MONTE CARLO SIMULATION OF A LIQUID SCINTILLATION COUNTER USING GEANT4 CODE

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ABSTRACT. This paper presents a first approach to the use of the GEANT4 Monte Carlo (MC) technique in liquid scintillation counting (LSC) applied to measurements in radiological laboratories. The GEANT4 software was developed by RD44, a worldwide collaboration of national institutes, laboratories, and large high-energy physics experiments. GEANT4 is a public software package composed of tools that can be used to accurately simulate the passage of particles through matter. The GEANT4 catalog of processes at optical wavelengths includes refraction and reflection at medium boundaries, bulk absorption, and Rayleigh scattering. Processes that produce optical photons include the Cherenkov effect, transition radiation, and scintillation.

The simulated setup includes a vial containing the scintillation cocktail in between 2 opposite photomultipliers tubes (PMTs) working in sum-coincidence mode. The decay of several beta emitters (such as ^{14}C and ^{3}H) can be simulated, as well as alpha or EC emitters. Additionally, significant information could be obtained, such as the energy deposited by decay into the scintillation cocktail or the light output generated into the scintillation cocktail. GEANT4 is a useful tool for efficiency calibration, stopping power calculations, or wall effect studies for different scintillation cocktails and geometries.

INTRODUCTION

Liquid scintillation counting (LSC) is an accurate technique for standardization of radionuclides (Broda et al. 2007). Different methods have been proposed for quantitative LSC measurement: the CIEMAT/NIST method (Grau Malonda and García-Toraño 1982) and the triple-to-double coincidence ratio (TDCR) method (Pochwalski and Radoszewski 1979). Both methods need critical data in order to determine accurately the activity of the standards. Calculation of the counting efficiency for a specific nuclide and LS counter, together with the computation of the energy spectrum transferred to the liquid scintillator, becomes essential to the standardization methods. Several models (Simpson and Meyer 1992; Grau Carles and Grau Malonda 2001) and computer codes (Garcia-Toraño and Grau Malonda 1985; Grau Carles 2006) have been used to calculate those data.

In this work, a first approach is presented for the use of the Monte Carlo (MC) technique, using the GEANT4 toolkit, in liquid scintillation counting (LSC). The MC simulation includes a number of processes, namely, beta-ray generation, energy deposition into the scintillation cocktail, light production, light attenuation, photoelectron generation, and signal amplification in 2 photomultiplier tubes (PMT) working in coincidence. The simulation is carried out in such a way that several parameters can be calculated for a nuclide, like counting efficiency, energy spectrum, or wall effects.

METHODS

Monte Carlo Simulation

The MC simulations have been carried out through GEANT4 code (Agostinelli et al. 2003). GEANT4 is a public toolkit for high-energy physics (HEP) experiments using an object-oriented environment and written in C++. GEANT4 is not only for HEP but also for cosmic rays physics, space science, and medical applications. In order to meet such requirements, a large degree of functionality and flexibility is provided for geometrical description, primary particle generation, physics processes, and visualization and analysis technologies.

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In GEANT4 code (version 8.2), highly complex setups and a rich set of solid types (simple solids, Boolean solids, BREPS [Boundary REPresented Solids]) containing different materials are available for describing the geometry setup of each experiment. Additionally, various utilities provided within the GEANT4 toolkit help for the generation of primaries particles in the simulation. GEANT4 allows the selection of particle type (all PDG data and even radioactive ions), energy, and momentum, together with its distribution into different areas or volumes.

The GEANT4 toolkit includes the simulation of electromagnetic physical processes from 1 keV to 100 TeV. The processes associated to gammas are the photoelectric effect, Compton scattering, pair production, and electron and muon pair production. For electrons and positrons, the processes included are ionization and delta ray production, *bremsstrahlung*, e+e– annihilation, and synchrotron radiation. Finally, the physical processes corresponding to all charged particles are made up of multiple scattering, transition radiation, as well as scintillation and Cherenkov radiation. These last 3 processes are vitally important to simulate a LSC counter using the GEANT4 toolkit. If a charged particle produced in the decay of the radionuclide traverses a dielectric material with velocity above the Cherenkov threshold or a scintillating material, an optical photon is produced. A photon is called optical when its wavelength is much greater than the typical atomic spacing, for instance when $\lambda \geq 10$ nm, which corresponds to an energy $E \leq 100$ eV. Next, the optical photons undergo 3 kinds of interactions: elastic (Rayleigh) scattering; absorption; and medium boundary interactions (refraction and reflection) along the geometry of the simulated setup.

