SnT 2025 8 SEPTEMBER ONLINE DAY 9 TO 12 SEPTEMBER AT HOFBURG PALACE, VIENNA & ONLINE
CTBT: SCIENCE AND TECHNOLOGY CONFERENCE

P3.6-049

Impact of Energy Calibration in X-Ray Region on Xenon Activity Concentration Calculation under Least-Squares-Based Net Area Calculation Method

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INTRODUCTION AND MAIN RESULTS

This study examined the sensitivity of xenon activity concentration calculation to energy calibration shifts in the X-ray region. Spike and sample spectra were analyzed using the Least-Squares-based net area calculation method.

To evaluate the effect, the X-ray energy calibration was systematically shifted between −2 and +2 channels while gamma peak areas were held constant. The analysis showed that even a single-channel shift can lead to significant deviations with the magnitude and direction depending strongly on the isotope composition of the spectra.

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Introduction

High resolution beta-gamma coincidence counting enables comparison of different radioxenon analysis algorithms. *Yoon et al.* [1] performed an intercomparison between Net Count Calculation (NCC) and Least-Squares-based net area calculation (LSQ) methods. That study observed up to 50% deviations in Xe-133 activity concentration when the X-ray energy calibration was shifted by 0.35 keV (approximately equivalent to a 2-channel shift). This work extends the effort, which examines how much deviation in the activity concentration may result from the calibration shifts.

Theoretical Background: Least-Squares-based Net Area Calculation

The International Data Centre (IDC) pipeline currently applies the LSQ method for xenon quantification from high resolution gamma spectra [2]. This approach estimates a vector X representing net peak areas of four xenon isotopes (Xe-131m, Xe-133m, Xe-133 and Xe-135). It requires i) Modelling X-ray counts and gamma contributions (Matrix A), ii) Observed gamma peak net areas, and iii) Spectrum counts in the X-ray region (Vector B). The matrix-vector equation, $AX \approx B$, is then solved using weighted least squares.

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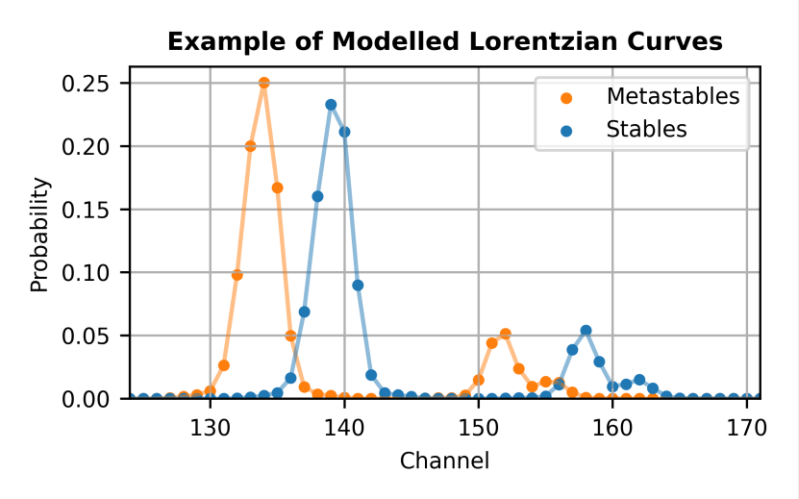
i) Modelled X-ray Counts and Gamma Contributions

In the LSQ method, Lorentzian functions represent the X-ray response for metastable (Xe-131m, Xe-133m) and stable (Xe-133, Xe-135) isotopes. At each channel, corresponding energy and resolution values are used to compute Lorentzian curves centered at X-ray energies. Each y-value constituting the Lorentzian function is weighted by its emission probability and scaled by a ratio that links X-ray and gamma responses under detector efficiency calibration as shown in the figure below. Summing these contributions across all X-ray channels yields Lorentzian multiplets.

