A Deconvolution of Gamma-Ray Spectra for Accurate Attenuation Studies

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Abstract: The peak fitting of gamma-ray spectra for estimating net/gross counting is complex because of the selection of interested full energy peak folded by Compton scattering peak and others. Therefore it is necessary to unfold the spectra by deconvolution using Maximum likelihood expectation maximization (ML-EM) method for accurate attenuation measurements in the range 356 keV - 1330 keV for NaI(Tl) gamma ray detector. The histogram data must have an accurate Guassian distribution of photon attenuated by scintillation material and coupled photomultiplier device which depends on response function of detector. The Monte Carlo simulation gives poor resolution. The Deconvolution using (ML-EM) has meets the ideal counting statistics of gamma rays of mono-energetic photons and validate by comparison of mass attenuation coefficients of aluminium absorber for given energies. The measured experimental values by using ML-EM simulation with theoretically reported values by Hubble and Seltzer[1] are in good agreement.

Keyword : Gamma ray, NaI(Tl) detector, deconvolution, mass attenuation coefficient.

Gamma rays are widely utilized in health physics, shielding, medicine, industry, and basic sciences. The mass attenuation coefficient of gamma rays is an important parameter of matter and while applying in these applications, the mass attenuation coefficient must be measured with better accuracy and resolution for good geometry. The spectrum analyzed before and after attenuation of the sample depends on a number of factors, such as S/N, resolution, and efficiency of the detector (Guadilla et. al., 2018).

The region of interest peak, distribution of scattered photons, and broadening peak are the main contributors to the deviation of radionuclide peaks, especially multi-emitters, by more than 3% to 4%, compared to theoretical values [1,2]. Several methods, algorithms, and techniques have been used in a number of studies. T. J. Kennet et. al. (1978)[3] uses an interactive procedure on Bayes' postulate is used for deconvolution in the limit of iteration index.

The analysis of spectra before and after attenuation of a sample depends on several factors, including the signal-to-noise ratio (S/N), resolution, and efficiency of the detector (Guadilla et al., 2018). The region of interest (ROI) peak, distribution of scattered photons, and peak broadening are primary contributors to deviations in radionuclide peaks, especially for multi-emitters. These deviations are often 3-4% greater than theoretical values (Kennet et al., 1978). Numerous studies have explored methods, algorithms, and techniques for deconvolution to address these issues. For instance, Kennett et al. (1978) utilized Bayesian deconvolution techniques, whereas L. Bouches (1995) compared various deconvolution methods under high S/N ratio conditions.

In this study, the ML-EM algorithm was applied to analyze gamma-ray spectra and improve peak resolution. This approach enhanced the accuracy of mass attenuation coefficients and refined peak measurements, especially for overlapping energy peaks.

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L Bouches(1995)[4] deconvolute using various methods. In the 3σ deviation of a large S/N ratio of 3s deviation considering the range and shape of the spectrum suggested for the Maximum Entropy method (Guadilla et al., 2018).
Braian L Evan (1999)[5] analyzed the Compton-scattered spectrum using maximum likelihood deconvolution algorithm in focus of resolution of photopeaks.
I J Marg (2006)[6] evaluate complex spectra with LM, MLEM, MEM methods with considering performance parameters, P. Paatero (2006)[5] used different deconvolution methods, such as stroke generalized least square successive approximation harmonic analysis.
Methodology :
Spectral deconvolution method :
The deconvolution of singlet or doublet gamma-ray spectra is crucial for calculating the precise peak area and counts of intersected energy peaks. The convolution process of photons into a count signal in the scintillation detector results in energy loss, primarily due to Compton scattering, the photoelectric effect, and pair production. The energy of the peak in the observed spectra is gross with poor resolution, and the convolution enhances the energy of the peak and resolution in terms of the channel of the multi-channel analyzer.

The observed pulse height and spectrum channel count, as detected through the convolution of the emitted spectrum from the source with the detector's response, are represented as follows:

$$M(E) = \int_0^{\infty} R(E, E_0).S(Eo)dE_0. \quad (1)$$

where M(E) is the measured spectrum and R(E,E_0) is the pulse height data distribution for various energy intervals as the response function.

