Comparative Study on Peak-Seeking Methods of the Mixed Radioactive Energy Spectrum

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Abstract

The Geant4 software is used to simulate the CsI detector to measure the mixed energy spectrum from three radionuclides in the nuclear waste barrel. In this paper, a variety of methods are used to perform peak-seeking analysis on the mixed energy spectrum generating from $^{60}$Co, $^{137}$Cs and $^{226}$Ra, the effects of each peak-seeking method are compared for this complex energy spectrum. In this comparative experiment, the results show that the morphological energy spectrum peak-seeking method is more suitable for the energy spectrum from a mixture of multiple radionuclides.

Subject Areas

Nuclear Engineering, Nuclear Physics, Particle Physics

Keywords

Radionuclide, Energy Spectrum, Peak-Seeking

1. Introduction

A large amount of nuclear waste is produced during the decommissioning of nuclear facilities. For security and effective management, these radioactive wastes need to be packaged and stored in waste barrels according to the actual situation. Plenty of nuclear wastes generated in the process of nuclear energy mining, production and application [1]. To formulate corresponding disposal measures, the key information about the radionuclides in the waste drums needs to obtain, such as kinds and content of radionuclides. However, the kinds of radionuclides in waste barrels are complex. The energy spectrum contains complex information of radionuclides, and it also contains the influence of statistical fluctuations and environmental background [2]. The kinds of radionuclides in the nuclear...
waste barrel could be determined based on the energy of the main peak and each verification peak through finding all peaks in the energy spectrum accurately.

Peak-seeking has always been a necessary process for nuclide identification. The determination of peak position and boundary affects directly the calculation of peak area, and it affects the accuracy of nuclide characterization furtherly [3]. The main problem is to search true peaks with nuclide discrimination from statistical fluctuations, Compton margins, environmental background and other uncertain energy spectrum information [4]. The peak-seeking method is based on the smoothed energy spectrum obtained by the detector. With the continuous research, the widely used peak-seeking methods include simple comparison method, Gaussian product method, derivative method, covariance method, symmetric zero area method and morphological energy spectrum peak finding method, etc. Among them, different peak-seeking methods have different advantages and disadvantages. This article mainly uses these methods to compare peak-seeking of mixed radioactivity spectrum.

2. Mixed Radioactive Energy Spectrum

Geant4 is developed by the European Organization for Nuclear Research in the C++ language development environment, which is mainly used to simulate the interaction process of particles in matter [5]. The G4 General Particle Source (GPS) in Geant4 is used to implement the definition of multiple particle sources in the simulation. In this work, the Geant4 program described three mixed radioactive sources and CsI detectors 6 cm away from them. And collecting the information deposited by the particle in CsI detector is to obtain the required energy spectrum. Figure 1 shows the mixed energy spectra from $^{60}$Co, $^{137}$Cs and $^{226}$Ra.

![The mixed nuclide spectrum](image-url)
3. Energy Spectrum Smoothing

The measured energy spectrum data contains not only the effective energy spectrum data representing the nuclide information, but also the electronic noise signal of the detector instrument and its own statistical fluctuations [6]. Before the peak-seeking, the measured original data needs to be smoothed, and the smoothed energy spectrum data needs to retain the characteristic information of the original spectrum as much as possible to achieve the best peak-seeking effect to improve the accuracy of radioactive nuclide identification. The energy spectrum smoothing methods mainly include Fourier transform method, multi-point smoothing method and exponential smoothing method. The least-square method has always been a widely used curve fitting smoothing method [7]. Xu et al. [8] proposed a background noise extraction method based on the least-squares linear curve fitting, it realizes the elimination of background noise and achieves a better smoothing effect. This method satisfies the characteristics of the sum of squares of the errors of all parameter points and fitting points, it achieves effective smoothness while retaining the original spectral characteristic information as much as possible. In this paper, the least-square method is used to smooth energy spectrum. Figure 2 are the original and smoothed by the least square method respectively.

4. Peak-Seeking

4.1. Simple Comparison Method

The simple comparison method of peak searching is a relatively simple analysis method for early energy spectrum data analysis. The peaks and the determination of peak positions are judged by simple comparison [9]. To meet the conditions: \[ \text{data}_{i−m} < \text{data}_i − k\sqrt{\text{data}_i} > \text{data}_{i+m} \], it could be characterized as a peak.

