# Simulation Method for CdZnTe Detector Efficiency Based on Ideal Models

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## Abstract

Efficiency loss occurs when using traditional Monte Carlo methods to calculate the detection efficiency of CdZnTe detectors. To apply passive efficiency calibration techniques to CdZnTe detectors, a calculation method for CdZnTe detection efficiency based on an ideal model (considering only the interaction processes between photons and the detector crystal and structural materials) is proposed. The reliability of the calculation method was verified using a 152Eu standard source sample, and the results demonstrate that the deviation between calculated results and reference values does not exceed 5%. This method can yield reliable efficiency calculation results without considering the complex process of incomplete charge carrier collection within the CdZnTe crystal, and demonstrates strong operability.

## Full Text

## Preamble

### Simulation Calculation of CdZnTe Detection Efficiency Based on Ideal Model

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## Abstract

[**Background**] Traditional Monte Carlo methods exhibit efficiency losses when calculating the detection efficiency of CdZnTe detectors. [**Purpose**] To apply sourceless efficiency calibration technology to CdZnTe detectors. [**Methods**]

We propose a calculation method for CdZnTe detection efficiency based on an ideal model that considers only photon interactions with the detector crystal and structural materials. [**Results**] The reliability of this method was verified using a $^{152}$Eu standard source, demonstrating that deviations between calculated results and reference values do not exceed 5%. [**Conclusions**] This method yields reliable efficiency calculations without requiring consideration of the complex processes of incomplete charge carrier collection within CdZnTe crystals, offering strong operability.

The full-energy peak source detection efficiency, hereinafter referred to as detection efficiency, is defined as the ratio of the number of characteristic $\gamma$-rays of a certain energy emitted by the sample per unit time to the full-energy peak counts recorded by the detector. This parameter is critical for radionuclide activity measurements using $\gamma$-spectrometry detectors. Sourceless efficiency calibration provides a convenient method for obtaining detection efficiency without requiring standard sources, relying solely on Monte Carlo calculations. This technique is widely applied in sample activity measurement [1-4].

**Keywords:** CdZnTe, detection efficiency, sourceless efficiency calibration
**Classification:** TL816.4

## Introduction

For common $\gamma$-spectrometry detectors such as HPGe, NaI(Tl), and $LaBr_3$, traditional Monte Carlo methods can achieve excellent agreement with experimental measurements by considering only photon interactions with the detector crystal and structural materials. This approach is known as the ideal model detection efficiency calculation method [5-11]. CdZnTe represents a new type of semiconductor $\gamma$-spectrometry detector offering strong energy resolution at room temperature and high detection efficiency for low-energy $\gamma$-rays, making it suitable for radionuclide activity measurements [12-15]. However, applying the ideal model to CdZnTe detectors results in significant efficiency losses [16-17], with calculated values substantially lower than measured efficiencies. Numerous factors contribute to this efficiency loss in CdZnTe detectors, including charge loss during carrier transport, “dead regions” created by crystal mounting equipment, “dead regions” near the anode, non-uniform electric field distributions caused by imperfect electrode deposition processes and crystal defects, all of which lead to incomplete charge collection and consequent full-energy peak efficiency losses [18]. Several studies suggest that Monte Carlo simulations of CdZnTe detection efficiency must model not only photon interactions with the CdZnTe crystal and detector structure but also carrier drift, electron cloud diffusion, electric field effects, charge induction and collection, electronic noise, and signal processing to achieve agreement with experimental values [19-21]. Such calculations are complex and difficult to implement.

This paper explores a simplified calculation method for CdZnTe detection efficiency based on the ideal model. By iteratively comparing with experimental data, we determine the effective height of a 10 mm\$$\times 10mm\times$\$5 mm CdZnTe detector and use this as an input parameter for the calculation model.