The spectrum measured M(E) can be described as,

$$M=RS \quad (2)$$

$$\begin{bmatrix} M_1 \\ \vdots \\ M_2 \end{bmatrix} = \begin{bmatrix} R_{11} & \dots & R_{1j} \\ \vdots & \vdots & \vdots \\ R_{i1} & & R_{ij} \end{bmatrix} \begin{bmatrix} s_1 \\ \vdots \\ s_j \end{bmatrix}$$

$$M_i(E) = \sum_{i,j=1}^{n} R_{ij} S_j \quad (3)$$

Where M_i is the true detector counts. R_{ij} is the is the response function of detector and S_j is discretized incident function.

Multiplying equation (3) by $(Rij)^{-1}$ inverse matrix of (R_{ij})

$$S = R^{-1}M \quad (4)$$

the response function of matrix has large span of energy/channel relative to the counts for monoenergetic gamma source. Measuring the response matrix encounters challenges such as noise, geometrical factors, and negative results, all of which contribute to issues with peak width.

The Spectral inverse problem by MLEM method removes/suppress the above problem. The main advantage of MLEM method of deconvolution algorithm resulting actual number of counts measured by detector.The MLEM algorithm monotonically converges to a likelihood solution, surpassing conventional least-squares methods. The deconvolution after MLEM algorithm gives true values similar to Poisson statistical[6] nature. Due to its very large condition number, the response matrix is almost singular. Consequently, computing its inverse is prone to numerous arithmetic errors, which result in the production of an identity matrix multiplied by the original matrix.

L.B. Lucy (1974)[11] introduced the MLEM technique, which was applied to tomography. The inverse problem of singular ill condition matrices is removed. The MLME maximizes the each bits/ interval of equal width in likelihood for appropriate counting statistics driven by spectra.

The iterative algorithm[10] and applied for true measured spectrum to obtain best fit. The method assumes use the Poisson distribution for each Independence variable. M_i of measured spectrum by detector having (n+1) response factor R_{ij}. It is assumed that x(k) is the best estimate of actual spectra and given by Shepp (1982)[10] as :

$$X_k^{(n+1)} = x_k^n \left\{ \frac{1}{\sum_{i=1}^{i} R_{ik}} \left[\frac{M_i}{\sum_{j=1}^{j} R_{ij} x_j^{(n)}} R_{ik} \right] \right\} \tag{5}$$

here i and j are row and column indices of response matrix. MLME algorithm calculate the new value of $X_i^{(n+1)}$in each iteration and it is continuous until the predefined tolerance value is reach. The tolerance value is determined by using the mean square differences between consecutive interations.

$$Tol = \sum_{j=1}^{j} \left(x_{j+1}^{(n)} - x_j^{(n)} \right) 2 \tag{6}$$

Experimental measurements :

In this study, we applied the MLEM deconvolution method to analyze the photo-peak data before and after gamma-ray attenuation. A NaI(Tl) (2"X2") scintillation detector coupled with an 8k-Multichannel analyzer was utilized in the attenuation experiment. The experimental narrow-beam geometry setup[2] was arranged. The attenuated and unattenuated spectra were obtained for 600 s and employed for deconvolution.
The study established the response function of the (2” x 2”) NaI(Tl) detector by setting up the target geometry. The detector was placed 26 cm from the aluminium entrance window.The detector is coupled to 8 K multichannel analyzer. The aim of the experiment to estimate the broadening parameter required to MCNPX simulation Gaussian distribution energy peak and secondly to validate the Monte Carlo simulation. The acquisition time of experiment was 600 sec. The radioactive nucleoids used in this study are given in table 1

The MELM algorithm was implemented using MATLAB software (version 2018a) to simulate the MCVP data. The resultant spectra are presented in Figure 2 for **singlet and** doublet energy sources ($Na^{22}$and CO^{60}, 511keV–1330keV), demonstrating the comparison of the convoluted and deconvoluted spectra in the aforementioned energy range.

