CONSTRUCTING THE RESPONSE FUNCTION FOR A BGO DETECTOR USING MCNP5 AND DEVELOPING THE DECONVOLUTION ALGORITHM IN THE LOW GAMMA ENERGY

By

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To my mother who is in heaven and to my father who has sacrificed everything for me.
ACKNOWLEDGMENTS

The Nuclear and Radiological Engineering Department of University of Florida was very unfamiliar with me when I came here for the first time. Now, I feel it is my home. I think life is a long journey. I have been on a hard but funny travel in America. During travel, you come to know the truth: you cannot take one step without other people’s help no matter how great you are. Therefore, the first thing you learn is how to appreciate the people who help you keep traveling.

Fortunately, my journey has been wonderful so far even though it was very hard to me sometimes. That means I am indebted to many people: Professor Allieza Haghighat would not be better for a lifetime teacher as well as an academic supervisor. I appreciate my co-adviser, Dr. Baciak for reviewing my paper. I was happy that I knew other faculties and staffs in the department. And also I have made too many good friends to mention in one page: Jorge, Vishal, Romel, Benoir, and others. Especially, I greatly appreciate my roommate Melissa for proofreading my thesis. Along with them, my strongest supporters are my family and friends in Korea. Without their sacrifice, I would not have been here. My mother would be very proud of me even in the heaven.

Many events have been mixed with bad, sad and good things: a bad thing is that my goal in America has yet to be accomplished, a sad thing is that my mother passed away two years ago, and a good thing is that I am in good health. I don’t need to be disappointed with the past nor too optimistic for the future because my journey is still going on. I will keep my voyage in America with much more efforts until my life ends. In conclusion, I might not be that smart because I have already started forgetting what I studied in a class, but I will never lose my gratitude of all of them.
# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>ACKNOWLEDGMENTS</td>
<td>4</td>
</tr>
<tr>
<td>LIST OF TABLES</td>
<td>7</td>
</tr>
<tr>
<td>LIST OF FIGURES</td>
<td>8</td>
</tr>
<tr>
<td>ABSTRACT</td>
<td>11</td>
</tr>
<tr>
<td>CHAPTER</td>
<td></td>
</tr>
<tr>
<td>1 INTRODUCTION</td>
<td>13</td>
</tr>
<tr>
<td>Characteristics of the Gamma Spectrum</td>
<td>13</td>
</tr>
<tr>
<td>General Deconvolution Methods for Gamma Spectrum</td>
<td>14</td>
</tr>
<tr>
<td>Response Function</td>
<td>17</td>
</tr>
<tr>
<td>Bismuth Germinate Oxide (BGO) Detector for the Gamma Spectroscopy</td>
<td>18</td>
</tr>
<tr>
<td>Objectives</td>
<td>18</td>
</tr>
<tr>
<td>2 CONSTRUCTION OF THE RESPONSE FUNCTION</td>
<td>23</td>
</tr>
<tr>
<td>Overview</td>
<td>23</td>
</tr>
<tr>
<td>Modeling of the BGO Detector Using the MCNP5 Code</td>
<td>26</td>
</tr>
<tr>
<td>Characteristics of the MCNP5 Code for Gamma Transport</td>
<td>27</td>
</tr>
<tr>
<td>Crystal Size</td>
<td>28</td>
</tr>
<tr>
<td>Source Position</td>
<td>28</td>
</tr>
<tr>
<td>Window Thickness</td>
<td>29</td>
</tr>
<tr>
<td>Angular Dependence</td>
<td>30</td>
</tr>
<tr>
<td>Comparison of the Experimental and MCNP5 Simulation Results</td>
<td>31</td>
</tr>
<tr>
<td>Experimental Setup</td>
<td>31</td>
</tr>
<tr>
<td>Energy Broadening</td>
<td>32</td>
</tr>
<tr>
<td>Comparison of the Experimental Results to the MCNP5 Predictions</td>
<td>34</td>
</tr>
<tr>
<td>Generation of the Response Matrix</td>
<td>36</td>
</tr>
<tr>
<td>3 DECONVOLUTION METHODS</td>
<td>55</td>
</tr>
<tr>
<td>Maximum Likelihood Estimation (MLE)</td>
<td>57</td>
</tr>
<tr>
<td>Expectation Maximization (EM)</td>
<td>59</td>
</tr>
<tr>
<td>Maximum Likelihood Expectation Maximization (MLEM)</td>
<td>60</td>
</tr>
<tr>
<td>Direct Inverse Method &amp; Gaussian Mixture Method (DIM-GMM)</td>
<td>62</td>
</tr>
<tr>
<td>Finite Mixture Model (FMM)</td>
<td>62</td>
</tr>
<tr>
<td>Gaussian Mixture Model and Parameter Estimation through the EM</td>
<td>64</td>
</tr>
<tr>
<td>Concept of the New DIM-GMM</td>
<td>67</td>
</tr>
</tbody>
</table>
4 RESULTS ...........................................................................................................................................73

Deconvolution of the Sample Spectrum Obtained from the MCNP Simulation .........................74
Comparison of the Deconvolution Effect of the MLEM and the DIM (Sources 1 and 2) ........................................................................................................................................74
Comparison of the Deconvolution Effect of the MLEM and the DIM-GMM (Source 3) ........................................................................................................................................75
Deconvolution of the Sample Spectrum Obtained from Experiments ........................................76
Comparison of the Deconvolution Effect of the MLEM and the DIM (Sources 1 and 2) ........................................................................................................................................76
Comparison of the Deconvolution Effect of the MLEM and the DIM-GMM (Source 3) ........................................................................................................................................78

5 DISCUSSION ........................................................................................................................................88

Response Function ..................................................................................................................................89
Deconvolution Methods ..................................................................................................................................91

6 CONCLUSION .........................................................................................................................................94

APPENDIX

A MCNP CODE FOR THE BGO DETECTOR MODELING .................................................................98
B C LANGUAGE CODE FOR ENERGY BROADENING EFFECT .................................................103
C LINEAR INTERPOLATION OF THE RESPONSE FUNCTION .................................................105
D MATLAB CODE FOR INTERPOLATION OF THE RESPONSE FUNCTION MATRIX .........................108
E MATLAB CODE FOR THE SPECTRAL DECONVOLUTION USING THE MLEM ALGORITHM ..................................................................................................................112
F C LANGUAGE CODE FOR THE SPECTRAL DECONVOLUTION USING THE GMM .................................................................................................................................114

LIST OF REFERENCES .................................................................................................................................119

