ON HIGH ENERGY CALIBRATION OF THE GAMMA RAY SPECTROMETER USING THE WHOLE SPECTRUIM PROCESSING APPROACH

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The Peak Net Area (PNA) method is the world-wide accepted technique for analysis of gamma-ray spectra [1]. It is based on the net area calculation of the full energy peak, therefore, it takes into account only a fraction of measured gamma-ray spectrum. On the other hand, the Whole Spectrum Processing (WSP) approach to the gamma analysis makes possible to use entire information being in the spectrum [2,3,4,5]. This significantly raises efficiency and improves energy resolution of the analysis. A principal step for the WSP application is building up the suitable response operator. Problems are put in an appearance when suitable standard calibration sources are unavailable. It may be occurred in the case of large volume samples and/or in the analysis of high energy range. Combined experimental and mathematical calibration may be a suitable solution.

A) WHOLE SPECTRUM PROCESSING MODEL

The whole spectrum processing (WSP) model is based on the response operator which is mathematically formulated by a vector model

$$\mathbf{d} = \mathbf{K_c}\,\mathbf{q}\,, \tag{1}$$

where $\mathbf{d}$ is a column vector of the measured physical spectrum, $\mathbf{q}$ is a column vector of the real incident spectrum, and $\mathbf{K_c}$ is a matrix of the complete response operator with dimension that corresponds to the length of physical and incident spectra.

As an aspect of statistical fluctuation in the gamma-ray spectra, a solution of (1) cannot be found by direct computation of the vector $\mathbf{q}$ (for example by direct inversion of $\mathbf{K_c}$), and indirect iterative computational methods must be employed. These methods are based on minimizing the residuum between physical and model spectra according to the vector $\mathbf{q}$. The model fitting methods can be classified into two main groups: a) the least squares (LS) approach, and b) the maximum likelihood (ML) approach. Then LS and ML residual functions may be expressed as

$$\Delta_{LS} = (\mathbf{d} - \mathbf{K_c q})^2, \text{ and } \Delta_{ML} = log(\mathbf{d}) - log(\mathbf{K_c q}). \tag{2}$$

Using the residual function of LS or ML ($\Delta = \Delta_{LS}$ or Δ_{ML}), the gradient method yields an iteration step for $\mathbf{q}$ that may by formulated as $\Delta\mathbf{q} = -\,\mathbf{w}.grad(\Delta)$, where the symbol „*grad*" represents derivates of the residual function according to all elements in the vector of $\mathbf{q}$ (gradient) and $\mathbf{w}$ is a length of the iteration step.

B) STRUCTURE OF THE RESPONSE OPERATOR

The response operator matrix $\mathbf{K_c}$ contains all interaction taking part in detection and propagation of gamma-rays. There are the three principal ways in which gamma- and X- rays interact with matter. These include a) photoelectric effect, b) Compton scattering, and c)

electron-positron pair production. In summary, all three processes produce energetic electrons and positrons which can be detected directly, or can initiate other electron processes to obtain an electric charge pulse that can be used in detection. Generally, each of the principal processes generates a characteristic response within a characteristic energy range of the physical spectrum.

However, the appropriate mono-energy standard sources are not available for each energy channel within energy range put under analysis (number of c). Only several energy response components can be directly acquired by calibration measurements or by Monte Carlo simulation computations (number of $n << c$) and put into standard response operator matrix of $\mathbf{K_n}$.

Whereas, it is not possible directly to generalize the standard response operator $\mathbf{K_n}$ to the complete response operator $\mathbf{K_c}$ needed for the WSP operation, the operator $\mathbf{K_n}$ have to be decomposed into a suitable latent structure where partial latent elements (factors) may be directly interpolated within the whole energy range. This factorization is based on technique of Scaling Confirmatory Factor Analysis (SCFA) and may be schematically formulated as

$$\mathbf{K_n} = [\mathbf{F} \mid \mathbf{C_n}]\, \mathbf{B_n}\,, \tag{3}$$

where $\mathbf{F}$ is a matrix of extracted latent factors, $\mathbf{C_n}$ is a matrix of scaling coefficients, $\mathbf{B_n}$ is a matrix of loading coefficients, and symbol $[\mathbf{F} \mid \mathbf{C_n}]$ represents scaling product of the factors. Then the latent interpolation $\mathbf{C_n} \rightarrow \mathbf{C_c}$ and $\mathbf{B_n} \rightarrow \mathbf{B_c}$ yields the complete response operator using the factor structure (3) as follows

$$\mathbf{K_c} = [\mathbf{F} \mid \mathbf{C_c}]\, \mathbf{B_c}\,. \tag{4}$$

The factor structure of the response operator corresponds to principal interactions of photons with matter and describes principal components of the physical gamma-ray spectrum such as peak of full energy absorption, single and multiple scattering continuum, backscattering peak, single and double escape peaks and so on.