The Compton scattered counts were added and shifted to Gaussian-shaped energy photo peaks. The net photo peak, FWHM, and resolution after the MELM in the energy range of 511keV–1.33keV are tabulated in Table 1.

For modeling of detector, the interesting between the detector and photons measured in pulse height counting simulation in Monte Carlo simulations. The detector structure was modeled precisely more in passive experiment photomultiplier tube (PMT) specifications.

The MCNPX counts a tally option generates parameters from MCNPX is Gussian Energy broadening (GEB) option. Gives the detector simulated data of unbroadeningin energy input to calculated breaking peak of spectral data and used specified tally inputs to solve equation,

$$fE = ce^{-\left(E - \frac{E_0}{A}\right)^2} \tag{7}$$

Where E is broadened energy, E_0 is unbroadened energy of the tally, C is normalization counts and A is Guassian width given as,

$$A = \frac{FWHM}{2\sqrt{ln2}} \tag{8}$$

The desired FWHM that is specified by the user provided counts a. b and c in equation 8 required by GEB tally.

$$FWHM = A + B\sqrt{E + CE^2} \tag{9}$$

The GEB parameters for this experimental setup were determined by using FWHM data of various gamma sources (Table -1) and by least square in OriginPro to calculate a b and c paramaters based on FWHM formulas the following parameters in the GEB option to generate detector region as,

A = -13.29326 keV b= 2.7863keV and c=-2.77739E-4keV

The Mass attenuation coefficients (μ/ρ) for aluminium absorber is measured by narrow beam geometry setup (Fig:1) . If a homogenous beam of gamma rays intensity (I) falls on absorber material, the detector detects the photons that passed through that absorber, then the dependence of detected radiation intensity (I_0) on the absorber thickness x is given by Beer-Lambert exponential law as

$$I=I_0 e^{-\mu x} \qquad (10)$$

Where I_0 and I are incident and transmitted intensity of photons respectively. The mass attenuation coefficient for a compound is given by Bragg's mixture rule

$$\frac{\mu}{\rho} = \sum w_i \left(\frac{\mu}{\rho}\right)_i \qquad (11)$$

where w_i and $(\mu/\rho)_i$ are the weight fraction and mass attenuation coefficient of the i_{th} constituent element respectively. Here, assay of 99.99% pure aluminium foils are used for attenuation measurement**.** Table 2 gives experimental values and reported values[1] after deconvolution of spectra. The comparison reveals a good agreement between the experimental and theoretical values1 of the mass attenuation coefficient.