BIOGRAPHICAL SKETCH ...............................................................................................................................123
<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2-1</td>
<td>Tally of two full energy peaks and their normalized tally by tally of 0° as a function of the angles for the non-shielded case ($^{60}$Co).</td>
</tr>
<tr>
<td>2-2</td>
<td>Tally of two full energy peaks and their normalized tally by tally of 0° as a function of the angles for the lead shielded case ($^{60}$Co).</td>
</tr>
<tr>
<td>2-3</td>
<td>List of experiments performed for examining the accuracy of Monte Carlo modeling.</td>
</tr>
<tr>
<td>4-1</td>
<td>Comparison of deconvolution results of the MLEM and the DIM over the sample spectra which are obtained from MCNP5-simulations for two different sources, source 1 ($^{54}$Mn) and source 2 ($^{22}$Na) respectively.</td>
</tr>
<tr>
<td>4-2</td>
<td>Comparison of deconvolution results of the MLEM and the DIM &amp; GMM over the sample spectra which MCNP5-simulates a source mixing with $^{54}$Mn, $^{22}$Na, and $^{137}$Cs (Source 3).</td>
</tr>
<tr>
<td>4-3</td>
<td>Comparison of deconvolution results of the MLEM and the DIM over the sample spectra which are obtained from experiments for two different sources, source 1 ($^{54}$Mn) and source 2 ($^{22}$Na) respectively.</td>
</tr>
<tr>
<td>4-4</td>
<td>Comparison of deconvolution results of the MLEM and the DIM-GMM over the sample spectra which are obtained from experiments for a source mixing with $^{54}$Mn, $^{22}$Na, and $^{137}$Cs (Source 3).</td>
</tr>
</tbody>
</table>
## LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-1</td>
<td>Typical gamma spectrum analyzed according to the spectrum attribute.</td>
<td>21</td>
</tr>
<tr>
<td>1-2</td>
<td>Typical forward method for deconvolution.</td>
<td>22</td>
</tr>
<tr>
<td>1-3</td>
<td>Typical inverse method for deconvolution.</td>
<td>22</td>
</tr>
<tr>
<td>2-1</td>
<td>Detection mechanisms for an actual scintillator detector and a MCNP5 simulation.</td>
<td>40</td>
</tr>
<tr>
<td>2-2</td>
<td>Tally and P/T as a function of crystal size ($^{137}$Cs source).</td>
<td>41</td>
</tr>
<tr>
<td>2-3</td>
<td>Tally and P/T as a function of source positions ($^{137}$Cs source).</td>
<td>41</td>
</tr>
<tr>
<td>2-4</td>
<td>Change of the solid angle as the source-to-detector distance increases.</td>
<td>42</td>
</tr>
<tr>
<td>2-5</td>
<td>Tally and P/T as a function of detector window thickness ($^{137}$Cs source).</td>
<td>42</td>
</tr>
<tr>
<td>2-6</td>
<td>Geometry of a source and a detector is illustrated for the non-shielded case: A $^{60}$Co source is rotated by 20 degree for every simulation.</td>
<td>43</td>
</tr>
<tr>
<td>2-7</td>
<td>Geometry of a source and a detector is illustrated for the lead shielded case: A $^{60}$Co source is rotated by 20 degree for every simulation.</td>
<td>43</td>
</tr>
<tr>
<td>2-8</td>
<td>Spectrum of $^{60}$Co as a function of the angles for the non-shielded case.</td>
<td>44</td>
</tr>
<tr>
<td>2-9</td>
<td>Spectrum of $^{60}$Co as a function of the angles for the lead shielded case.</td>
<td>44</td>
</tr>
<tr>
<td>2-10</td>
<td>The BGO detector and gamma source are supported with the low density epoxy board.</td>
<td>45</td>
</tr>
<tr>
<td>2-11</td>
<td>Experimental setup for measuring the gamma rays from the disk source.</td>
<td>45</td>
</tr>
<tr>
<td>2-12</td>
<td>Three different response function of a 1x1 detector are depicted; MCNP5 without the Gaussian energy broadening, MCNP5 with the Gaussian energy broadening and the experiment.</td>
<td>46</td>
</tr>
<tr>
<td>2-13</td>
<td>Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 1”x1”, for different detector-source distances.</td>
<td>47</td>
</tr>
<tr>
<td>2-14</td>
<td>Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3”x3”, for different detector-source distances.</td>
<td>48</td>
</tr>
<tr>
<td>2-15</td>
<td>Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 1”x1”, for different detector-source distances.</td>
<td>49</td>
</tr>
</tbody>
</table>
Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3”x3”, for different detector-source distances.

Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3”x3”, for different detector-source distances.

Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3”x3”, for different detector-source distances.

Examples of response functions which are constructed using the numerical interpolation with and without the energy broadening.

Comparison of 662 keV spectrum obtained from interpolation and 662 keV spectrum reduced from convolution of the response function and a source.

How statistic methods define source data and measured data and how MLE and EM estimate parameters given a source data.

Spectra before and after it is deconvolved.

Descriptions of how the DIM-GMM works.

Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the MCNP5-simulated sample spectrum on source set 1, $^{54}$Mn.

Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the MCNP5-simulated sample spectrum on source set 2, $^{22}$Na.

The MCNP5-simulated sample spectrum for a mixture of $^{54}$Mn, $^{22}$Na, $^{137}$Cs on source set 3.

Unfolding spectrum of source set 3 for the MCNP5-simulated sample spectrum by the MLEM algorithm.

Unfolding spectrum of the MCNP5-simulated sample by the DIM on source set 3.

The GMM separates peaks of the spectrum which was obtained by the DIM at Figure 4-5.

Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the experimentally generated spectrum on source set 1, $^{54}$Mn.

Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the experimentally generated spectrum on source set 2, $^{22}$Na.

Comparison of the MCNP5 and measured sample spectra for $^{22}$Na and $^{54}$Mn sources.

Experimentally generated sample spectrum for a mixture of $^{54}$Mn, $^{22}$Na, $^{137}$Cs on source set 3.
4-11 Unfolding spectrum of source set 3 for the experimentally generated sample spectrum by the MLEM algorithm .................................................................87

4-12 Unfolding spectrum of the experimentally generated sample spectrum by the DIM on source set 3.........................................................................................87

C-1 Linear expansion of the response function of the low energy ..........................................................107

C-2 Linear compression of the response function of the low energy ......................................................107
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In our study, all the general procedures necessary for extracting useful information from the measured gamma spectrum of a BGO detector and point radioisotope sources have been discussed with regard to the MCNP modeling and the deconvolution methods. The sensitivity of the BGO detector was studied by using the MCNP5. From simulation results, the MCNP5 code was verified for its feasibility of the spectral analysis. The detector response function is subject to the detector system condition: such as crystal material, crystal size, photon energy, and source position. Therefore, various detector responses were modeled on the conditions of the detector system. A response function matrix was constructed on the basis of the MCNP5 simulation results. All the results were compared with the experimental ones.

In terms of the inverse problem, the deconvolution of the measured gamma spectrum is identical to development of the algorithm for deriving the stable solution from the intrinsically ill-posed deconvolution problem. Despite its slow convergence, deconvolution algorithms based on statistical iteration have recently drawn much attention as the powerful alternative for resolving the above problem. Thus, we have tested two well known statistical deconvolution methods, the MLEM (Maximum Likelihood Expectation Method) and the GMM (Gaussian
Mixture Method) for the deconvolution of the measured gamma spectrum. The new deconvolution method called “DIM-GMM” was developed which consists of the DIM (Direct Inverse Method) and the GMM (Gaussian Mixture Model). Those methods have shown good performance.
CHAPTER 1
INTRODUCTION

Characteristics of the Gamma Spectrum

Gamma rays are high energy photons, which are radiated from de-excitation of the nuclei or from sub-atomic interactions. Each nuclide has its own characteristic energies corresponding to the energy level of its nuclear state. Due to this property, the gamma energy has been used for a variety of spectral applications.

One of the most favorable methods to detect gamma rays is to use scintillation detectors. As with other detectors, the detection mechanism in scintillation detectors relies on indirect measurement. This involves very complicated processes which consequently cause undesired signals. The basic principle can be described as follows: an energetic radiation photon ionizes the detector crystal proportional to its incident energy. Then, ionized electrons produce visual photons through so called fluorescence. These photons are guided into a PMT (Photo Multiplier Tube), and the PMT converts them into an electric signal which contains information on the radiation source.

In addition to perturbation from the detector, other external effects such as backscatter and cosmic rays contribute to the formation of the gamma spectrum. Thus, the actually measured spectrum makes a more complicated shape which stems from convolution of unwanted peaks and backgrounds as well as photo-peaks of interest as shown in Figure 1-1. Accordingly, proper analysis of the gamma spectrum is closely connected to the study of detection system’s characteristics. If the measured spectrum is analyzed in terms of spectral attributes [1], it can be classified into the following:

- **Photo-peaks**: the full energy peak of interest which is generated by the photoelectric effect.
• **Compton backgrounds**: they are produced by Compton scattering, single and double escape peaks generated by pair production, and x-ray escapes created by the photoelectric effect.

• **Compton-scatters and background radiations**: the general gamma spectrum is inevitably deconvolved with Compton scatters coming from an interaction between the original radiation source and materials surrounding the detector crystal, and backgrounds radiations which are due to external factors such as cosmic rays and terrestrial sources.