Matrix A is constructed from these multiples. Its upper rows represent the counts from the modelled Lorentzian multiplets, and the last four rows correspond to the gamma region, where gamma peak of each isotope is expressed as a unit contribution.



ii) Gamma Net Peak Area (SCAC-based Calculation)

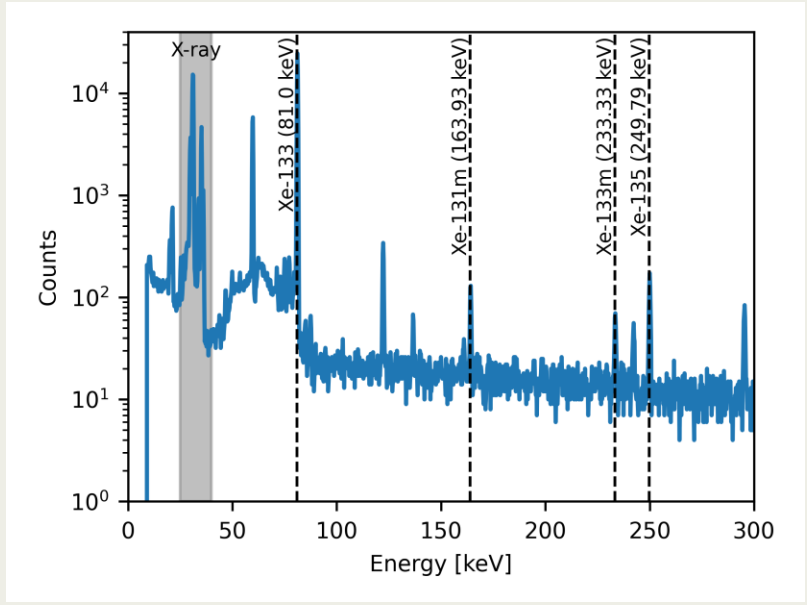
Gamma net peak areas are calculated using the Single Channel Analyzer Curve (SCAC) derived from a multi-channel spectrum. For a peak having the centroid at channel i, its net area is calculated by assuming that the peak is a perfect Gaussian shape with the net height of $SCAC_i$ - $Baseline_i$.

iii) Spectrum Counts in the X-ray Region

Counts at channel i is calculated as

$$Spectrum_i - Baseline_i$$

Vector B contains the baseline-subtracted X-ray counts as the leading elements and the SCAC-based gamma net peak areas as the last four elements.



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The weight matrix W is a diagonal matrix $W_{kk} = 1/\sigma_k^2$ where σ_k is uncertainty
The vector X is obtained by weighted least squares.

$$X = (A^T W A)^{-1} A^T W B$$

This yields optimal estimates of isotope-specific peak areas, which is later converted to activity concentrations.

Method

This study retrieved spike and sample spectra from the last ten years, having xenon isotope activity concentrations above 1 mBq/m^3. The spectra were grouped into four cases based on isotope combinations present in each spectrum. This approach was made under the assumption that multi-isotope cases may exhibit distinct response behaviors. While gamma peak areas were kept constant, the X-ray energy calibration was artificially shifted in discrete steps (-2, -1, +1 and +2 channels). The IDC production calibration served as the reference (zero-shift). Deviations in concentrations were calculated and evaluated in each shifted scenario for individual cases.

Case	Xenon Isotopes in Spectrum	Number of Analyzed Spectra
1	Xe-133	723
2	Xe-133, Xe-131m	20
3	Xe-133, Xe-131m, Xe-133m	25
4	Xe-133, Xe-133m, Xe-133m, Xe-135	9