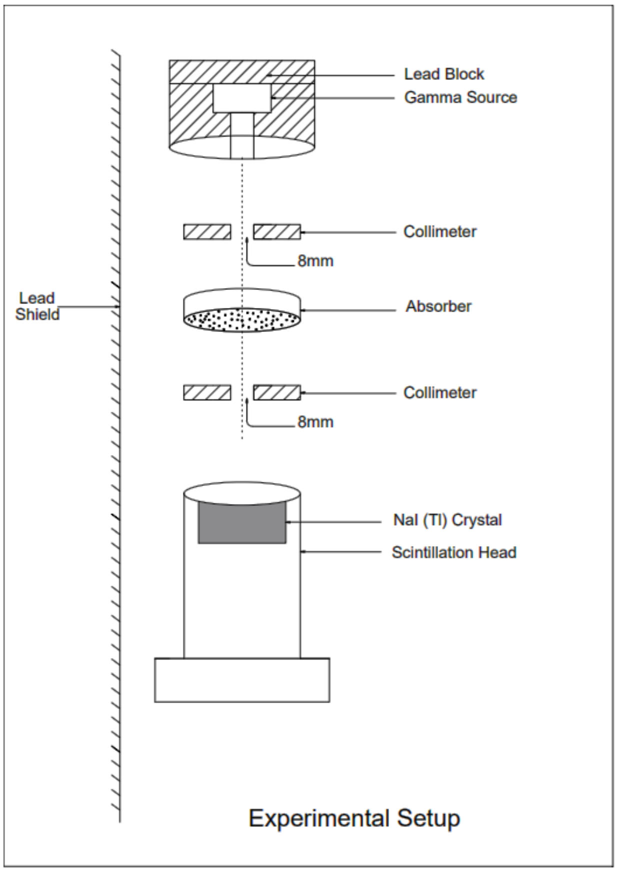
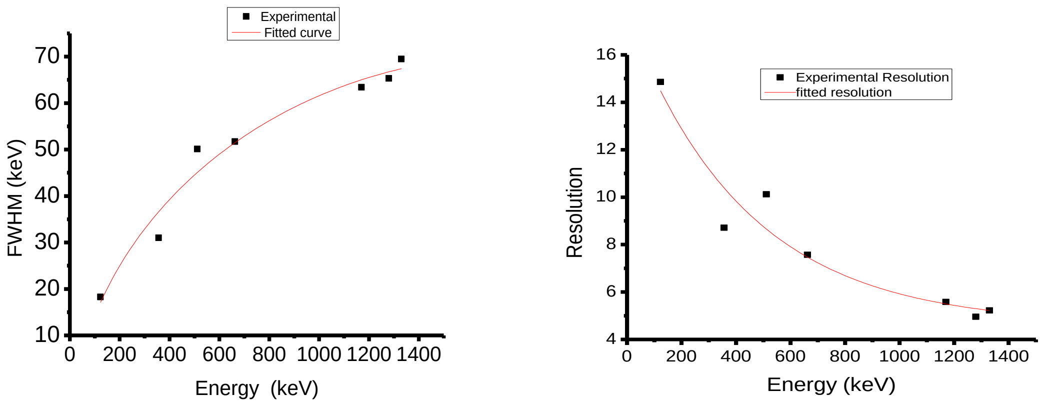


Fig. 1 . Experimental setup to measure Mass attenuation coefficients (μ/ρ) of aluminium absorber

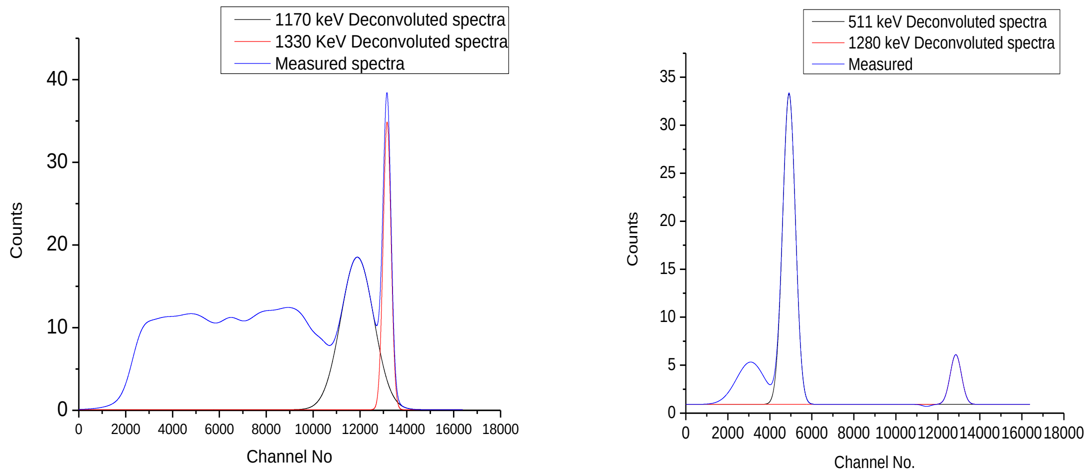
Table 1. Resolution and FHWM of NaI(Tl) detector for MCNPX and Deconvoluted Spectrum in energy range 3561130 keV.

