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Iterative optimisation of Monte Carlo detector models using measurements and simulations

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ABSTRACT

This work proposes a new technique to optimise the Monte Carlo models of radiation detectors, offering the advantage of a significantly lower user effort and therefore an improved work efficiency compared to the prior techniques. The method consists of four steps, two of which are iterative and suitable for automation using scripting languages. The four steps consist in the acquisition in the laboratory of measurement data to be used as reference; the modification of a previously available detector model; the simulation of a tentative model of the detector to obtain the coefficients of a set of linear equations; the solution of the system of equations and the update of the detector model. Steps three and four can be repeated for more accurate results. This method avoids the "try and fail" approach typical of the prior techniques.

1. Introduction

The increase of computing power available to the average workstation in the recent years allows a shift from the laboratory to the desktop of development and calibration of in vivo measurements systems (e.g. whole- and partial-body counters): where measurements with real detectors and sources were previously used, now simulations of equivalent setups can be performed. The shift brought several advantages, such as the possibility of simulating not yet available measurement configurations which may later be selected and implemented in the laboratory [1], or the immediate availability of custom radioactive sources and of calibration phantoms not available in physical form.

The simulations are performed with Monte Carlo software such as MCNPX [2] or GEANT [3]. These tools simulate the transport of radioactive particles of broad ranges of energies through the matter, from the source to the detector. The model of the detector is a limiting factor for the overall quality of the simulations, but the set-up of accurate detector models is a time consuming task, because sometimes the technical drawings provided by the manufacturers are accurate only for the front region of the detector (sometimes not even there [1]).

Different setups involve radioactive sources located not only at the front side of the detector, but also on the side of the active crystal (e.g. a Marinelli beaker or a liver contamination in the case of a partial-body measurement of lungs). For these cases an improved Monte Carlo model has to be developed.

Different techniques are available in the literature for the optimisation of detector models for Monte Carlo simulations. Among the least accurate techniques, one consists in precomputing the effects of different small changes applied to a reference model. The set of changes that improves the final agreement of the simulations is then chosen as new reference or as final model [4].

Another technique [5] uses radiographic images of a detector unit to update the corresponding virtual model. This method can determine visible parameters such as position, size and shape, but it requires a complex instrumentation (a measurement facility suitable for ^{60}Co radiographies) and it is not suited to estimate the dead layer thickness, an important parameter for simulating low-energy X- and gamma-radiation.

The technique disclosed in [6] consists of a manual "try and fail" approach where a manual addition of layers or cylinders is required. This technique is limited to axially symmetric models.

The method that best allows to reproduce the experimental results is described in [7]: the final deviations between measurements and simulations are below 3% for any energy and source configuration.

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[1] The opinions expressed in this paper are those of the author, an examiner at the European Patent Office (EPO). They should not be construed as necessarily the policy of the European Patent Office (EPO), or imply any commitment by the EPO to any particular course of action.

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However, this method requires a special measurement geometry, involving a tungsten collimator, a very high number of measurement points and a significant user effort.

The present work describes a method that overcomes most of the deficiencies of the described techniques and that improves the accuracy of detectors models efficiently with respect to time and effort. Moreover, it is not limited to detectors with an axially symmetric geometry.

2. Instruments and method

The method here described consists of four steps. In the first step experimental measurements are carried out, in the second step a series of input files is generated, in the third step Monte Carlo simulations are performed using the most up-to-date detector model and in the fourth step the model is updated using the measurement data and the results of the simulations. Steps three and four can be iteratively repeated until the desired accuracy is achieved.

The detectors used for this work are Canberra XtRa HPGe detectors, characterised by a closed-end coaxial p-type crystal and by a dead layer 0.3–0.4 μm thick on the front side and 0.6–0.9 mm thick on the lateral side. The crystal is held in place with a copper holder 0.8-2.7 mm thick [1] and with screws in unknown number and shape. A simplified drawing representative of a detector and of the setup later used for the measurements is shown in Fig. 1 (the inner details such as the crystal holder are not shown).

To ensure the accurate and reproducible positioning of the point sources during the measurements, a custom plate made of PMMA was manufactured. The plate (element 'c' in Fig. 1) was mounted on top of the detector case (see Fig. 1) and could be rotated around the axis of the detector to probe the detection efficiency at different angles. The mounting means were thin enough not to shadow the crystal during the measurements. This ensured the most reproducible input data.