### 1.1 Method

High-energy $\gamma$-rays interact deeper within the CdZnTe crystal on average, producing larger electron clouds and undergoing more interactions, which increases the probability of incomplete charge collection and results in greater full-energy peak efficiency loss. For quasi-hemispherical CdZnTe detectors, the magnitude of efficiency loss for different $\gamma$-ray energies depends on crystal height. Through analysis, we can attribute this efficiency loss to an effective reduction in CdZnTe crystal height. Under the ideal model framework, we determine this effective height through iterative comparison with point source experimental data. By establishing an ideal calculation model based on actual measurement geometry and using the crystal effective height as an input parameter, we can significantly reduce deviations between calculated and measured values.

When a sample is positioned on the central axis of a cylindrical detector, the ideal model calculates the point source detection efficiency as illustrated in Figure 1 [Figure 1: see original paper]. The primary parameters affecting the calculation results are the CdZnTe crystal width (x, z) and height (y), the distance between the crystal upper surface and the inner surface of the housing (h), the housing thickness (a), and the source-to-detector surface distance (SD). For calculations, the CdZnTe cross-section is treated as square (x=z). The sensitivity of efficiency calculations to parameter variations differs depending on SD. By systematically adjusting these parameters to bring calculated efficiency values into agreement with experimental values, we obtain an optimal parameter set where the height $y_0$ represents the crystal effective height. At this optimum, the deviation between calculated and measured values becomes minimal—a process known as detector characterization. According to GB/T16145-2022, sourceless efficiency calibration for sample activity calculations requires that efficiency deviations from traceable measurements not exceed 15%. To ensure more reliable results, we adopt a stricter criterion of \$ \$6% deviation as the condition for parameter optimization.

The experiment employed a DT-01C11005 quasi-hemispherical CdZnTe detector from Ditech. The manufacturer-specified CdZnTe crystal dimensions are 10 mm\$$\times 10mm\times 5mm, sealedinacylindricalaluminumhousingmeasuring30mm\times$\$70 mm with wall thicknesses of 1 mm and 0.5 mm. The crystal surface is positioned 3 mm from the inner surface of the detector housing. Tested performance shows 1.5% energy resolution for the 661.66 keV $\gamma$-ray from $^{137}$Cs. The electronic signal processing system uses a Canberra Lynx multi-channel analyzer, which provides high voltage, amplifies pulse signals, and records pulse-height spectra. Data acquisition was performed using Canberra's Genie2000 $\gamma$-spectrometry software, which allows configuration of high voltage, shaping time, and signal amplification.

To cover a broad $\gamma$-ray energy range, the experiment requires four standard point sources with accurately known activities: $^{241}$Am, $^{152}$Eu, $^{137}$Cs, and $^{60}$Co. This is a prerequisite for calculating CdZnTe detection efficiency using this method. To validate the efficiency calculations, we prepared a $^{152}$Eu aqueous solution source (ø30 mm$×$15 mm). Table 1 summarizes the standard source information used in the experiment. The activity uncertainties for point sources are nominal values from manufacturer certificates, while the uncertainty for the volume source was estimated based on the standard solution uncertainty and preparation process.

We used the MCNP5 code to simulate CdZnTe detector efficiency, employing the F8 tally to record $\gamma$-ray spectra entering the crystal. The ideal calculation model considers only photon interactions with the CdZnTe crystal and detector structure, excluding carrier drift, electron cloud diffusion, electric field effects, charge induction and collection, and other processes.

## 2 Results and Analysis

We measured the detection efficiency for $^{241}$Am, $^{137}$Cs, $^{60}$Co, and $^{152}$Eu point sources at various distances from the CdZnTe detector surface (SD = 1.5 mm, 46.5 mm, 96.5 mm). Simultaneously, we calculated the detection efficiency under corresponding conditions using MCNP5 with the detector's nominal parameters (a = 0.5 mm, h = 3 mm, x = 10 mm, y = 5 mm, z = 10 mm). Based on deviations between measured and calculated values, we made fine adjustments to parameters a, h, x, z, and y. Among these five parameters, modifying h, x, and z alters the detector solid angle relative to the source, affecting the full-energy peak count rate for all $\gamma$-ray energies. The sensitivity to these parameters increases as SD decreases, with identical trends across different $\gamma$-ray energies. Changing a and y affects different energy $\gamma$-rays to varying degrees, independent of SD. We employed two calculation modes: Mode 1 adjusts only h, x, and z while keeping a and y at nominal values; Mode 2 adjusts all five parameters. All parameter adjustments were made in 0.1 mm increments.

