ARTICLE IN PRESS

Applied Radiation and Isotopes xxx (xxxx) xxx-xxx



Contents lists available at ScienceDirect

Applied Radiation and Isotopes



journal homepage: www.elsevier.com/locate/apradiso

SUMCOR: Cascade summing correction for volumetric sources applying MCNP6

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HIGHLIGHTS

- Code SUMCOR developed for cascade summing correction is described.
- MCNP6 is used to track individual points inside the volumetric source.
- Cascade summing correction is based on the matrix formalism.
- Results are compared with two intercomparisons organized by the ICRM-GSWG.

A R T I C L E I N F O

Keywords: Cascade summing Monte Carlo Gamma-ray emission HPGe MCNP6

ABSTRACT

The main features of code SUMCOR developed for cascade summing correction for volumetric sources are described. MCNP6 is used to track histories starting from individual points inside the volumetric source, for each set of cascade transitions from the radionuclide. Total and FEP efficiencies are calculated for all gamma-rays and X-rays involved in the cascade. Cascade summing correction is based on the matrix formalism developed by Semkow et al. (1990). Results are presented applying the experimental data sent to the participants of two intercomparisons organized by the ICRM-GSWG and coordinated by Dr. Marie-Cristine Lépy from the Laboratoire National Henri Becquerel (LNE-LNHB), CEA, in 2008 and 2010, respectively and compared to the other participants in the intercomparisons.

1. Introduction

There is a continuing effort inside the ICRM (International Committee for Radionuclide Metrology) community to improve the codes for calculating cascade summing corrections, for samples of different geometries and decay scheme characteristics. Reports on comparisons were presented at the 2009, 2011, 2013 and 2015 ICRM meetings, showing the evolution of the codes.

Following this effort, the Nuclear Metrology Laboratory (LMN -Laboratório de Metrologia Nuclear), in São Paulo, developed a code for cascade summing correction for volumetric sources called SUMCOR. The present paper describes the main features of this code and the results obtained with data supplied by Dr. Marie-Cristine Lépy from the Laboratoire National Henri Becquerel (LNE-LNHB), CEA. These data were sent to the participants of two intercomparisons, which are described in Lépy et al. (2010, 2012).

2. Methodology

2.1. Monte Carlo simulation

Code MCNP6 (Goorley et al., 2013) was used for all simulations. Fig. 1 shows the model used for simulation of point sources at different distances from the detector window, as depicted by code VISED (Carter and Schwarz, 2005). In this picture the source was located at 2 cm. All detailed geometric aspects and materials described in reference Lépy et al. (2010), including the radiographs, were considered.

It was noticed that the presence of the PPMA (poly(methyl methacrylate)) holder around the source gives rise to a pronounced scattering in the calculated spectrum, mainly at intermediate gamma-ray energies (around 400–700 keV) where the Compton Effect is dominant. As a consequence, the total detection efficiency is larger when compared to the value calculated without the PPMA holder.

For volume sources, two source-detector models were created: the first (called Model 1) describes all aspects of the source and detector systems, and the source location is defined at a random point sampled

http://dx.doi.org/10.1016/j.apradiso.2017.09.014

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Received 9 March 2017; Received in revised form 4 September 2017; Accepted 10 September 2017 0969-8043/ @ 2017 Elsevier Ltd. All rights reserved.

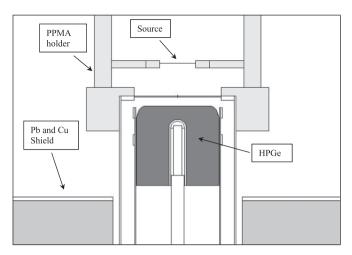


Fig. 1. Partial view of the source-Detector Model 1 for MCNP6 as drawn by code VISED (Carter and Schwarz, 2005). For volume sources, the PPMA holder has been replaced by the radioactive solution container.

inside the source volume; the second (called Model 2) is identical to Model 1 except the source location which is defined to cover all the source volume. In both models, the PPMA holder used for point sources has been replaced by the containers and contact materials (Mylar, PPMA and copper) used in the intercomparison for volume sources, as described in reference Lépy et al. (2012).

Using Model 1, for each point location, 10^5 histories were followed for each gamma-ray or X-ray present in the cascades and a total of 50 points were sampled from a uniform distribution inside the source volume. For the volumetric source, applying Model 2, 10^6 histories were followed for each gamma-ray or X-ray present in the cascades. More histories were followed for Model 2 because the calculation was performed only once, whereas for Model 1 it was performed fifty times for different points inside the source volume.