• **Detector resolution**: Due to the statistical fluctuations which are primarily related to a collection of visible photons, the full photo peaks broaden to form the Gaussian distribution.

• **Geometry of a source and a detector**: Location of a sample source and a detector affects the shape of the spectrum.

Because of the above factors, the measured spectrum will not completely coincide with the original radiation source. The spectral shape will vary even for the same radiation source according to the crystal materials and size, and the sample-detector geometry used. Therefore, many additional processes are required before and after measurements in order to extract only the necessary information from such a complicated spectrum.

**General Deconvolution Methods for Gamma Spectrum**

Various unfolding models for the effective data analysis have been introduced depending on objectives of spectral applications [2]. However, making a correct estimation of the source information from the observed data is not an easy task because obtained data loses its original information in the real detection system due to effects discussed in the previous section.
From the classical viewpoint, the methodology to approach the gamma spectrum analysis can be divided into two types, forward method and inverse method [3] [4]. Mathematically, it can be expressed as

\[ M = R \cdot S + \epsilon \]  

where \( M \) indicates the measured data, \( S \) represents the source data, and \( R \) is the detector response function. All measurement errors or uncertainties are symbolized with \( \epsilon \). Given a model function well-characterizing the physical system, the forward method estimates the true spectrum (source spectrum) by best fitting the model to the measured data. However, the inverse method predicts the true spectrum (source information) given results of the measured spectrum.

In the traditional forward method, the procedure for deconvolution is as follows: first develop a model function which best characterizes the physical system, and estimate the data using the model function, then compare the estimated data with the measured spectrum, and repeat that process by an iteration technique until it converges. Figure 1-2 depicts the typical mechanism of the forward method. Advantages of the forward method are that it provides stability of a solution and time savings while its disadvantage is that the forward method has difficulty resolving the overlapped peaks. Total peak area method (TPA) [5], peak search method [6] and stripping method [7] can be categorized as examples of the forward method.

The way to approach deconvolution in the frame of the inverse problem is based on correlation of cause (source data) and effect (measured spectrum) in Figure 1-3. Mathematically, it appears to be very simple to solve this inverse problem. However, in reality it presents the mathematical challenge because the real world is often ill-posed [8]. The concept of the well-posed or ill-posed problem was first introduced by Hadamard in his 1902 paper. The well-posed problem is defined as follows: Given a measured spectrum (M),
i) There exists a solution (S).

ii) The solution is unique.

iii) The relation of the solution and the measured data is continuous.

If the inverse problem does not satisfy above conditions, it is defined as ill-posed. Usually, most inverse problems are ill-posed. This means either a solution does not exist, or it is not unique unlike the forward problem, which provides a unique solution. Moreover, the solution could be unstable even if the inverse problem is well-posed. Specially, this phenomenon is termed as ‘ill-conditioned’ [9]. In this unstable system, even a small change of the system can cause a large amplification of the original data. Therefore, general algorithms for the inverse problem seek an approximate solution in a numerical way rather than an exact solution. One of those examples is the least squares method (LSM) which was introduced by Carl Friedrich Gauss in 1805. Its basic idea is to find the minimization of a sum of squares of difference between observed value and value given by the model:

\[ s = \arg \min_{s \in S} \| R \cdot s - M \|^2 \quad (1-2) \]

where M includes measurement error \( \varepsilon \).

The LSM is the very classical method for deconvolution of the gamma spectrum [10, 11]. In many cases, it encounters an oscillatory behavior of the deconvolved spectrum due to the ill-conditioned system so it often produces an unphysical result [12].

Many mathematical algorithms have been developed in order to reduce this oscillatory effect. Regularization is the fundamental method which has improved instability of a solution and accomplished the meaningful approximate solution by introducing additional information [13]. Eq.1-3 shows the Tikhonov regularization, which has been the most commonly used regularization method for ill-conditioned problems [14].
\[ s = \arg \min_{s \in S} \{ \| R \cdot s - M \|^2 + \alpha \| s \|^2 \} \]  

(1-3)

The second term called ‘regularization term’ in the right side of Eq.1-3 is artificially introduced for enforcing smooth constraints on the system and, as a consequence, obtaining the unique stable solution. However this constraint parameter, \( \alpha \), inevitably causes biased estimates. Therefore, the optimized constraint parameter should be determined by taking into consideration the balance between artificial effects and noise problems [12].

A statistical method is an example for the inverse technique [14]. The main idea of an inverse technique is to consider that the measured data is a random variable which follows a Gaussian or Poisson distribution and the technique allows for determination of the necessary parameters associated with these distributions. Thus, they assume that the obtained sample is independent and identically distributed. Then, the best model which characterizes that distribution is designed with parameters. Using the maximum likelihood methods, it estimates the parameters which make that distribution most likely. The Expectation maximization (EM) [15], and the maximum likelihood expectation method (MLEM) [16] are typical examples of the statistical methods.

**Response Function**

The response of scintillation detectors has been studied for a long time because of their importance to gamma spectral analysis as well as investigation of detector characteristics [17, 18, 19]. An observed spectrum does not illustrate the original data information, but rather the distorted data that is perturbed by the detector system. In other words, the measured spectrum could not be used for spectral applications without the deconvolution process. The response function includes information on the data which is lost through the detection process. Thus, the result of the spectral deconvolution greatly depends on the response function used by the
deconvolution algorithm. For that reason, it is important to generate an accurate response function in the spectral deconvolution process.

In principle, the detector response function is defined as a probability distribution \( R(E, E') \), indicating that a photon source emitted with energy \( E' \) is measured as a pulse height with energy \( E \). Strictly speaking, the detector response function is involved only in photon interactions within the detector such as photoelectric interaction, Compton scattering, and pair production that are caused by incidence photons of interest. However, the actual response function includes other external factors such as Compton backscatter and cosmic rays [20].

**Bismuth Germinate Oxide (BGO) Detector for the Gamma Spectroscopy**

Despite having some drawbacks such as low detection efficiency, and high susceptibility to radiation damage, a semiconductor detector such as a HPGe (High Purity Germanium) detector has a huge advantage over scintillator detectors in gamma spectroscopy analysis because of its excellent resolution (~2 keV at 1 MeV) [21]. However, the high detection efficiency of a BGO detector and its ease of use outweigh its low energy resolution in a certain physical environment [22, 23] compared to that of the HPGe detector. Furthermore, a certain effective unfolding algorithm even allows the BGO detector to achieve as high a resolution as the HPGe detector [24]. For that reason a BGO detector of high efficiency has been often selected as the detection system for many applications despite its poor detector resolution [25].

**Objectives**

The objectives of this thesis are to construct a response function for a BGO detector using the MCNP5 code, then find the optimized interpolation technique for the response function over the different detector system conditions based on the response function obtained, and finally develop a new computational algorithm for deconvolution of the measured spectrum in the BGO detector for a radioisotope source. All the processes have been discussed in this study.
The spectrum deconvolution requires a complicated and multistage procedure for the proper data analysis since the observed spectra arise from convolution of various photon interactions in the detector system. The detector response function contains all the information concerning transformation of the original source. Therefore, the accurate construction of the response function requires the most work prior to beginning development of the deconvolution algorithm.

In this study, we constructed the response function library using MCNP5 simulations while taking into consideration the experimental factors that have critical effects on the sensitivity of a detector: the BGO crystal size, the detector radiation source position, radiation energy of the radioactive source. The simulated results were then compared with experimental results, and the feasibility of the MCNP5 simulations were discussed. Based on the MCNP5 simulation results, the response function matrix was built for deconvolution of the measured gamma spectrum.

Selection of the deconvolution method depends on the characteristics of the spectral applications being used. There has not been such an algorithm which works well for all spectral applications: for example, library least squares shows a good performance for identification of the radioisotopes only if an accurate library is provided [26]. The total peak method is a good alternative unless the full energy peaks are densely overlapped in the measured spectrum [27]. As long as the accurate response function is given, the peak stripping method is a very powerful method [28, 29].