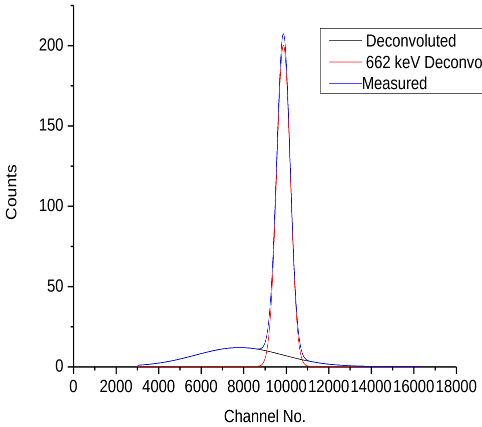
Nuclide	Energy (keV)	MCNPX Spectrum	Deconvoluted Spectrum	Resolution(%) (keV)	Photo peak Energy Shift (E_{DECON}-E_{MCNpX}) (keV)
		Measured FWHM (keV)	Fitted FWHM (keV)		
^{133}Ba	356	31.045	39.29367	8.707865	35
^{22}Na	511	50.122	49.92401	10.12211	95
^{137}Cs	662	51.724	58.80992	7.571299	12
^{60}Co	1170	63.412	82.91839	5.583248	80
^{22}Na	1280	65.324	87.38921	4.954063	40
^{60}Co	1330	69.502	89.35773	5.225714	24

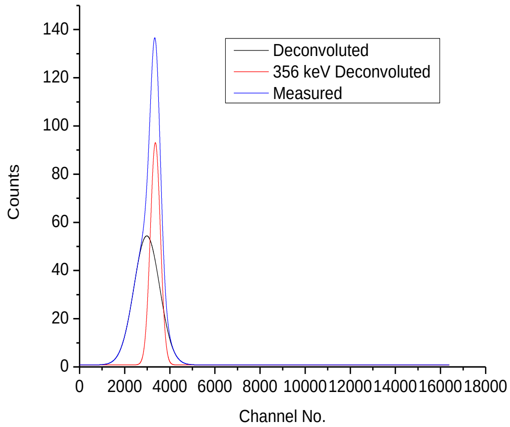
The resolution of NaI(Tl) detector depends upon the each and every assembled part. The energy response function can be is obtained by using histogram of available sources.



Graph 1 Measured gamma ray spectrum FWHM and resolution Vs. gamma ray energies 356-1330keV.







Graph 2 : Histogram of gamma ray spectra after MCNPM and Deconvoluted simulation for ^{133}Ba, ^{137}Cs, ^{22}Na, ^{60}Co nuclides.

Table 2. Theoretical and experimental values of mass attenuation coefficients (μ/ρ) for aluminium absorber.

Energy (Kev)	mass attenuation coefficients (μ/ρ) (cm^2/gram)		% Deviation[1]
	Experimental values	Theoretical values[1,2]	
356	0.06603	0.06578[1] ……..	0.3800
511	0.08478	0.08348[1] 0.08466[2]	-1.5572
662	0.07537	0.07467[1] 0.07547[2]	0.9374
1170	0.05690	0.05679[1] 0.05620[2]	-0.1936
1280	0.05309	0.05429[1] 0.05102[2]	2.2103
1330	0.05280	0.05325[1] 0.05298[2]	0.8459

Results and discussion

This study established the response function of NaI(Tl) detector using Monte Carlo Simulation. The application of MLEM deconvolution significantly improved in photo-peak resolution, particularly in singlet and doublet peaks as presented in Table 1. The deconvolution will assist more precise Compton scattering study, mass attenuation coefficient estimation and aids in identifying the unknown energy peak of gamma spectra.

The interactive algorithm relies on MLEM net counting accuracy. This method is particularly useful for PHA analysis across a wide range of Compton scattering photo-peak attenuations, including photoelectric peak attenuation in the K and L shell in HPGe detectors*.

The mass attenuation coefficient for Al absorber is shown in Table 2. Shows good agreement with theoretical values. Therefore, MLEM deconvolution method applied in this work validates the work.

* The Shifting of photo-peak energies due to the detector response function is observed considerably at higher energy.

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