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Equivalence of computer codes for calculation of coincidence summing correction factors



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HIGHLIGHTS

• Measured and calculated true coincidence corrections differ in recent study.

• We checked for equivalence of computer codes that can perform such calculations.

• Codes compared with each other for a set of well-defined detector and sample models.

• Satisfactory agreement between the codes for a p-type detector model.

• Large differences for an n-type detector model and X-ray emitting radionuclides.

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ABSTRACT

The aim of the study was to check for equivalence of computer codes that can perform calculations of true coincidence summing correction factors. All calculations were performed for a set of well-defined detector and sample parameters, without any reference to empirical data. For a p-type detector model the application of different codes resulted in satisfactory agreement in the calculated correction factors. For high-efficiency geometries in combination with an n-type detector and a radionuclide emitting abundant X-rays the results were scattered.

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1. Introduction

In a recent intercomparison exercise on the calculation of coincidence summing correction factors in gamma-ray spectrometry (Lépy et al., 2012), considerable differences between the measured and calculated results were observed in some cases. It was therefore decided to carry out a study aimed at checking for equivalence of computer codes that can perform such calculations. In case significant differences were uncovered between the codes, the goal was to quantify them. This should help separate the effects

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of differences between the codes themselves from other effects that affect the calculated coincidence factors, such as imperfections in the detector and sample models. Different codes were therefore set up in this work to perform calculations of coincidence summing correction factors for a set of well-defined sample and detector parameters, without any reference to empirical data. The selected coincidence summing codes were only confronted with each other, without any intention of eventually favouring one over the other. Rather, the differences between them were supposed to shed light on how reliable such calculations are in ideal circumstances.

The computer codes selected for the study were (in alphabetical order) EFFTRAN (Vidmar, 2005; Vidmar et al., 2011), EGS4 (Nelson et al., 1985; Byun et al., 2004; Johnston et al., 2006), EGSnrc (Kawrakow and Rogers, 2006), ETNA (Lépy et al., 2006; Lépy,

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Ferreux and Pierre, 2012), GEANT 3.21 (Brun et al., 1987), GEANT4 (Agostinelli et al., 2003; Hurtado et al., 2009; Capogni et al., 2010), GESPECOR (Sima et al., 2001, Arnold and Sima, 2006; Sima and Arnold, 2008, 2012), PENELOPE (Salvat et al., 2008; Laederman and Decombaz, 2000) and VGSL (Plenteda and De Geer, 2002; Waters, 2002; Karhu et al., 2006). All of these codes are well established in the community of gamma-ray spectrometry users. Several of them have built-in modules for the simulation of nuclear decay or specific addons for this purpose and come complete with associated decay-scheme libraries, which simplify their use. In Capogni et al., 2010, a comparison was made between GEANT3.21 and GEANT4 with regard to the calculation of coincidence summing correction factors for a chosen sample-detector geometry and for radionuclides of general interest in gamma-ray spectrometry.

In the present work, a set of well-defined detector and sample geometries was considered – a large p-type and a similar n-type closed-end coaxial HPGe detector were simulated in combination with a point source, a pillbox soil sample, an extended water solution sample and a cellulose filter. For each of the possible detector-sample combinations, coincidence summing correction factors were obtained by pure calculation for selected lines of Co-60, Y-88, Cs-134, Ba-133, Eu-152 and Na-22. The emphasis of the study was on routine application of coincidence summing corrections in environmental measurements and only the main gamma lines of each nuclide were therefore considered.

The choice of the nuclear decay schemes data was deliberately left to the users of the individual codes, because such data form an essential constitutive part of each code. The same is true for the interaction mechanisms implemented in the codes and the particletracking energy cut-offs. In general, individual codes were used with their respective default parameters whenever possible.

2. Method

The main result of all the computations was a series of the coincidence summing correction factors for a given detector, sample, radionuclide and its gamma line. The correction factor was defined as a ratio of the expected number of counts in the fullenergy peak of an equivalent (same energy and photon emission probability), ideal mono-energetic gamma emitter, free of all coincidence effects, and the number of counts in the corresponding fullenergy peak of the real emitter. As such, the resulting coincidence summing correction factor is always larger than unity for lines dominated by summing-out events, and smaller than unity for summing-in dominated lines. Whenever an analysis of a measured spectrum of the radionuclide in question is carried out, the area of the peak corresponding to the given gamma line should be multiplied with the coincidence summing correction factor defined in this way to correct for the systematic coincidence effect.

The parameters of the two simulated closed-end coaxial HPGe detectors, a p-type and an n-type one, are given in Table 1. The two detectors were identical, except for the thickness of their respective dead layers. The characteristics of the sources are listed in Table 2. No source containers were simulated, because this detail was not considered essential for the general purpose of the study. In all the cases, a complete cylindrical symmetry of the setup was assumed.

A schematic presentation of the setup for the case of the point source and the p-type detector model is shown in Fig. 1.

The characteristics of various materials used in the constructions of the detector and sample models are given in Table 3.

A lead shielding was also included in the simulations. It had both a diameter and a height of 400 mm and its thickness on all sides was 50 mm. No lining or graded shielding was included. The detector was placed centrally within the lead shielding, with the geometrical centres of the shielding itself and of the detector crystal coinciding.

Table 1

Detector parameters. All dimensions are given in millimetres (mm). The housing diameter is in all cases the same as the window diameter.

Parameter	Detector A	Detector B
Crystal material	Ge	Ge
Crystal diameter (including the side dead slayer)	60	60
Crystal length (including the top dead layer)	60	60
Dead layer thickness (top and side)	1	0
Hole diameter	10	10
Hole depth	40	40
Window diameter	80	80
Window thickness	1	1
Window material	Al	Al
Crystal-to-window distance	5	5
Housing length	80	80
Housing thickness	1	1
Housing material	Al	Al

Table 2

Sample parameters. All dimensions are given in millimetres (mm).

Parameter	Water	Point	Soil	Filter
Sample diameter Sample thickness Sample material Sample-to-window distance	90 40 Water 1.0	- - 1.0	60 20 Dirt 1.0	80 3 Cellulose 1.0



Fig. 1. A schematic presentation of the setup for the case of the point source and the p-type detector model. All dimensions are in millimetres (mm).

Table 3

Characteristics of various detector and sample materials. All densities are given in g/cm³.

Material	Density	Chemical formula
Ge	5.323	Ge
Al	2.70	Al
Water	1.0	H ₂ O
Dirt	1.4	SiO ₂
Cellulose	0.3	$C_6H_{10}O_5$

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