Deconvolution algorithms based on statistical iteration have recently drawn much attention especially in the field of medical imaging [30, 31]. Some researchers have obtained a good result
when applying it to the energy spectrum analysis. Especially, Meng et al. have demonstrated the MLEM algorithm is superior to other deconvolution methods[24].

Our study introduced a newly developed deconvolution method and compared it to the MLEM algorithm. The new deconvolution method consists of two steps. In the first step, the ill-posed response function with energy broadening is decomposed into a response function matrix without energy broadening and an energy broadening matrix, and measured spectrum is reproduced through the inverse calculations of the response matrix without energy broadening. In the second step, this preprocessed spectrum is deconvolved using the GMM (Gaussian Mixture Method) [32].
Figure 1-1. Typical gamma spectrum analyzed according to the spectrum attribute: 1) indicates the ideal spectrum of Cs-137, 2) illustrates the real gamma spectrum, and 3) - 5) show the spectrum shape when the real spectrum is decomposed corresponding to physical effects.
Figure 1-2. Typical forward method for deconvolution

Figure 1-3. Typical inverse method for deconvolution
CHAPTER 2
CONSTRUCTION OF THE RESPONSE FUNCTION

Overview

One of the goals of the current research is the development of a response function for a BGO detector using the MCNP5 code. The detector response function is subject to various physical factors and surrounding environments such as crystal materials, crystal size, detector-source distance and so on. This implies that a different detector response function matrix needs to be constructed whenever the detection system is changed. It is highly irrational and inefficient because it takes enormous time and effort to build the response function matrix for every case. If sensitivity of the detector response has property of linearity over change of the physical parameter, we can build a correlation of the sensitivity and the parameter change and thus estimate the response function of other parameters based on that correlation. For example, suppose we have constructed response functions of two different crystal sizes, 1x1 inch and 3x3 inch. We could interpolate the response function of a crystal size of 2x2 inch without additional simulation or experiment by finding a correlation between the detector sensitivity and the crystal size.

For the first time, we simulated performance of the BGO detector using the MCNP5 code under various physical conditions in the detection system in order to examine feasibility of the MCNP5 code in modeling the BGO detector [APPENDIX A]. After that, a response function matrix was constructed of 1500 different energies between 1 keV to 1500 keV on the basis of the MCNP5 simulation results. Note that the response functions were produced for a few energies and the response functions for the rest of energies were obtained using an interpolation technique.
In general, three methods are known for generating the response function: the experimental method [33-34], the semi-empirical method [35, 36], and the Monte-Carlo simulation [37, 38] method. Typically, the experimental method is not practical for development of the response function because the number of single mono-energetic radioactive sources required is limited. In addition, most of the radioactive sources emit more than one single gamma energy, which makes it more difficult to estimate the detector response for a single energy. From the 1970s through the 1990s the semi-empirical approach had been widely used where the analytical function is established regarding all the possible physical characteristics of a mono-energetic photon interaction. Its parameters are calculated from the least square fits to several response function spectra obtained from experiments, and then this semi-empirical function is used to generate the response function of other gamma energies. With the advent of remarkable developments in the computer technology and the particle transport algorithm technique, Monte Carlo simulation codes such as MCNP5 [39] and GEANT4 [40] have been favored for construction of the response function since it saves time and effort in production of the response function.

In the frame of the mathematical approach, the observed spectrum can be expressed in the integral form such as:

\[
M(E) = \int_{0}^{\infty} R(E,E')S(E')dE' + \varepsilon(E)
\]

where \(M(E)\) denotes the measured spectrum at energy \(E\), \(S(E')\) indicates the radioisotope source at energy \(E'\), and \(R(E,E')\) represents the response function operator which transfers a photon from spectrum \(S(E')\) to spectrum \(M(E)\). \(\varepsilon(E)\) is the measurement error.

In a radiation detection system, energetic photons are recorded through a series of electronic processing. The electric signal whose amplitude is proportional to the photon energy deposited in the detector crystal is generated from the interaction of an incident gamma ray and
the crystal material. Each signal is digitized by the ADC (Analog-Digital-Convertor) and then counted in registers (channels) corresponding to the digitized pulse height [41]. Consequently, the actual measured spectrum is represented in a discrete form. The degree of discretization depends on the number of the ADC channels used. Considering this characteristic of the radiation detection system, the integral form of Eq. 2-1 can be rewritten as the summation of the discrete energies:

$$M(E) = \sum_{E'=0}^{\infty} R(E', E') s(E') + e(E)$$

(2-2)

Eq. 2-2 can be expressed in matrix notation as follows:

$$M = R \cdot S + \varepsilon$$

(2-3)

where $M$ is a vector ($m \in R^m$), $S$ is a vector ($s \in R^n$), $\varepsilon$ is a vector ($\varepsilon \in R^n$), and $R$ is a matrix ($R \in R^{m \times n}$). The dimension of vector $M$ is not necessarily the same as that of vector $S$, but we treat only the same dimension for simplicity of a problem. Thus, the dimension of the response function matrix $R$ is assigned a $n \times n$ matrix.

From a viewpoint of the imaging system, the detector response matrix would be the point spread function [42], which convolves with a point source and spreads it out. The complicated shape of the observed spectrum is subject to the features of the response function matrix, i.e., the detector system. If the response function matrix can be decomposed according to causes of the convolution, then there is an obvious merit in handling a deconvolution problem. Unlike the experiment-based response function matrix, the simulation-based response function matrix can be decomposed into two parts: the response function matrix without energy broadening and the energy broadening matrix.
\[
\begin{bmatrix}
m_1 \\
m_2 \\
\vdots \\
m_N \\
\end{bmatrix} = \begin{bmatrix}
r_{1,1} & r_{1,2} & \cdots & r_{1,N} \\
r_{2,1} & r_{2,1} & \cdots & \cdots \\
0 & r_{2,1} & \cdots & \cdots \\
0 & 0 & \cdots & \cdots \\
0 & 0 & 0 & r_{N-1,N} \\
0 & 0 & 0 & 0 & r_{N,N} \\
\end{bmatrix} \begin{bmatrix}
s_1 \\
s_2 \\
\vdots \\
s_N \\
\end{bmatrix}
\]

\[M = R \cdot S + \varepsilon = (\bar{R} \cdot B) \cdot S + \varepsilon\]  (2-6)

where \(\bar{R}\) is the detector response matrix without the energy broadening and \(B\) is the energy broadening matrix.

The reason for splitting the response function into two matrices is associated with the methodology for the spectrum deconvolution. The detector response is generally ill-posed at Eq. 2-4, but this ill-posed response matrix can be transformed into a well-posed response matrix by the decomposition process. As shown in Eq. 2-5, the response matrix without energy broadening is a triangular matrix when it is decomposed; implying that it is well-posed. In the present study, we produced two types of response function matrixes: with energy broadening and without energy broadening. One is used for the MLEM method and the other for a new combination of the DIM and the GMM.

**Modeling of the BGO Detector Using the MCNP5 Code**

Primary features of the gamma spectrum are closely related to the detector properties and geometry of the detection system. Unfortunately, many features are not simulated by the MCNP5
code. For example, flat continuum and asymmetry of the tail of a photo peak which arise from leakage of electrons and detector imperfection within the crystal [20, 43]. Nevertheless, the MCNP5 code has shown good performance for many detector related simulations. This is because in many cases such detailed description of the detector physics is not that critical for modeling a detector. Therefore, we are interested in critical factors that affect the detector sensitivity such as crystal size, source position, detector window thickness, and source-detector angle. Such a study will contribute to the efficient development of a computational algorithm for construction of the response function matrix using the MCNP5 code and, at the same time, provide in-depth understanding of detection mechanism of the scintillation detector.

