The simulated spectra of ^{228}Th (and daughters in equilibrium), ^{58}Co , and ^{228}Ac are shown in Figure 2. These represent simulations of 1.1, 3, and 3.2 million decays, respectively.

The background simulations above resulted in calculated detector efficiencies which allowed the determination of the concentrations of the modeled radionuclides. The thorium chain, measured to be at or near equilibrium, was found to be $0.07\ \mu\text{Bq/g}$, and the observable peaks from 238 keV to 2615 keV all agreed well with the relative intensities in the simulation. The ^{58}Co , formed by fast cosmic secondary neutrons spalling the copper while on the Earth's surface, was $98\ \mu\text{Bq/g}$. The poor statistical quality of the peaks used for this analysis caused a 30% uncertainty in these concentrations.

The spectrum resulting from the stripping of these backgrounds was within error bars of that obtained without the copper Marinelli shield, confirming that a single detector component containing about $300\ \mu\text{Bq/g}$ ^{210}Pb dominated the background. In addition, a new ^{210}Pb limit in the surrounding lead shielding material was obtained by taking the difference between the stripped spectrum and spectra obtained without the copper inner shield. The limit from alpha

counting for this lead was $<300\ \mu\text{Bq/g}$. Attributing the entire difference to ^{210}Pb in the outer shield reduced this limit to $<9\ \mu\text{Bq/g}$.

4. CONCLUSIONS

The observed 4% variation in the blind test, resulting from careful adjustment of the entire set of dimensional parameters, substantiates the "5% error" rule-of-thumb frequently used by scientists casually simulating 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.

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