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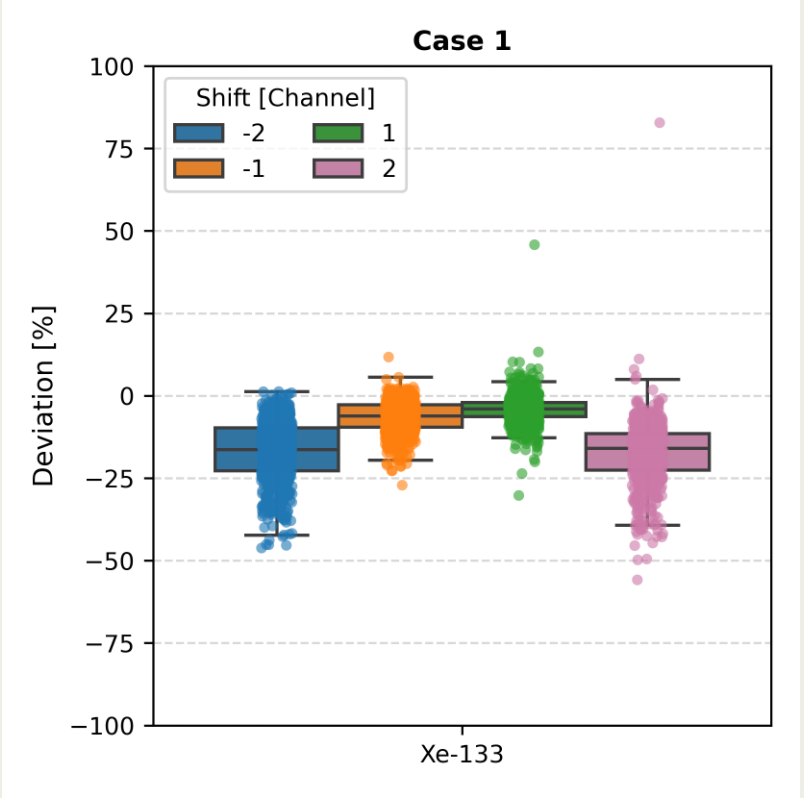
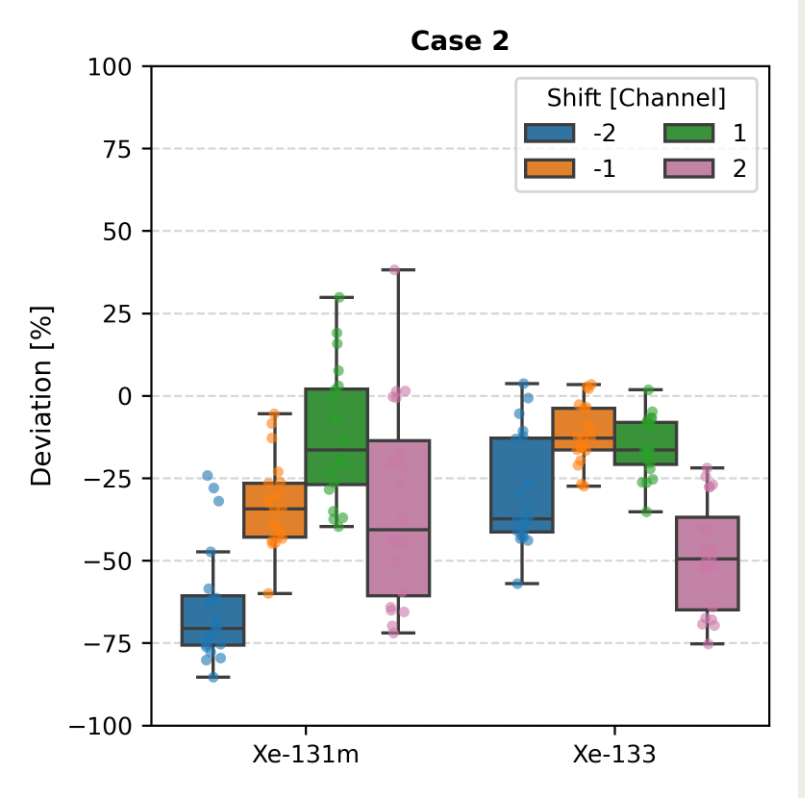
Results





Case 1: Deviations were moderate compared to Cases 2 to 4. However, even a one-channel shift produced notable bias, demonstrating sensitivity to calibration even in the single-isotope case.

Case 2: Larger deviations were observed, in some cases exceeding −75%. The presence of both metastable and stable isotopes increased sensitivity to calibration shifts, especially for Xe-131m.