For SD = 1.5 mm measurements, each full-energy peak accumulated over 10,000 counts, yielding counting rate uncertainties $ $1% (k=2). Under these conditions, the efficiency measurement uncertainty is dominated by uncertainties in the standard source activity and $\gamma$-ray emission probabilities. With activity uncertainties of 2.5% and emission probability uncertainties <1%, the overall efficiency measurement uncertainty can be estimated as 3%. For SD = 46.5 mm and 96.5 mm measurements, the small CdZnTe crystal volume and low detection efficiency for high-energy $\gamma$-rays make the full-energy peak counting rate uncertainty the dominant contributor, reaching approximately 5% for $\gamma$-rays above 661.66 keV. The $^{152}$Eu high-energy $\gamma$-rays have low emission probabilities, resulting in relatively large count uncertainties; therefore, we selected only the 121.78 keV, 244.70 keV, and 344.28 keV $\gamma$-ray full-energy peaks for analysis.

Figure 2 [Figure 2: see original paper] shows the simulated efficiency curves and measurement results using nominal parameters for SD = 1.5 mm, 46.5 mm, and 96.5 mm. While calculation uncertainties do not exceed 1% for SD = 1.5 mm, they increase with SD. Due to limited computational resources, the uncertainty for high-energy efficiency calculations reached 5.5% at SD = 96.5 mm.

The results demonstrate substantial deviations between efficiency values calculated using nominal parameters and experimental measurements. The discrepancy is relatively small at low energies but increases with $\gamma$-ray energy, reaching a maximum deviation of 58.8% for the 1173.24 keV $\gamma$-ray. At SD = 1.5 mm, the deviation for 59.54 keV $\gamma$-rays is 11.54%, decreasing significantly at SD = 46.5 mm and 96.5 mm, indicating that parameters affecting the detector solid angle (h, x, z) are inaccurate, with greater impact at smaller SD. However, the deviation for higher-energy $\gamma$-rays does not decrease with increasing SD. Analysis reveals that the discrepancy arises not only from inaccurate h, x, and z values but also from the effective thickness y of the CdZnTe crystal, which appears to be the primary cause of increasing deviation with $\gamma$-ray energy. For low-energy $\gamma$-rays at small SD, parameters affecting the solid angle dominate the efficiency calculation, whereas for high-energy $\gamma$-rays at large SD, the effective thickness y becomes the dominant factor.

Based on this analysis, we performed iterative efficiency calculations using Mode 1 (adjusting only h, x, and z) and compared results with measurements. Figure 3 [Figure 3: see original paper] presents the optimal efficiency curves obtained using Mode 1 under different SD conditions (a = 0.5 mm, h = 3.5 mm, y = 5 mm, x = 10.1 mm, z = 10.1 mm).

Figure 3 shows that adjusting only h, x, and z cannot produce satisfactory results. Since these parameters only affect the detector solid angle relative to the source, their adjustment merely “shifts” the efficiency curve vertically without achieving good agreement across all experimental points. Therefore, Mode 2 (adjusting all parameters a, h, x, z, and y) is required.

Through iterative calculations under various parameter conditions and comparison with experimental results, we obtained good agreement between calculated and measured values for the parameter set: a = 0.5 mm, h = 3.5 mm, y = 3.5 mm, x = 10.1 mm, z = 10.1 mm. In this optimal set, h, x, and z differ slightly from nominal values, likely due to detector installation and crystal manufacturing processes. However, parameter y is only 70% of the nominal value—a deviation unlikely to result from manufacturing alone, but rather primarily from efficiency loss due to incomplete charge collection caused by carrier recombination, crystal “dead regions,” and other factors. Here, $y_0$ = 3.5 mm represents the effective height of the 10 mm\$$\times 10mm\times$\$5 mm quasi-hemispherical CdZnTe detector. Figure 4 [Figure 4: see original paper] shows the efficiency curves calculated using Mode 2 under different SD conditions (a = 0.5 mm, h = 3.5 mm, y = 3.5 mm, x = 10.1 mm, z = 10.1 mm), and Table 2 lists the deviations between Mode 2 calculations and experimental values.