2.2. Cascade summing correction

This correction was calculated applying the matrix formalism described by Semkow et al. (1990) which are the results shown in the tables. Additional calculations were performed using Menno Blaauw's equations (Blaauw and Gelsema, 2003) but the running time using turned out to be much longer, when compared to the matrix formalism. The summing correction factors calculated by these two formalisms were in good agreement with each other. For the LS-Ratio calculations, the matrix formalism was modified in order to follow the prescription given by Blaauw and Gelsema (2003).

The summing correction factor was calculated as the weighted average value from all individual points inside the source volume. The weighting factor was the corresponding FEP (full energy absorption peak efficiency - ε_p) of the corresponding transition in the cascade, as follows:

$$\overline{F}_{S} = \frac{\sum_{i=1}^{N_{p}} F_{S\,i} \varepsilon_{p\,i}}{\sum_{i=1}^{N_{p}} \varepsilon_{p\,i}}$$

$$\tag{1}$$

Where:

- N_P is the total number of random points inside the source volume;
- ε_{pi} is the full energy absorption peak (FEP) efficiency for each
- random point, for the corresponding transition in the cascade; F_{Si} is the summing correction factor for each random point, for the
- corresponding transition in the cascade; Points closer to the detector have higher peak efficiencies; therefore
- the weighted mean obtained by Eq. (1) corresponds to a larger

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correction when compared to the simple mean. This can be considered the best estimate to the summing correction factor included in the tables.

All relevant decay data for the radionuclides involved were taken from NUCLEIDE (Vanin et al., 2004; Bé et al., 2013). They are: energy levels; transition probabilities; total and K shell conversion coefficients; X-ray fluorescence yields and metastable half-lives. These data were input and stored in the code corresponding arrays.

For the case of electron capture decay nuclides, the K X-rays were included but the contribution from other shells was not considered. For beta minus decay the contribution from electrons were not considered as well. A future improvement to SUMCOR is planned to include L Xrays and beta ray contributions. For beta plus decay and volume sources, the present version of SUMCOR may be used by adding the corresponding annihilation quanta to the corresponding positron decay levels in the decay scheme. This is possible because the annihilation process occurs near the positron decay location. For point sources, the present version of SUMCOR code is not suitable because the annihilation process may occur outside the source location, changing the 511 keV annihilation photon detection efficiency.

2.3. SUMCOR calculation procedure

Fig. 2 is a block diagram showing the main features of code SUMCOR. In this figure, the following parameters are defined:

NP	is the number of random points inside the source volume;
NT	is the number of transitions in the cascade;
FEPP	is the full energy absorption peak (FEP) efficiency for
	each random point, for each energy in the cascade;
TEFP	is the total efficiency for each random point, for each
	energy in the cascade;
FSUMP	is the cascade summing correction factor for each random
	point, for each energy in the cascade;
LSRATIO	is the Linear to Square Ratio for each random point, for
	each energy in the cascade;
FEPV	is the full energy absorption peak efficiency for the
	volume source (Model 2);
TEFV	is the total efficiency for the volume source (Model 2);
FSUMV	is the cascade summing correction factor for the volume
	source (Model 2).

The running process follows several steps. Initially, the source-detector system Model 1 is selected in MCNP6 and a random point is sampled inside the volumetric source. For each X-ray or gamma-ray energy present in the input data, the total and FEP efficiencies are calculated for that point by MCNP6 and the results for all transitions are stored. Then the cascade summing correction factor is calculated for that point, considering all cascades.

Subsequently, a new random point is sampled and this process is repeated until the last point is sampled (i = NP). The weighted average summing correction factors and their standard deviations are calculated, considering all sampled points inside the source and all gammatransitions in the cascades. These are the results shown in all the tables of the present work, applying Eq. (1). At this stage, the average total and FEP efficiencies are calculated, as well as the LS-Ratio described by Blaauw and Gelsema (2003), considering all sampled points.

Next, the source-detector system Model 2 is selected for the MCNP6 code and the total and FEP efficiencies are calculated for the volumetric source, for all transitions. Then the cascade summing correction factor is calculated for all cascades, following the same formalism applied previously, but only once considering the volumetric source efficiencies. The cascade summing correction is calculated using the total and FEP efficiencies for Model 2 taken from the output of MCNP6 for all transitions. This procedure is biased because it considers simple average

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