Cascade summing corrections for HPGe spectrometers by the Monte Carlo method

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Abstract

Cascade summing corrections for application in HPGe gamma ray spectrometry have been calculated numerically by the Monte Carlo method. An algorithm has been developed which follows the path in the decay scheme from the starting state at the precursor radionuclide decay level, down to the ground state of the daughter radionuclide. With this procedure, it was possible to calculate the cascade summing correction for all gamma ray transitions present in the decay scheme. Since the cascade correction requires the values of peak and total detection efficiencies, another code has been developed in order to estimate these parameters for point and cylindrical sources. The radionuclides $^{60}\text{Co}$, $^{133}\text{Ba}$ and $^{131}\text{I}$ were used for testing the procedure. The results were in good agreement with values in the literature.

Keywords: Monte Carlo; Summing; Gamma-ray

1. Introduction

Gamma spectrometry using HPGe detectors is widely used due to the excellent energy resolution of this kind of detectors. In particular, it can be used for the activity determination of gamma-emitting radioactive sources whenever the full-peak efficiency calibration curve is known, from which the efficiency value for each single gamma ray energy is obtained by interpolation.

However, in this application, the total efficiency is also needed (Knoll, 1988). The measured peak efficiency curves must be corrected for cascade summing which occurs whenever two or more gamma rays from the same decay event are detected simultaneously inside the detector crystal (Lépy et al., 1986; Debertin and Schöttig, 1979; Schima and Hoppes, 1983; Morel et al., 1983). This effect increases with the detection efficiency, therefore, it becomes important for large crystals and short source-to-detector distances. Since this effect is not related to the source strength, it can be significant even for very small source activities reaching values up to 40% depending on the radionuclide and detection conditions (Debertin and Schöttig, 1979).

In the present work the peak and total efficiencies have been numerically calculated by the Monte Carlo method and compared with experimental results. This Monte Carlo code can be used for both point and cylindrical sources.

The cascade summing correction involves the decay scheme characteristics and detection efficiencies which can be incorporated into an analytical expression (Schima and Hoppes, 1983). In the present work, a second Monte Carlo algorithm has been developed which follows each path in the decay scheme from the beginning state at the precursor radionuclide decay level, down to the ground state of the daughter radionuclide. With this procedure it was possible to calculate the cascade summing correction for all of the gamma-ray transitions present in the decay scheme.
2. Calculation method

2.1. Cascade summing algorithm

Each step in the decay scheme is selected by random numbers taking into account the transition probabilities and internal conversion coefficients. The selected transitions are flagged according to the type of interaction that has occurred, giving rise to total or partial energy absorption events inside the detector crystal. Once the final state has been reached, the selected transitions were accounted for verifying each pair of transitions which occurred simultaneously.

A code named COINCIG calculates the cascade summing correction using total and peak efficiencies calculated by the Monte Carlo method or obtained experimentally. A flow diagram of this code is shown in Fig. 1.

Two arrays are used as input data: the first one for each excited state, the energies of the depopulating gamma rays, their total transition probabilities and their conversion coefficients. The beta or electron-capture transition probabilities are also included. The second matrix corresponds to the total and peak efficiencies for all gamma ray energies involved, previously calculated by the Monte Carlo method or obtained experimentally.

The first step selects a beta (or electron-capture) transition by means of a random number which determines the daughter excited state. Then a second random number is selected to determine which gamma transition will occur.

The condition for gamma detection is verified by means of the following equation:

\[ r < f_{op} \frac{\varepsilon_T}{(1 + z)} \]  \hspace{1cm} (1)

where \( r \) is a random number in the interval \([0,1]\), \( f_{op} \) is an optimization factor (greater than one) to speed up processing (Cashwell and Everett, 1959; Sóbol, 1976); \( \varepsilon_T \)
is the total efficiency; $z$ is the internal conversion coefficient of the transition.

The factor $f_{op}$ is introduced because the efficiencies are usually much smaller than one. Therefore, without this factor, many events would be lost from detection. The upper limit for $f_{op}$ is such that Eq. (1) is never greater than one. After all transitions are considered, this factor is incorporated in the final correction as described later (Cashwell and Everett, 1959; Sôbol, 1976).