Table 2 reveals that at SD = 1.5 mm, the deviations for 121.78 keV and 244.70

keV $\gamma$-rays are relatively large at 25.0% and 21.5%, respectively. This is primarily due to cascade coincidence between the 121.78 keV (emission probability 35.6%) and 244.70 keV $\gamma$-rays (emission probability 7.6%) from $^{152}$Eu with the 40.12 keV X-ray (emission probability 37.7%), which reduces full-energy peak count rates and causes larger deviations. Figure 5 [Figure 5: see original paper] shows the $\gamma$-ray spectrum of $^{152}$Eu measured with the CdZnTe detector at SD = 1.5 mm, clearly revealing coincidence peaks at (121+40) keV and (244+40) keV. For other $\gamma$-ray energies, calculated efficiencies agree well with measurements, with deviations \$ \$6%.

## 3 Experimental Validation

To validate the reliability of the ideal model CdZnTe efficiency calculation method, we prepared a $^{152}$Eu aqueous solution standard source sample (ø30 mm\$×15*mm)witharef erenceactivityof*6.85×10^{4}\$ Bq. The activity uncertainty, primarily attributable to uncertainties in the standard solution activity, solution mass measurement, and preparation procedure, was estimated as 5% (3% from the standard solution certificate and 4% from mass measurement and preparation). The sample container was a cylindrical organic glass cup with 3 mm wall thickness. We first calculated the CdZnTe detector efficiency using the ideal model, then analyzed the sample activity using these efficiencies, and finally compared the results with the reference activity to verify calculation accuracy. To assess the impact of cascade coincidence effects, spectral measurements and efficiency calculations were performed at SD = 0 and SD = 95 mm. Table 3 lists the activity calculation results for the $^{152}$Eu aqueous solution standard source under both conditions.

The data in Table 3 demonstrate that at SD = 95 mm, cascade coincidence effects become negligible, and the calculated $^{152}$Eu aqueous solution sample activities deviate from standard values by \$ \$5% across different $\gamma$-ray energies, confirming that using effective height as the CdZnTe crystal input parameter in the ideal model yields reliable results for volume sources. At SD = 0, coincidence summing between the 121.78 keV $\gamma$-ray and the 40.12 keV X-ray from $^{152}$Eu causes the activity calculated using the 121.78 keV full-energy peak to be 8.4% lower than the reference value, while results from other $\gamma$-ray energies agree well with reference values. Since CdZnTe detectors exhibit high efficiency for low-energy X-rays or $\gamma$-rays but low efficiency for high-energy $\gamma$-rays, coincidence effects between low-energy photons must be considered when measuring radionuclide activities, while coincidence effects between high-energy $\gamma$-rays can be neglected.

When using Monte Carlo methods to calculate CdZnTe detector efficiency, ideal models based on manufacturer nominal parameters show large deviations from measured values, increasing with $\gamma$-ray energy. Laboratories equipped with standard point sources of $^{241}$Am, $^{137}$Cs, $^{60}$Co, and $^{152}$Eu can determine the effective height of CdZnTe crystals through measurements at various SD distances, thereby obtaining reliable detector efficiencies. This method avoids complex modeling of carrier drift, electron cloud diffusion, electric field effects, charge induction and collection, electronic noise, and signal processing following $\gamma$-ray interactions in CdZnTe crystals, providing a relatively simple calculation process that establishes a technical foundation for applying sourceless efficiency calibration to CdZnTe detectors.

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*Note: Figure translations are in progress. See original paper for figures.*