A source holder also consisting of PMMA (element 'd' in Fig. 1) is fixed to the plate. The holder provides two different positions for the point source (element 'e' in Fig. 1) at 39 mm and 142 mm from the front plane of the detector case. Radially the source holder can be mounted at two radii at 100 mm or 200 mm from the centre line of the detector; the actual distance from the surface of the case is about 50 mm smaller due to the diameter of the casing (element 'a' in Fig. 1). As the crystal is about 70 mm long and is shifted 5 mm from the front plane of the detector case, the source was positioned at 39 mm below the detector surface. Fig. 2 shows an actual measurement configuration with the holder mounted.

The Monte Carlo software used is MCNPX 2.7.0 [2]. The simulations were run in "photon" mode, where an explicit tracking of the secondary electrons is avoided and their energy is deposited in the place of the interaction photon-matter. This simplification made the simulations over a magnitude faster without affecting the final results: the difference between the two approaches was found to be within the statistical uncertainty. This happens because the ranges of electrons in the materials used and at the energies involved are shorter than the minimum size of the detector geometry. For example, the range for 60 keV electrons in copper, aluminium, germanium is $R(e^-)_{Cu} = 1.06 \times 10^{-5}$ m, $R(e^-)_{Al} = 2.91 \times 10^{-5}$ m and $R(e^-)_{Ge} = 1.87 \times 10^{-5}$ m.

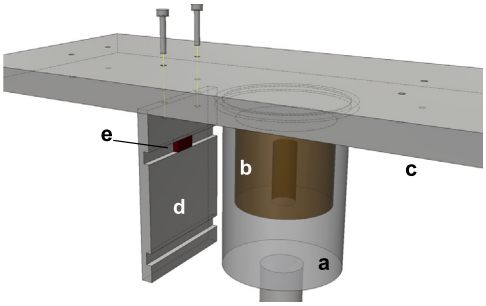

Fig. 1. Simplified drawing of the measurement setup, not to scale: (a) detector case; (b) crystal; (c) PMMA plate with holes for screws; (d) point source holder and screws for mounting to the PMMA plate; (e) point source inserted in a slit of the holder. The bottom side of the plate has means for holding the plate in position on top of the detector case, while keeping the plate free to rotate.

Fig. 2. Detector with the PMMA plate mounted on top and the source holder hanging from the PMMA plate. The holder has an additional white part not relevant for the purpose of this work.

The simulations were run with 10^7 particles to reduce the statistical uncertainty to about 1%, comparable to the value for the real measurement data.

The handling of the detectors and the calculation of the peak area in the resulting spectra was performed using the software Canberra Genie-2K [8]. The calculation of the peak area was performed using the algorithm "step", as provided by Canberra, corresponding to a quadratic curve that better represents the shape of the background of a gamma peak [8].

2.1. Step I: measurements

Once mounted the PMMA plate on top of the detector case, a reference position was defined and the source holder was fixed in the position corresponding to a radius of 100 mm, the smallest one. As already mentioned, the point source (element 'e' in Fig. 1) was placed in the upper slit, at 39 mm from the front plane of the detector case.

Three point sources were used for the measurements: ^{241}Am, ^{133}Ba and ^{137}Cs. ^{133}Ba emits multiple lines, but only the line at 81.0 keV was considered, the other ones being too weak to be detected properly or too energetic to interact significantly with the dead layer.

The measurement time was variable, according to the activity of the source and to the efficiency of the detector at the different energies. A maximum statistical uncertainty at the main peak of 1% was reached in 240 s for ^{241}Am and in 120 s for ^{133}Ba and ^{137}Cs. The resulting peak area was converted from counts per measurement to detection efficiency.

Each point source was measured in 16 configurations around the detector, at angles 22.5° apart. A sketch of the measurement setup is shown in Fig. 3.

2.2. Step II: generation of the inputs

The MCNPX model of the detector, initially built according to the technical drawings, was modified by selecting four uniformly spaced planes (i.e. 45° apart) from the sheaf of planes originated from the detector axis. These four planes divided the lateral dead layer into eight sectors (see Fig. 3). The angular offset of the sectors