If the gamma ray is detected, the total-efficiency event counter is increased and the corresponding event is flagged. The same procedure is followed with the peak efficiency. In this case, the detection condition is given by

$$ r < \frac{E_p}{E'_T} $$

where $E_p$ is the peak efficiency.

This procedure is repeated until the daughter radio-nuclide ground state is reached. Once all gamma rays from a given disintegration are emitted, the flags are verified and the cascade summing events are taken into account.

The equations for counting the events are:

$$ s_g = -\sum_{ij} \beta_{ij} \gamma_{ml}, $$

$$ s_{ml} = -\sum_{m,l} \beta_{ml} \gamma_{ij}, $$

$$ s_g = \sum_{i,j} \beta_{ij} \beta_{ml}, $$

where $\beta$ is the peak efficiency detection flag for a given transition (0 or 1), $\gamma$ is the partial absorption flag for a given transition (0 or 1), $i,j$ are the initial and final states of first gamma ray emitted, $m,l$ are the initial and final states of second gamma ray emitted.

Eqs. (3) and (4) correspond to cascade summing events where one gamma ray is totally absorbed while the other one is partially absorbed, thus subtracting a count from the total absorption peak. In Eq. (5), there are events where both gamma rays are totally absorbed, adding up a count to the $(i,l)$ transition or sum peak.

Once the ground state is reached, the cascade sum correction is calculated by

$$ c_g = 1 + \frac{s_g}{f_{op} N_g}, $$

where $c_g$ is the cascade sum correction for transition $i,j$, $N_g$ is the number of total absorption events for transition $i,j$.

2.2. Monte Carlo efficiency calculation

Since the cascade summing correction requires total and peak efficiencies, an additional Monte Carlo code, MCEFFIC, has been developed in the present work for estimating these parameters. This code includes Compton multiple scattering and the scattered photon energy is calculated applying the Klein–Nishina differential cross section (Cashwell and Everett, 1959) with the scattering angle, $\theta$, given by

$$ \cos \theta = 1 + \frac{1}{E - E'}, $$

where $E$ and $E'$ are the incident and scattered photon energies, respectively (in $m_0c^2$ units).

The value of $E'$ is given by (Cashwell and Everett, 1959)

$$ E' = \frac{E}{1 + s + (2E - s)r^3} $$

where

$$ s = \frac{E}{1 + 0.5625E} $$

and $r$ is a random number in the interval $[0,1]$.

Eq. (8) is valid in the $E \leq 4m_0c^2$ energy range ($\leq 2$ MeV). For the $4 < E \leq 10$ energy interval, an additional component was included in $E'$

$$ E'_c = E' + \frac{1}{2}(E - 4)r^2(1 - r)^2. $$

Secondary electrons were assumed to have zero range and annihilation gamma ray emission was considered isotropic. Escape of annihilation photons has also been considered.

This preliminary version of COINCIG does not take into account coincidences with X-rays. Therefore, it can be used when X-ray detection efficiency is low. Improvements in the code are planned to include this feature.

3. Results and discussion

Measurements have been performed for a HPGe detector 2.60 cm in diameter and 5.02 cm high using a calibrated $^{60}$Co source. Table 1 shows a comparison between the measured and calculated total efficiency. The agreement was around 10%.

Another comparison has been made between the code COINCIG and an analytical expression given by Schima (Schima and Hoppes, 1983). The results obtained for

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Experimental</th>
<th>Monte Carlo</th>
<th>Cascade summing correction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1173</td>
<td>0.05289 (53)</td>
<td>0.0559</td>
<td>0.9450 (32)</td>
</tr>
<tr>
<td>1332</td>
<td>0.04934 (50)</td>
<td>0.0537</td>
<td>0.9425 (32)</td>
</tr>
</tbody>
</table>

*Figures in parentheses are the uncertainty in the last digits.
$^{133}$Ba and $^{131}$I, in the same geometry as above, are shown in Table 2. The agreement between the results is excellent and is limited by the Monte Carlo statistics (typically from 0.1 to 1%, depending on the transition).

General tables based on radionuclide decay scheme are used without the need of detailed consideration of the path for each transition with respect to the others in the scheme, as usually required by standard methods. Therefore, once the decay scheme table is ready, the cascade summing correction can be easily calculated for all transitions by code COINCIG.