Simulation Setup

The simulated setup consists of a LS counter system (Quantulus 1220^{TM}) and a Wheaton^{TM} borosilicate glass vial of 20 mL. The counter is made up basically of 2 PMTs (model Hamamatsu^{TM} R331-05) working in coincidence, and the materials and dimensions of the window and the photocathode are included into the simulation (J Furness, personal communication, 2008). The simulated vial contains a standard of ^{14}C and ^{3}H (PerkinElmer unquenched LSC standards 1215-111) into 10 mL of a xylene-based LS cocktail.

Output Pulse-Height Spectrum

The optical photons reaching the photocathode produce photoelectrons (n_P) depending on their wavelength and according to the quantum efficiency of the PMT (Hamamatsu Corp. 1998). The photoelectron amplification in the first dynode is simulated assuming statistical Poisson distribution with a mean value of $n_p d_1$ (d_1 is the dynodic gain). This step is repeated for every dynode, and a pulse of electrons is obtained at the anode of the PMT. The signals from both PMTs are checked for coincidence and a final pulse is obtained.

In order to test the simulation results, the computed pulse-height spectra are linearly transformed into a channel spectra using adjustable parameters associated with the linear amplifier of the electronic chain.

RESULTS AND DISCUSSION

The method has been applied to the simulation of the response of a Quantulus system with 2 PMTs working in coincidence for ^{3}H and ^{14}C for different values of the figure of merit (FOM). This parameter is defined as the ratio between the deposited energy into the liquid scintillator by the interacting particle and the number of photoelectrons emitted by the photocathode (Horrocks and Studier 1961). The obtained results are shown in Figures 1 and 2. For the unquenched standard samples, the calculated values are shown in Table 1. The agreement between the calculation and experiment is remarkably good, in spite of the approximations adopted for the geometry setup. The calculated and experimental spectra are compared in Figures 3 and 4 for ^{14}C and ^{3}H, respectively. A good agreement is also obtained in the comparison of the spectra.

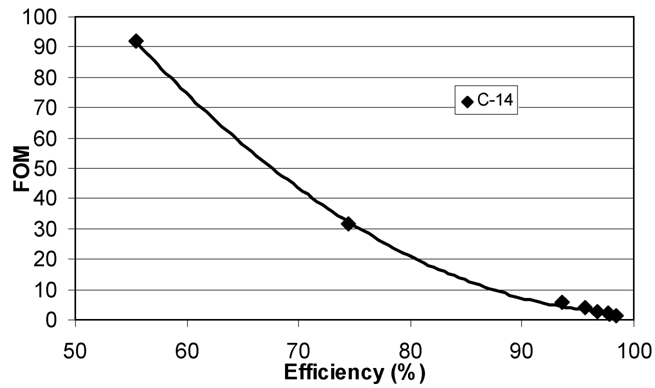

Figure 1 FOM factor vs. calculated efficiency for ^{14}C in a Quantulus system

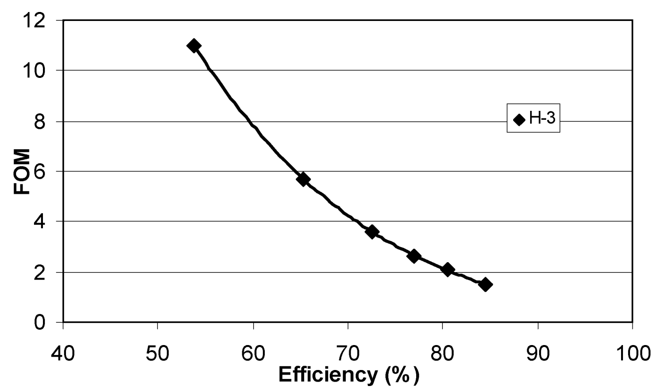

Figure 2 FOM factor vs. calculated efficiency for ^{3}H in a Quantulus system

TAble 1 Experimental and calculated efficiency for ^{3}H and ^{14}C.