C) CALIBRATION OF THE RESPONSE OPERATOR

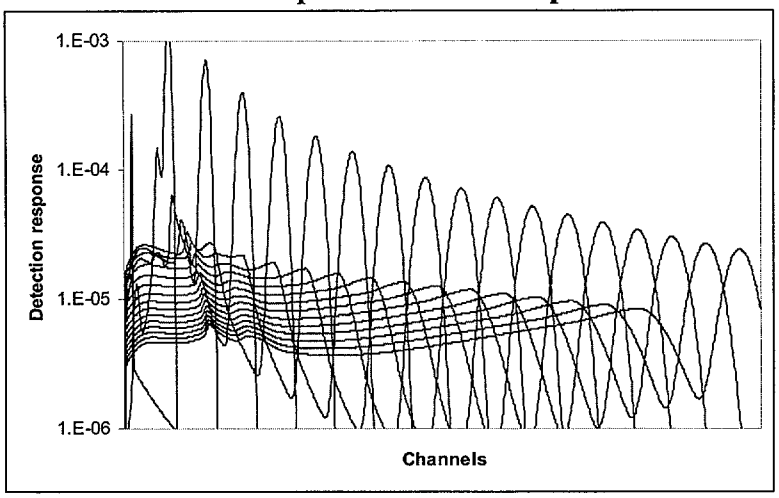
The calibration of the response operator may be formulated using a matrix equation as follows

$$\mathbf{S} = \mathbf{K_n}\, \mathbf{G}\,, \tag{5}$$

where $\mathbf{S}$ is a matrix of physical standard spectra as columns obtained by measuring the known standard sources (experimental calibration), or by Monte Carlo simulation (mathematical calibration), $\mathbf{G}$ is a matrix of known reference values for each of the standard spectra and for each of n energies used in calibration.

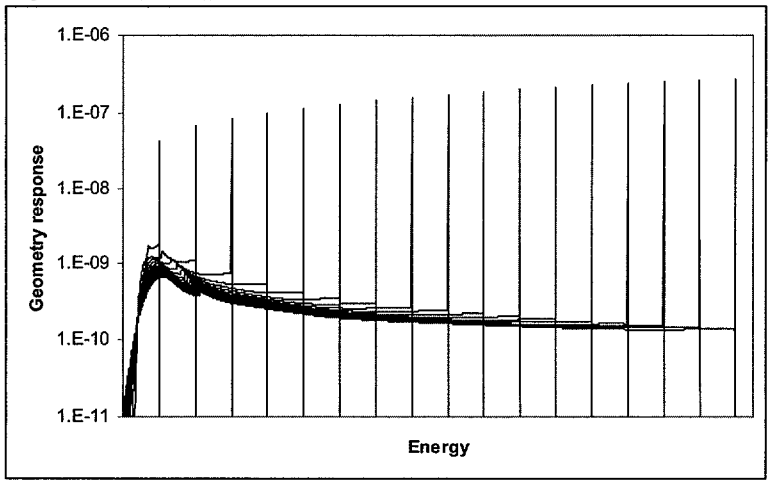
The experimental calibration may be used only when appropriate calibration standard sources are available. Generally, it can be employed for point and some voluminous standard sources such as standard Marinelli beakers, for instance. In Fig. 1, the detection response operator for gamma-ray spectrometer (2x2 inches NaITl detector, photomultiplier with UniSpec base) is depicted. The response functions were obtained by experimental calibration using point standard sources at 15 cm distance of the detector head [6]. The energy range of response functions was up to 2 MeV.