In this section, characteristics of the gamma spectrum in the BGO detector are modeled considering aforementioned physical parameters. The detector performance is assessed with the peak to total ratio (P/T). The P/T is a physical quantity referred to as the ratio of the full energy peak count to the total count recorded by a detector, which is generally used to measure the detector intrinsic efficiency [44].

**Characteristics of the MCNP5 Code for Gamma Transport**

As shown in Figure 2-1, a gamma ray produces visible light through so called scintillation process within the BGO detector. Those visible lights are low energy photons whose number is proportional to energy deposited. The energy of a scintillation photon is around 480 nm or 2.58 eV, and the number of scintillation yields is around 9000 photons/MeV for the BGO crystal. The reflector guides them into the PMT where they are converted into electrons which contribute to the electronic signal. On the other hand, the MCNP5 code is not designed to transport the visible photons. Once the gamma ray is determined to interact with a crystal by the Monte Carlo algorithm, the energy deposited in the crystal is regarded as absorbed at that spot without further transporting the visible photons that are induced from the interaction of the gamma rays and the
detector crystal as illustrated in Figure 2-1b. Thus, the MCNP5 code does not account for uncertainties which are involved in scintillation yields, leak of photons, and quantum electrons while they contribute to the energy resolution in the real detector. For this reason, the MCNP5 simulation shows a salient difference from a spectrum obtained from an experiment. The energy broadening effect should be treated after a simulation in order to compare to the experimental output.

**Crystal Size**

Three gamma spectra were generated for three different crystal sizes for a $^{137}$Cs point source located at 4 cm away from the center of the detector window. Their crystal diameters and heights are 1′ x 1′, 2′ x 2′, and 3′ x 3′. The P/T (peak-to-total ratio) is affected much more by the crystal volume-to-surface ratio rather than the crystal size [45]. The most influential factor on the P/T is the escape of the Compton-scattered photons which lead to enhancing the Compton background. From the geometrical viewpoint, a large volume-to-surface ratio suppresses the Compton background and increases the full energy peak. Therefore, if the volume-to-surface increases, the P/T increases. Figure 2-2 shows the P/T obtained from the MCNP5 simulation increases (from 0.606 to 0.764) as the crystal volume-to-surface ratio enlarges.

**Source Position**

For this analysis, we are considering a $^{137}$Cs isotropic point source located at 2 cm, 10 cm and 20 cm from the center of the detector window. Figure 2-3 shows the spectra obtained in these three configurations.

The shape of a spectrum is highly dependent on the change of the source-to-detector distance since the source-to-detector distance has a large effect on the absolute efficiency. On the other hand, the P/T does not depend significantly on the source-to-detector distance while it is closely connected to the incident energy, the volume-to-surface ratio, and the detector dimension.
Such a feature is observed in Figure 2-3. As a source is located farther away from the detector, intensity of the full energy peak notably decreases (from 0.1404 to 0.0006) due to reduction in absolute efficiency arising from the smaller solid angle, but the P/T doesn’t change significantly, i.e. 0.76 to 0.797.

A slight increment of the P/T can be explained by the solid angle difference in Figure 2-4. The gamma-rays which are more parallel to the centerline of the crystal at the lower solid angle result in less leakage out of the crystal and consequently, less Compton background and higher P/T.

**Window Thickness**

Three detector windows of thicknesses (0.02”, 0.04”, and 0.12”) were considered for a $^{137}$Cs point source located at 0.1 cm from the center of the detector window. For the detector window, only aluminum was considered because the reflector of visible photons is transparent to high energy photons.

The most prominent feature due to increment of the window thickness is increment of the spectrum intensity in the multi-scattering region. A considerable number of photons lose their energy in the detector window before being absorbed into the detector crystal. As a result, the photons losing their energy contribute to the spectrum intensity in the multi-scattering region. Figure 2-5 shows the expected window effect based on the MCNP5. As the detector window is thickened, the multi-scattering intensity increases, but the photo peak area decreases by 35.4 % from 0.16689 to 0.10775.

In comparison to the change in photopeak intensity, the change in the window thickness did not make as a large impact on the P/T as on the photopeak intensity for the range of thickness
tested. P/T decreases from 0.662 to 0.611 when the thickness of the detector window is increased.

Angular Dependence

In order to simulate the angular effect in the photon detection, five angles (0°, 20°, 40°, 60°, and 80°) were selected. Unlike in the previous models where photons were incident on the front of a BGO detector, in the angular dependence simulation photons can be projected onto the side of the detector as well as its front face. Thus, two cases were considered in Figures 2-6 and 2-7: one is to treat photons incident on both the front and the side faces, and the other is to treat only photons incident on the front face. For implementing the latter model, a couple of lead bricks were placed on the side face of the detector window to block photons from being projected on the side face in Figure 2-7. ⁶⁰Co was considered as a point source located at 25 cm from the center of the detector window and was rotated by 20 degree.

On the non-shielded model, the intensity of the full energy peak gradually increases corresponding to increment of the angle as shown in Figure 2-8. This result arises from the fact a large angle allows for more incident photons. Table 2-1 shows that the peak intensity of two peaks increases by 26 % for an 80 degree angle as compared to 0 degree angle case. A slight difference of the intensity between two peaks (1173.3 keV and 1332.5 keV) can be attributed to the detector efficiency.

The lead-shielded model shows the apparent discrepancy between the non-shielded spectrum and the shielded spectrum. First, the x-ray peak arising from the lead shield is observed which is not found in the non-shielded spectrum as shown in Figure 2-9. Secondly, the full energy peak intensity diminishes as the incident angle is enlarged on the contrary to the non-shielded model. This complete different phenomenon stems from the fact that the decrease of the
solid angle gives rise to reduction in the incident photons. Compared to the peak intensity of an angle of 0 degree, it decreases by 85 % at an 80 degree angle. The peak intensity hardly changes by an angle of 20 degree, but a rate of change in the peak intensity is much higher at the large angle than that in the non-shielded model as shown in Table 2-2. P/T was not treated in this simulation because of the mathematical difficulty in calculation of the number of the incident photons.

Comparison of the experimental and MCNP5 simulation results

Experimental Setup

Several experiments were done to test the accuracy of the MCNP5 modeling results. Also, various experimental setups were presented to study any correlation between the detector sensitivity and considered physical parameters: source type (\(^{137}\)Cs, \(^{60}\)Co), detector size, distance (2 cm to 20 cm) between the radioactive source and the BGO detector, and angles between the radioactive source and the BGO detector centerline (0° to 80°).

Table 2-3 summarizes four experimental sets which are presented for the variety of the physical conditions corresponding to the MCNP5 modeling. Experimental sets 1, 2, and 3 are involved in the study of detector performance, where two isotopes, three BGO crystals of the different sizes, and fourteen different geometries are utilized.

Experimental set 4 is designed for two purposes: verifying the response function obtained from the MCNP5 modeling, and providing a test spectrum for spectral deconvolution. The modeling set 4 will be discussed in Chapter 3. Three different BGO scintillators were selected which have the crystal sizes of 1” x 1”, 2” x 2”, and 3” x 3”. The same detector window thickness of 0.05 cm was considered for all detectors. Four radioisotopes were employed: \(^{137}\)Cs, \(^{60}\)Co, \(^{22}\)Na, and \(^{54}\)Mn, whose activities are 1±20% \(\mu\)Ci [46].Figure 2-10 depicts the experimental
setup in which a BGO detector and a radioisotope source are supported with the low density epoxy board.

The data collection and processing follow the typical data acquisition system as illustrated in Figure 2-11. The BGO detector was connected to the standard NIMs (Nuclear Instrumentation Modules) [41] and the data was collected using a multi-channel analyzer (MCA) and ORTEC Maestro software. The energy calibration was performed using a 32 keV x-ray and a 661.6 keV photopeaks emitted from $^{137}$Cs and 1173.2 keV and 1332.5 keV photopeaks emitted from $^{60}$Co in off-line analysis. To compare the experimental results to the MCNP prediction, the total count of each channel was normalized by the total number of activation counts of the radioactive source during the given acquisition time.