The simple Monte Carlo approach yielded total efficiencies with 10% accuracy. This value is usually satisfactory and may be considered as the main source of error in the cascade summing correction. The calculated peak detection efficiency was higher than the experimental efficiency by 10% at 50 keV and 40% at 3000 keV. However, the probability of simultaneous total absorption of two gamma rays at high energies is very low. Therefore, the contribution of the peak efficiency error to the cascade summing uncertainty is usually small.

Further refinements in the code are planned in order to reduce the uncertainty in the calculated efficiencies. Nevertheless, experimental peak efficiencies can be easily obtained for the code COINCIG to yield accurate cascade summing corrections.

The uncertainties in the summing correction shown in Tables 1–3 do not include the uncertainty in the efficiency because the same value of efficiency was applied in the analytical method (Schima and Hoppes, 1983). Therefore, the comparisons are only relative. Non-correlated errors in the efficiency can be taken into account by changing the input efficiencies randomly according to a Normal distribution having the same standard deviation estimated for the efficiency and observing the variation in the calculated cascade summing correction. A complete description of total uncertainties must take into account the covariance analysis which is planned for future versions of code COINCIG.

### Table 2
Calculated total and peak efficiencies for $^{133}$Ba

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Total efficiency</th>
<th>Peak efficiency</th>
<th>Cascade summing correction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Present work</td>
</tr>
<tr>
<td>53.151</td>
<td>0.1607</td>
<td>0.1484</td>
<td>0.8639 (29)</td>
</tr>
<tr>
<td>79.615</td>
<td>0.1543</td>
<td>0.1294</td>
<td>0.89580 (63)</td>
</tr>
<tr>
<td>80.998</td>
<td>0.1523</td>
<td>0.1268</td>
<td>1.2889 (73)</td>
</tr>
<tr>
<td>160.613</td>
<td>0.1261</td>
<td>0.0705</td>
<td>0.8727 (70)</td>
</tr>
<tr>
<td>223.239</td>
<td>0.1124</td>
<td>0.0411</td>
<td>0.8902 (33)</td>
</tr>
<tr>
<td>276.39</td>
<td>0.1059</td>
<td>0.0284</td>
<td>0.93196 (86)</td>
</tr>
<tr>
<td>302.854</td>
<td>0.1013</td>
<td>0.0233</td>
<td>0.95437 (91)</td>
</tr>
<tr>
<td>356.005</td>
<td>0.0987</td>
<td>0.0176</td>
<td>1.1457 (17)</td>
</tr>
<tr>
<td>383.852</td>
<td>0.0951</td>
<td>0.0146</td>
<td></td>
</tr>
</tbody>
</table>

bFigures in parentheses are the statistical uncertainty in the last digits.

### Table 3
Calculated total and peak efficiencies for $^{131}$I

<table>
<thead>
<tr>
<th>Energy (keV)</th>
<th>Total efficiency</th>
<th>Peak efficiency</th>
<th>Cascade summing correction</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>Present work</td>
</tr>
<tr>
<td>80.193</td>
<td>0.1545</td>
<td>0.1299</td>
<td>0.9018 (24)</td>
</tr>
<tr>
<td>177.21</td>
<td>0.1220</td>
<td>0.0615</td>
<td>0.9223 (98)</td>
</tr>
<tr>
<td>284.287</td>
<td>0.1042</td>
<td>0.0271</td>
<td>0.9398 (27)</td>
</tr>
<tr>
<td>318.093</td>
<td>0.0998</td>
<td>0.0207</td>
<td>0.918 (29)</td>
</tr>
<tr>
<td>325.78</td>
<td>0.1004</td>
<td>0.0205</td>
<td>0.900 (20)</td>
</tr>
<tr>
<td>364.48</td>
<td>0.0969</td>
<td>0.0153</td>
<td>1.00642 (32)</td>
</tr>
<tr>
<td>502.99</td>
<td>0.0882</td>
<td>0.0090</td>
<td>1.074 (21)</td>
</tr>
<tr>
<td>636.973</td>
<td>0.0833</td>
<td>0.0061</td>
<td>1.00065 (55)</td>
</tr>
<tr>
<td>722.893</td>
<td>0.0817</td>
<td>0.0051</td>
<td>1.0085 (43)</td>
</tr>
</tbody>
</table>

cFigures in parentheses are the statistical uncertainty in the last digits.
References