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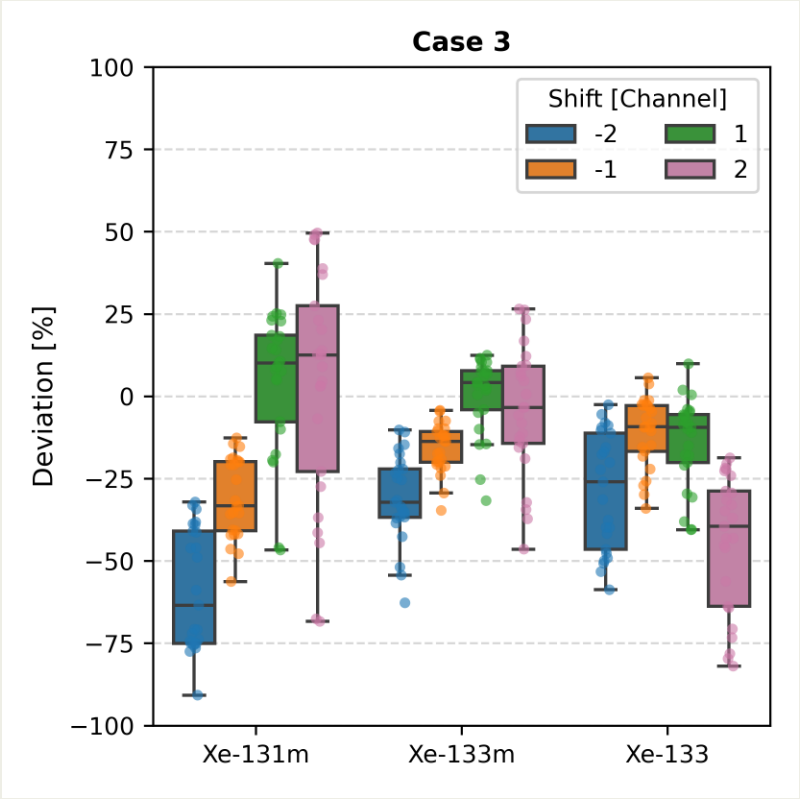
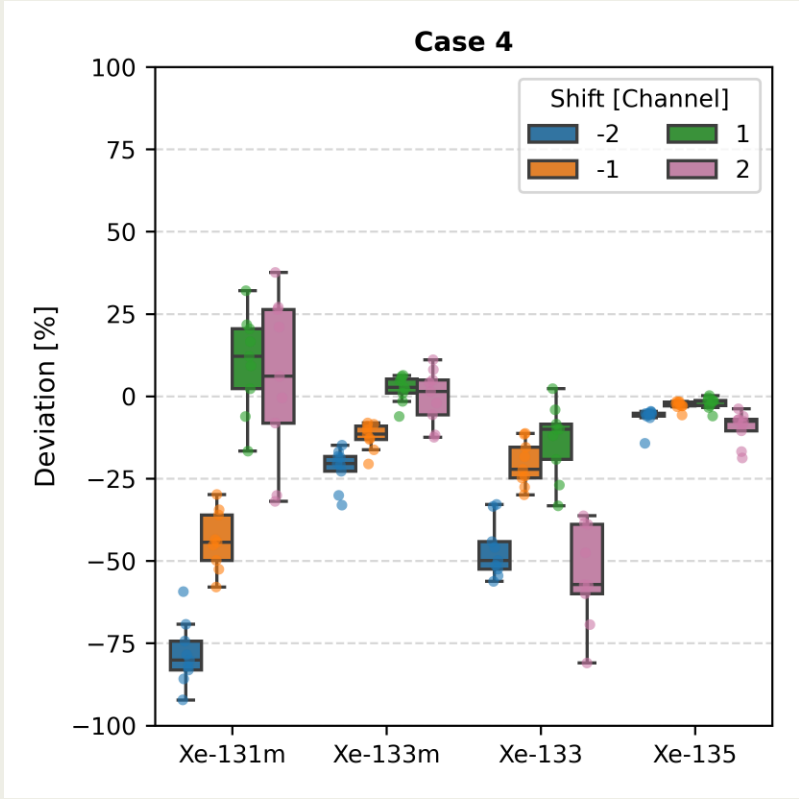


Case 3: Deviations became more pronounced and variable as multiple isotopes contributed to overlapping X-ray multiplets. Although Xe-131m and Xe-133m share the Lorentzian response, Xe-133m is less affected by calibration shift than Xe-131m. This is likely because Xe-131m has a smaller gamma branching ratio, making its area estimate more sensitive to calibration shifts.



Case 4: The most complex mixture showed the broadest range of deviations. Xe-135 was the least affected isotope, whereas Xe-131m exhibited extreme negative deviations under -2 channel shift. The relative insensitivity of Xe-135 can be explained by its larger gamma branching ratio, which reduces the influence of the calibration shift on its area estimation. In contrast, isotopes with smaller gamma branching ratios are more strongly impacted by shifts, leading to larger deviations.

Conclusions

This study demonstrates that accurate energy calibration in the X-ray region is essential for reliable xenon quantification by the LSQ method. Even a single-channel shift can introduce substantial deviations in calculated activity concentrations. While the effect is relatively modest for single-isotope spectra, it becomes pronounced in multi-isotope mixture spectra and for isotopes with smaller gamma branching ratios. These findings highlight the importance of accurate energy calibration in the X-ray region to ensure the robustness of activity concentration calculation.

References

[1] S. Yoon, J. Merešová, B. Liu “Intercomparison of Radioxenon Activity Analysis methods for High-Resolution Beta-Gamma Coincidence Spectra, International Noble Gas Experiment Workshop 10 – 14 June 2024, Vienna Austria.
[2] H. Honore, (2008) autoSaint source code (version 1.0)

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