The BGO detector was isolated from its surroundings in order to inhibit external backgrounds as much as possible. However, a measured spectrum intrinsically includes following three types of background counts: external backgrounds which originate from any other gamma source except for the radioisotope source, backscatter due to surrounding materials, and the electronic noise. In this experimental analysis, only the external background was taken into account. External background measurements were performed before and after the main experiment. Their average value was subtracted from the measured data.

**Energy Broadening**

The measured data is a result of convolution of many physical phenomena and fully absorbed energies of the radioactive sources: Compton scattering, backscatter, cosmic-ray, electric noise, and energy broadening. Since the energy broadening which is involved in statistical fluctuation makes a significant impact on the convoluted spectrum, the energy resolution effect should be accurately treated for modeling the BGO detector. However, MCNP5
does not provide the transport of visible photons which are the primary attribute of the energy broadening.

In the current study, the energy broadening was artificially estimated after the MCNP5 simulation on the assumption that the full energy peak forms a Gaussian distribution considering the following formula [47]:

\[ FWHM = a + b\sqrt{E + cE^2} \]  \hspace{1cm} (2-7)

where FWHM denotes full-width-half-maximum. Note that coefficients of a, b, and c may change depending on the detector type and experimental setup. For an example, parameters for a detector of 2x2 BGO crystal are determined as \( a = 4.87125 \), \( b = 2.87358 \), and \( c = 0.00026 \). The Gaussian energy broadening effect can be applied to each tally scored in the pulse height tally (F8) by sampling from the following Gaussian function:

\[ f(E) = Ce^{-(E-E_o)^2/\sigma^2} \]  \hspace{1cm} (2-8)

where \( E \) is the energy broadening, \( E_o \) indicates the energy without broadening effect and \( C \) represents the normalized constant. The variance \( (\sigma^2) \) of the energy broadening is obtained from the following equation:

\[ \sigma = \frac{FWHM}{2\sqrt{\ln2}} \]  \hspace{1cm} (2-9)

Actually, the F8 tally presents the Gaussian energy broadening option (GEB) in MCNP5 [39]. We, however, did not use the GEB option. Instead, we made the Gaussian energy broadening code which includes the above FWHM formula because of two objectives [APPENDIX B]. First, the resolution correction after the MCNP simulation provides a better efficiency for building a large number of the response functions. Secondly, for deconvolution the response function...
matrix needs to be decomposed into the response matrices without and with the energy broadening.

Figure 2-12 describes the result of the Gaussian energy broadening correction of the MCNP5 simulation, where three different detector responses are compared to each other: i) MCNP5 without Gaussian energy broadening, ii) MCNP5 with Gaussian energy broadening, and iii) the experiment. Originally, the MCNP5 code did not give a complete description on the exponential tail in the low energy side of the Gaussian energy peak. Such a deformation of the Gaussian peak can be attributed to the following: incomplete charge collection due to crystal imperfection, and the leak-out of Auger electrons and x-ray escape [43, 48]. Only the x-ray escape is taken into account in the MCNP5 simulations. However, Figure 2-12 exhibits that the energy-broaden MCNP5 and experimental results are in a good agreement except for backscatter, which is not treated in the MCNP5 modeling.

**Comparison of the Experimental Results to the MCNP5 Predictions**

The spectra obtained from the MCNP5 simulation were compared with the experimental results for different BGO crystal sizes, for different source-detector positions, for different detector-source angles, and for different radioactive sources.

Figures 2-13 (a-f) and Figures 2-14 (a-f) show the results of modeling set 1 which correspond to the BGO crystal sizes of 1x1 and 3x3 for the $^{137}$Cs, and for detector-source distance between 2 cm and 20 cm. A small difference is observed around the Compton edge where the spectrum of the experiment is a little bit higher than that of the MCNP5 simulation result. This can be attributed to the Compton backscattering, which is not modeled in the MCNP5 simulation. This effect magnifies at the crystal size of 3” x 3”, because increments of the detector size diminish the multi-scattering.
Figures 2-15 (a-f) and Figures 2-16 (a-f) show the results of modeling set 2 which correspond to the BGO crystal sizes of 1” x 1” and 3” x 3” for the $^{60}$Co source, and for detector-source distance between 2 cm and 20 cm. In the modeling set 2 for the crystal size of 3” x 3”, the full energy photopeak of the experiment is found lower than that of the MCNP5 prediction in Figures 2-16 (a-f). This might be associated with the sum peak. It has been reported in literature [49] that the loss of the peak efficiency due to the coincidence summing effect is around 3% for $^{60}$Co. As the number of radiation counts increases – the number of radiation counts in the modeling set 2 (two gamma lines, 1173.2 keV and 1332.5 keV) is twice in the modeling set 1 (one gamma line, 661.6 keV) for the same elapsed time, a large amount of signal processing loads are imposed on the detection system. It, consequently, leads to increment of a data loss due to the sum peak of 1173.2 keV and 1332.5 keV. Such reasoning is supported by the fact that difference in the full energy peaks between the two results maximizes at the shortest detector-source distance (2 cm) where more radiation photons are incident on the detector.

The results of modeling set 3 are given in Figures 2-17 (a-e) and Figures 2-18 (a-e), which correspond to the BGO crystal size of 2” x 2” for the $^{60}$Co source, and six detector-source angles. In modeling set 3, the full energy peak of the experiment does not exhibit as large difference from that of the MCNP5 prediction for modeling of set 2. Since the distance between a source and a detector (25 cm) for the modeling set 3 is longer than the distance used for the modeling set 2 (2 cm to 19 cm), the data loss due to the sum peak is not considered large enough to cause the inconsistency between the experimental and the MCNP5 result. On the whole, the MCNP5 simulations accurately reproduce the angular dependence characteristics of the BGO detector for two cases, the non-shielded model and the lead shielded model.
For the model sets 1, 2, and 3, all the results show that the Monte Carlo predictions are in good agreement with experiments. The visible light self-absorption within the scintillator crystal becomes a dominant factor as the crystal size increases. This behavior cannot be represented by MCNP5 since visible photons are not transported. Nevertheless, the reason that MCNP5 and the experimental results show a good agreement is due to the fact that loss of the visible photons during particle transport does not contribute to counts but to the detector resolution. In other words, the energy broadening of the MCNP5 result is estimated by using the value of the detector resolution obtained from the experimental values.

**Generation of the Response Matrix**

We constructed the response function matrix for the BGO detector with a crystal size of 1” x 1” where the mono energetic source is located 15 cm away from the center of the detector window. Considering the energy range of the sample radioactive sources (Maximum gamma energy is 1332.5 keV emitting from $^{60}$Co), a matrix dimension of the response was developed as 1500 x 1500 whose elements have 1 keV bin.

The response function relies on the geometry of the model as well as on the intrinsic features of the detector. It means that a new response function matrix is required whenever the detector or the geometry changes. It is a very time-consuming work to build the response functions of 1500 different energies. Thus, the numerical interpolation was adopted to cope with that problem [50, 51]. 14 different energies from 200 keV up to 1500 keV at intervals of 100 keV were selected and the response function corresponding to each energy was simulated using MCNP5. Below 200 keV, two intervals were used: 10 keV and 20 keV. Then, the response functions of energies between two selections were linearly interpolated [APPENDIX C, APPENDIX D]. The response function matrix obtained from the MCNP5 modeling and the
linear interpolation does not include energy broadening. Therefore, the Gaussian code was used for building the response matrix with the energy broadening. Figure 2-19 shows several response functions with and without the energy broadening, which are linearly interpolated.