![Figure 2. The smooth spectrum.](image)
$k$ is the peak-seeking threshold, which is generally between 1 and 1.5. And channel corresponding to the maximum value from $data_{i-m}$ to $data_{i+m}$ is peak position. The spectrum after peak-seeking is showed as Figure 3.

### 4.2. Gaussian Product Function Method

The Gaussian function is usually used to describe the shape of the peak of the spectrum, due to the peak reflects the statistical properties of the system noise and statistical fluctuation process [2], and it conforms to the normal distribution.

$$G(i) = \frac{A}{\sqrt{2\pi\sigma^2}} e^{-\left[(i-i_0)^2/2\sigma^2\right]}$$

Based on the Gaussian function, a new function is defined by adjacent data points. It is obvious that the first-order Gaussian function depends only on the width $H$. As shown in Equation (2):

$$P_{m=i} = \frac{G(i)G(i+m-2)}{G(i-2)G(i+1)} = \exp\left(\frac{11.092}{H^2}\right)$$

where, $m$ is the step length of the peak-seeking and it is also the order of the Gaussian function, which determines the sensitivity of the peak-seeking. With $m$ increasing, the sensitivity gradually increases, however, it is not suitable to determine the peak position after increasing to a certain value. Theoretically, the peak is determine by the $P_{m=i}$. When $P_{m=i}(i) = 1$, it is not a peak, when $C > 1$, it is a peak. Figure 4 is the peak-seeking result when $m = 1.5$.

### 4.3. Derivative Method

Derivative method [10] was proposed by Mariscotti in 1967, and its basic principle is regarding the energy spectrum as a continuous curve, using the characteristics of the shape of the energy spectrum curve near the peak position, the peak position can be accurately determined from the slope and curvature of the energy spectrum curve [11]. This method could intuitively reflect the data characteristics of the continuous curve change, and it could easily find the peak position and calculate the peak boundary to calculate the peak area accurately during the nuclide identification. In this paper, the first derivative to find the peak of the smooth spectrum. The principle is to calculate the derivation from the front end of the energy spectrum to the end. If the derivative value changes from a positive value to a negative value, it means there is a peak. This formula is described as followed:

$$\overline{data_i'} = \frac{1}{K} \sum_{j=i-m}^{i} (A_j data_{i+j})$$

The peak located at $i$ when the derivative value changes from positive to negative at zero crossing. Figure 5 is the result of peak-seeking by the first derivative method.

### 4.4. Covariant Method

The basic idea of the covariant peak finding method is to gradually fit the peak line function to the actual spectrum, the fitting result is used to distinguish true
and false peaks. Those with a higher degree of fit are true, and those with a lower degree of fit are judged as false. Calculate $h_i$ by gradually sliding fitting at $w = 2m + 1$.

$$h_i = \frac{\sum_{j=0}^{m} g_j \sum_{j=0}^{m} C_j data_{i,j} - \sum_{j=0}^{m} g_j \sum_{j=0}^{m} C_j \sum_{j=0}^{m} g_j data_{i,j}}{\sum_{j=0}^{m} g_j \sum_{j=0}^{m} g_j C_j^2 - \left(\sum_{j=0}^{m} g_j C_j\right)^2}$$  \hspace{1cm} (4)

where $h_i$ is the peak height, $g_j$ is the weighting factor, $C_j$ is the peak shape function (Including Gaussian function, Cauchy function, cosine function, hyperbolic secant function).

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**Figure 3.** Simple comparison method.

**Figure 4.** Gaussian product function method.
The calculation formula of fit is defined as:

\[ R_i = \frac{h_i}{\Delta h_i} \]  

(5)

\[ \Delta h_i = \left[ \frac{\sum_{j=m}^{m-1} g_j}{\left( \sum_{j=m}^{m-1} g_j \sum_{j=m}^{m-1} g_j C_j - \left( \sum_{j=m}^{m-1} g_j \right)^2 \right)^{\frac{1}{2}}} \right]^2 \]  

(6)

where \( \Delta h_i \) is the partial variance of the fitting process. The peak is judged according to the degree of fit \( R_i \), \( R_i \) is the maximum value and when \( R_i > R_{th} \) (where, \( R_{th} \) is described as a threshold, and depends on the half-width \( H \) and the number of points selected \( W \), generally between 2 and 5) the peak lies in the corresponding channel. The detail is showed in Figure 6.