	Efficiency (%) ^{3}H	Standard uncertainty	Efficiency (%) ^{14}C	Standard uncertainty
Experimental	66.0	0.5	96.0	0.8
Simulation	65.3	0.6	95.6	0.9

Finally, the MC technique was applied to study the wall effects occurring when a high-energy electron may leave the scintillator without losing all its energy. This effect must be taken into account in the calculation of the counting efficiency. The calculations were made for a ^{90}Y source into a 20-mL scintillation vial. The beta particle may be affected by the different physical processes like transition radiation, scintillation, and Cherenkov. The beta energy spectra of ^{90}Y and the calculated spectra where the wall effect has been evaluated are presented in Figure 5. It is clear from the figure that the spectrum distortion is significant.

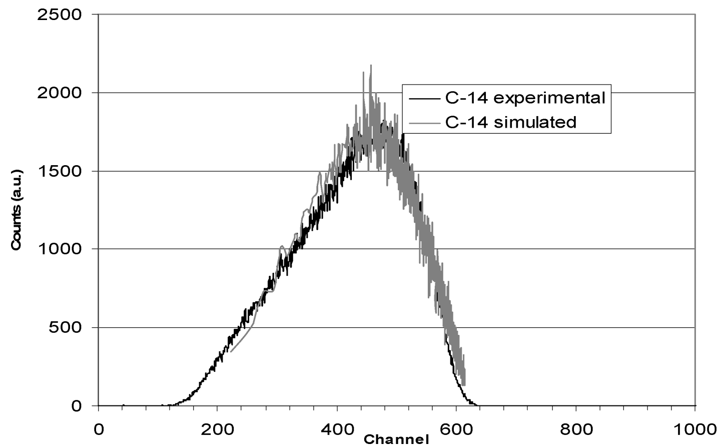

Figure 3 Calculated and measured spectra of ^{14}C

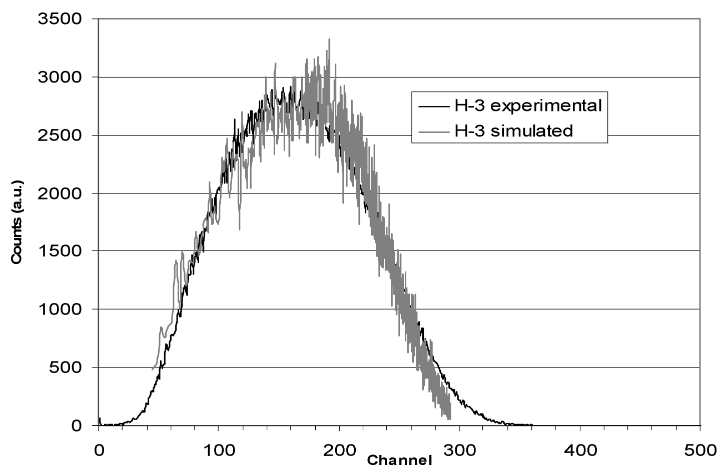

Figure 4 Calculated and measured spectra of ^{3}H

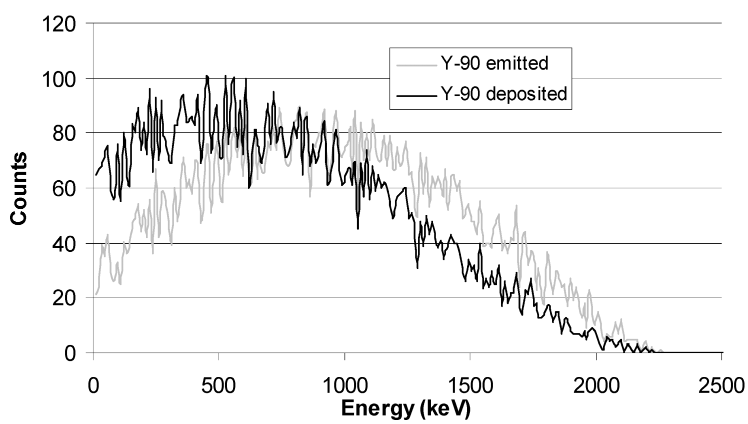

Figure 5 Theoretical and wall-effect-distorted beta spectra of ^{90}Y

CONCLUSION

We conclude that the MC simulation proposed accurately describes both the spectral shapes and the counting efficiencies of beta emitters as measured with a Quantulus LSC system, as well as other phenomena like the wall effect. Additional work toward improving the simulation setup containing the optical chamber, and to extending to alpha and EC emitters, is currently under study.

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