To verify the response matrix built, the monoenergetic energy of 662 keV, which is the equivalent of gamma lines resulting from $^{137}$Cs, was convolved with the response matrix and its result was compared with the spectrum directly produced by the MCNP5 simulation. They are consistent with each other in Figure 2-20.
Table 2-1. Tally of two full energy peaks and their normalized tally by tally of 0° as a function of the angles for the non-shielded case ($^{60}$Co).

<table>
<thead>
<tr>
<th>Source position (degree)</th>
<th>Non-shielded 2x2 crystal Peak area</th>
<th>Normalized by value of 0°</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1173.2 keV</td>
<td>1332.5 keV</td>
</tr>
<tr>
<td>0°</td>
<td>0.00065</td>
<td>0.00060</td>
</tr>
<tr>
<td>20°</td>
<td>0.00067</td>
<td>0.00062</td>
</tr>
<tr>
<td>40°</td>
<td>0.00071</td>
<td>0.00065</td>
</tr>
<tr>
<td>60°</td>
<td>0.00077</td>
<td>0.00070</td>
</tr>
<tr>
<td>80°</td>
<td>0.00083</td>
<td>0.00075</td>
</tr>
</tbody>
</table>

Table 2-2. Tally of two full energy peaks and their normalized tally by tally of 0° as a function of the angles for the lead shielded case ($^{60}$Co).

<table>
<thead>
<tr>
<th>Source position (degree)</th>
<th>Lead-shielded 2x2 crystal Peak area</th>
<th>Normalized by value of 0°</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1173.2 keV</td>
<td>1332.5 keV</td>
</tr>
<tr>
<td>0°</td>
<td>0.00066</td>
<td>0.00060</td>
</tr>
<tr>
<td>20°</td>
<td>0.00066</td>
<td>0.00060</td>
</tr>
<tr>
<td>40°</td>
<td>0.00058</td>
<td>0.00054</td>
</tr>
<tr>
<td>60°</td>
<td>0.00039</td>
<td>0.00037</td>
</tr>
<tr>
<td>80°</td>
<td>0.00010</td>
<td>0.00010</td>
</tr>
<tr>
<td>Set</td>
<td>Source</td>
<td>BGO Detector, crystal sizes</td>
</tr>
<tr>
<td>-----</td>
<td>-------------------------</td>
<td>----------------------------</td>
</tr>
<tr>
<td>1</td>
<td>Cs-137 (1 ± 20% $\mu$Ci)</td>
<td>1&quot;x1&quot;, 3&quot;x3&quot;</td>
</tr>
<tr>
<td>2</td>
<td>Co-60 (1 ± 20% $\mu$Ci)</td>
<td>1&quot;x1&quot;, 3&quot;x3&quot;</td>
</tr>
<tr>
<td>3</td>
<td>Co-60 (1 ± 20% $\mu$Ci)</td>
<td>2&quot;x2&quot;</td>
</tr>
<tr>
<td>4</td>
<td>Na-22, Mn-54, Cs-137 (1 ± 20% $\mu$Ci)</td>
<td>2&quot;x2&quot;</td>
</tr>
</tbody>
</table>
Figure 2-1. Detection mechanisms for an actual scintillator detector and a MCNP5 simulation.
Figure 2-2. Tally and P/T as a function of crystal size ($^{137}$Cs source).

Figure 2-3. Tally and P/T as a function of source positions ($^{137}$Cs source)
Figure 2-4. Change of the solid angle as the source-to-detector distance increases: the smaller a solid angle, the more parallel the incident photon.

Figure 2-5. Tally and P/T as a function of detector window thickness ($^{137}$Cs source)
Figure 2-6. Geometry of a source and a detector is illustrated for the non-shielded case: A $^{60}$Co source is rotated by 20 degree for every simulation.

Figure 2-7. Geometry of a source and a detector is illustrated for the lead shielded case: A $^{60}$Co source is rotated by 20 degree for every simulation.
Figure 2-8. Spectrum of $^{60}$Co as a function of the angles for the non-shielded case.

Figure 2-9. Spectrum of $^{60}$Co as a function of the angles for the lead shielded case.
Figure 2-10. A BGO detector and a gamma source are supported with the low density epoxy board.

Figure 2-11. Experimental setup for measuring the gamma rays from the disk source.
Figure 2-12. Three different response function of a 1” x 1” detector are depicted: MCNP5 without the Gaussian energy broadening, MCNP5 with the Gaussian energy broadening and the experiment.
Figure 2-13. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 1” x 1”, for different detector-source distances.
Figure 2-14. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3” x 3”, for different detector-source distances
Figure 2-15. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 1” x 1”, for different detector-source distances.
Figure 2-16. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 3’’ x 3’’, for different detector-source distances.
Figure 2-17. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 2” x 2”, for different detector-source angles without a shield.
Figure 2.18. Comparison of the experimental results to calculated spectra with and without broadening for BGO crystal of size 2' x 2", for different detector-source angles with a lead shield.
Figure 2-19. Examples of response functions which are constructed using numerical interpolation with and without energy broadening
Figure 2-20. Comparison of 662 keV spectrum obtained from interpolation and 662 keV spectrum reduced from convolution of the response function and a source.
The purpose of deconvolution in gamma spectroscopy is to extract the original source information from the measured data which is perturbed by the detector system. From the viewpoint of the inverse problem, the largest difficulty in deconvolution arises from the non-existence of a unique solution or instability of a solution due to an ill posed or an ill-conditioned problem [52]. These troubles hinder a deconvolution method from deriving the exact solution, and instead lead it to seek the physically meaningful approximate solution within permissible uncertainties.

There are two types of approaches to handle with this approximate problem: deterministic deconvolution and statistical deconvolution [53]. A basic idea of the deterministic method is to construct a model and fit the observed data to estimate the unknown source data. It looks for the most probable parameters by data-matching of the measured data and calculated data. As discussed in the previous chapter, LSM or regularization method can be regarded as the deterministic deconvolution method [12].

In contrast, the statistical model assumes that the observed data is distributed from a random sampling. A model is constructed which characterizes the distribution and its associated parameters. This model is called the probability distribution function. Once the probability distribution function is built, it seeks estimators, i.e., parameters which make the measured spectrum most likelihood [54].

Both methods do not exhibit a large difference from the point of model parameterization. The two models are actually related with each other. The distinctive difference comes from interpretation of the model over the observed data. The former seeks the optimum parameter of
the model to best describe the observed spectrum, while the latter finds the parameter of the highest probability distribution model to generate the observed spectrum.

The biggest advantage of the deterministic approach is its simplicity to treat a problem but it has not provided a satisfactory outcome for high dimensionality of the data. This drawback is mostly attributed to the lack of information. The regularization method makes considerable improvement by introducing additional information. However, determination of a functional and a regularization parameter considerably limits its application to the spectral deconvolution [8].

By contrast, statistical deconvolution resolves aforementioned issues more efficiently than the deterministic model. Also, it is an appropriate methodology to treat nuisance problems such as errors in the measured data and uncertainties of a model since its principle is the inference estimation based on statistics concepts, i.e., variance and means-square error.

Many methodologies have been developed for the deconvolution of a measured spectrum in terms of statistics: maximum entropy method (MEP) [55], genetic algorithm (GA) [56], maximum likelihood expectation maximization (MLEM) [16] and expectation maximization (EM) [57]. Statistical methodologies for deconvolution are based on statistical theory such as maximum likelihood estimation (MLE) [58] and Bayesian model.

In the present study, we have utilized the MLEM for deconvolution since it has already demonstrated good performance on spectral deconvolution. Gaussian mixture model (GMM) has been introduced for development of a new model. The GMM has been coupled with the direct inverse method (DIM) for the deconvolution of the gamma spectrum. We term this new methodology as “Direct inverse method and Gaussian mixture method (DIM-GMM)”.