4.5. Symmetric Zero Area Method

The symmetric zero-area method utilizes the symmetric window function and the smoothed energy spectrum for convolution transformation, and threshold processing is carried out on the transformed data to obtain the spectral peak position [12]. After the transformation, the convolution transformation of the linear basis will be zero, and only the places where there are peaks will not be zero. Therefore, the transformed spectrum could intuitively reflect the change in peak shape. And the mathematical equation is defined as follows:

\[ \hat{Y}_i = \sum_{j=m}^{m} C_j data_{i+j} \]  

(7)

where \( \sum_{j=m}^{m} C_j = 0 \), \( C_j = C_{-j} \) realized symmetry. Convolution transformation
is developed when $W = 2m + 1$. The transformation function of the symmetric zero areas can be a square wave function or a peak-like function, where the whole square wave function is defined as follows:

$$C_j = \begin{cases} -b & -m \leq j < -(H-1)/2 \\ a & -(H-1)/2 \leq j \leq (H-1)/2 \\ -b & (H-1)/2 < j \leq m \end{cases}$$

(8)

where $H$ is center width. And the peak-like function is the difference between a specific function $G_j$ and a constant $d$. $G_j$ could be described as Gaussian function, Cauchy function, cosine square function, hyperbolic secant function, Gaussian second derivative function, etc. And $d = \frac{1}{W} \sum_{j=-m}^{m} G_j$. In order to make the sensitivity of peak searching independent of the statistics of the measured spectrum, the standard deviation of the transformed spectrum is generally used as the peak searching unit. The criteria are as follows:

$$SS_i = \frac{\hat{Y}_i}{\Delta \hat{Y}_i} = \frac{\sum_{j=-m}^{m} C_j data_{i,j}}{\left( \sum_{j=-m}^{m} c_j^2 data_{i,j} \right)} > f$$

(9)

where $f$ is the peak-seeking threshold, when $SS_i > 0 \land SS_i > f$, it could conclude that it is a peak. The peak position is at the channel corresponding to the positive value and the peak boundary is determined by the adjacent negative peaks on both sides, as shown in Figure 7.
4.6. Morphological Energy Spectrum Peaking

The morphological peak finding method is a new method based on the characteristics of image processing morphological changes. Its basic principle is to perform a morphological transformation of energy spectrum by selecting appropriate structural elements. The basic steps are: Firstly, the opening operation of the corrosion operation and the expansion treatment are performed to obtain the filtered energy spectrum. That A is corroded by structure B shows as follows:

\[
A \otimes B = \{ r \times B \} \subseteq A
\]

(10)

where the arithmetic symbol \( \otimes \) means “Corrosion calculation” to eliminate unwanted signals. Then, white hat transformation is performed to get new energy spectrum data. The formula for A to be expanded by B is as follows:

\[
A \oplus B = \{ r \times \hat{B} \} \cap A
\]

(11)

where the symbol \( \oplus \) means to fill in image holes and eliminate small noise. Finally, after removing false peaks according to the peak width setting, the peak-seeking is performed, and the determined peak position is output to the original energy spectrum to complete the entire peak search. And here is a peak criterion, \( L_i > W \), where \( L_i \) is peak-width to be found.

The peak-seeking algorithm based on morphology combines the advantages of image processing technology, and the low accuracy of traditional algorithms is avoided [13]. The accuracy is high in peak-seeking of the energy spectrum, and the method has the effect of identifying overlapping peaks to a certain extent. Figure 8 shows the result of the method.
5. Conclusion

This paper compares five traditional peak-seeking methods and a new peak-seeking method based on morphology by using the mixed energy spectrum generated by multiple nuclides. The results have shown that simple comparison method have been difficult to reach the peak-seeking requirements of the complex energy spectrum, and the peak-seeking effect is relatively poor. And only four peaks can be found in the smoothed energy spectrum, and lost the peak of 300 or so. In the result of the debugged Gaussian function, five peaks were found, which is different from the first method in the second peak. Similar to the results of the derivative method, covariant method and the symmetric zero area method, the peak positions are also roughly the same in Gaussian product function method, but the resolution effect of reunion is poor. And the positions of the third and fourth peaks in the searched peaks cannot be determined very well, especially in the area where the third peak has two peaks. These traditional methods perform better than the first two methods, but they still have poor peak-seeking effects in the complex energy spectrum. The peak-seeking method based on morphology is better adapted to the complex energy spectrum, and its effect is also the best in this comparative study. It can be further concluded that the morphological method is more suitable for peak-searching in the mixed energy spectrum obtained by multiple nuclides.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.
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