Figure 1. Experimental detection response functions depicted with 100 keV step



For non-standard voluminous detection geometry, there one has to use a mathematical calibration based on Monte Carlo simulation such as MCNP code, for example. The code was applied for simulation of photon transport from 200 liters drum that was situated 100 cm from the detector. Spectral fluence rates of photons at the place of the detector centre were calculated by MCNP Tally 4. The geometry response functions obtained from the simulation are shown in Fig. 2

Figure 2. MCNP geometry response functions shown with 100 keV step



However, the mathematical calibration makes possible to simulate only detection and propagation of the gamma-rays within the detector body and the detector surroundings. In order to involve also electric charge pulses processing into the spectral response, one must combine both methods of calibration. Generally, the experimental calibration is suitable to apply for processes within the detector (lonely detection and following electronic processing) and the mathematical calibration is reserved for processes around the detector. Then, the combined calibration may be mathematically formulated as follows

$$\mathbf{K_c} = \mathbf{K_D}\,\mathbf{K_G}, \tag{6}$$

where $\mathbf{K_D}$ is detection response operator (DRO) matrix characterizing detection of photons within the detector, and $\mathbf{K_G}$ is geometry response operator (GRO) matrix including absorption processes within a voluminous radioactive sample put under gamma analysis and propagation of gamma-rays from the source to the detector, respectively.

D) CALIBRATION IN THE HIGH ENERGY RANGE

Apart from non-standard large volume detection geometry, application of the combined calibration method is required also in the high energy range where deficit of available standard sources above 2 MeV is accordingly occurred. The detection response functions of the 2x2 inches NaI(Tl) detector calculated by MCNP (Detector Tally 7) are shown in Fig. 3 for energy range of 2 MeV and in Fig. 4 for 10 MeV range.

Figure 3. MCNP detection response functions shown with 100 keV step (2 MeV range)

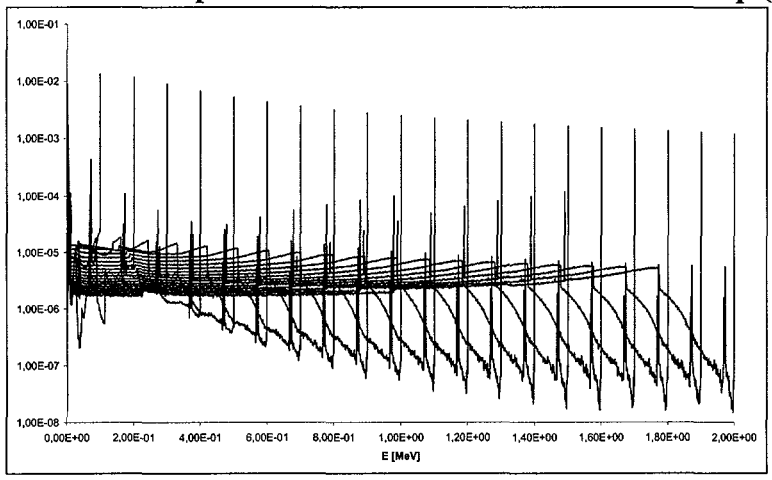
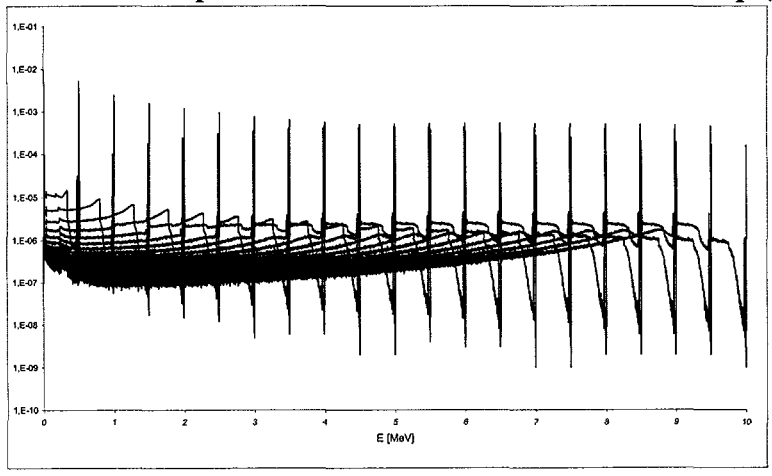


Figure 4. MCNP detection response functions shown with 500 keV step (10 MeV range)



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