In this Chapter we will discuss the statistic theories which are applied to the MLEM and the GMM.
Maximum Likelihood Estimation (MLE)

The objective of spectral analysis is to infer quantitative or qualitative information from the measured data. In gamma spectroscopy such information cannot be obtained directly from the measured spectrum. The maximum likelihood estimation (MLE) is a fundamental data analysis tool which is utilized for extracting information of interest from the observed data. This method is based on a statistical approach which is used to estimate parameters of a model. It was originally proposed by Sir Roland A. Fisher in 1912 [59] and has been widely used for various applications including the analysis of gamma spectra [60, 61, 62].

The basic procedure of the MLE is illustrated in Figure 3-1. When the source data is collected through measurement, two different types of data are generated: measured data and missing data. The measured data is referred to as incomplete data in terms of statistics, which implies it loses some information when the source data is transformed into measured data. This is why the source data is termed as complete data which can be recovered via only the indirect method. The missing data, which is unobservable [22] and is often called the hidden or latent data, is used by the expectation maximization algorithm which will be discussed later. The MLE deals with the measured data or incomplete data.

The MLE assumes that the measured spectrum is obtained from a sampling of random variables which are independent and identically distributed. Based on this assumption, a statistical parameterization model called a probability density function is constructed. The density function characterizes the distribution of the random variables:

\[ p(y_1, y_2, \ldots, y_N | \Theta) \]  

Because the observed samples are independent, the probability density function (pdf) can be expressed as a product of the probabilities of each data point; i.e,
\[ p(y_1, y_2, \ldots, y_N | \Theta) = p(y_1 | \Theta)p(y_1 | \Theta) \ldots p(y_N | \Theta) = \prod_{i=1}^{N} p(y_i | \Theta) \quad (3-2) \]

The pdf specifies characteristics of the probability that the sample distribution is \( Y = (y_1, y_2, \ldots, y_N) \) given parameter \( \Theta \). The Poisson distribution or Gaussian distribution has been often used as the pdf [63]:

\[ p(y | \mu) = \prod_{i=1}^{N} \frac{\mu_i^{y_i} e^{-\mu_i}}{y_i!} \quad (3-3) \]

where \( \mu \) denotes the mean of the Poisson distribution, and

\[ p(x | \mu, \sigma) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma_i}} e^{\left(\frac{(x_i - \mu_i)^2}{2\sigma_i^2}\right)} \quad (3-4) \]

where \( \mu \) and \( \sigma \) indicate the mean and the standard deviation of the Gaussian distribution.

Unlike the deterministic method which looks for parameters by fitting a model to the measured data, the MLE method finds the parameters taking advantage of a statistical quantity, i.e., the likelihood function [55]. Mathematically, the probability density function and the likelihood function are treated as the same:

\[ L(\Theta | y_1, y_2, \ldots, y_N) \equiv p(y_1, y_2, \ldots, y_N | \Theta) \quad (3-5) \]

However, the likelihood function searches for the estimator which makes the probability density the highest for an observed data. The estimator is obtained by maximizing the likelihood function, i.e.,

\[ \Theta^* = \arg \max_{\Theta} L(\Theta | Y) \quad (3-6) \]

Log likelihood is often used for calculation of estimators instead of the likelihood for ease of calculation:
\[ \theta^* = \arg \max_{\theta} \log L(\theta|Y) \quad \text{or} \]
\[
\frac{\partial \log L(\theta|Y)}{\partial \theta} = \frac{\partial}{\partial \theta} \log \prod_{i=1}^{N} p(y_i|\theta) = 0
\] (3-7)

The value \( \theta^* \) calculated from Eq. 3-7 is called the maximum likelihood estimator (MLE).

**Expectation Maximization (EM)**

The methodology of the MLE presents some advantages in terms of the fact that it uses advanced statistical inference techniques. Thus, it has been applied to various models and different types of data. Nevertheless, some problems still arise in parameter estimations. Usually, the likelihood function is mathematically intractable to maximize the likelihood or find this likelihood estimator. This drawback is mainly due to high dimensionality of a data and non-linearity of a model. In addition, information of interest is the unobservable complete data, or missing data, rather than unknown parameters of the incomplete data in gamma spectroscopy. It means that the incomplete data log likelihood in the MLE does not provide the source data information, and also the complete data log likelihood in the MLE cannot be used because the source data information is not given. The MLE algorithm is not an advisable choice for problems for which the measured data is incomplete.

Therefore, in order to treat these problems, expectation maximization (EM) algorithm is used. The EM associates the observed incomplete data with the complete data in a way that estimation of the likelihood function is computationally tractable. The general formulation of the EM algorithm was introduced by Dempster, Laird, and Rubin in 1977 [15]. Its most salient feature, distinguishing from the MLE, is that it maximizes the complete data log likelihood via a numerical iteration technique. The general procedure of the EM algorithm is performed by two successive steps, E (Expectation) step and M (Maximization) step. The E step is the process to
relate the incomplete data and the complete data. Given the observable incomplete data (Y) and initial parameters (Θ⁰), the conditional expectation value of the complete data log likelihood is defined as

\[ Q(\Theta, \Theta_{g+1}) = E[\log p(X, \Theta | Y, \Theta_{g+1})] \]  

(3-8)

In the M step, one iterates on the value of \( \Theta \) parameter until a maximum value of Q is achieved, i.e.,

\[ \Theta_{g+1} = \arg \max_{\Theta \in \Omega} Q(\Theta | \Theta^g) \]  

(3-9)

**Maximum Likelihood Expectation Maximization (MLEM)**

The maximum likelihood expectation maximization (MLEM) is the special case of the EM algorithm. The MLEM algorithm was proposed by Shepp and Vardi [16] for reconstruction of medical images in emission tomography. It has been used in the field of medical imaging [31, 64], and has exhibited good performance in spectral deconvolution [24, 65].

The main principle is explained by the following procedure: suppose that the measured spectrum is subject to a Poisson distribution, the pdf characterizing the measured data is constructed on the basis of a Poisson distribution. In the MLEM method, the likelihood of the pdf is maximized using the MLE algorithm. A numerical iterative equation is derived from this MLE process. This equation is identical to the expectation step of the EM method. The final step is to maximize the equation as the EM method does.

In the MLEM, it is important to note how to relate the measured data (incomplete data) with unknown source data (complete data) in order to obtain the best estimator. The MLEM defines the source data as the estimator, and utilizes the given response function which is associated with the source data by following equation:
\[ s^*(d) = \sum_{b=1}^{B} s(b)R(b, d) \]  \hspace{1cm} (3-10)

where \( s(b) \) indicates the number of photons of the energy bin \( b \) emitted from the radioactive source, and the response function matrix \( R(b,d) \) represents the probability that a photon of the energy bin \( b \) emitted from the source is detected at energy bin \( d \) in the detector. \( s^*(d) \) is the mean of the photons detected at the energy bin \( d \) in the detector.

The mathematical theory is developed via the following procedure: the pdf is expressed as

\[ p(m^*|s) = \prod_{d=1}^{D} e^{-s^*(d)} \frac{s^*(d)^{m^*(d)}}{m^*(d)!} \]  \hspace{1cm} (3-11)

where \( m^*(d) \) denotes the measured spectrum at the energy bin \( d \) in the detector.

The log likelihood associated with the pdf is given as

\[ \log L(s) = \log p(m^*|s^*) = \prod_{d=1}^{D} e^{-s^*(d)} \frac{s^*(d)^{m^*(d)}}{m^*(d)!} \]  \hspace{1cm} (3-12)

To estimate \( s \) corresponding to maximum of the log likelihood, we differentiate Eq. 3-12 with respect to \( s(b) \):

\[ \frac{\partial \log L(s)}{\partial s(b)} = - \sum_{d=1}^{D} R(b, d) + \sum_{d=1}^{D} \frac{m^*(d)R(b, d)}{\sum_{b'=1}^{B} s(b')R(b', d)} = 0 \]  \hspace{1cm} (3-13)

Multiplying both sides of Eq.3-13 by \( s(b) \), then

\[ s(b) \left. \frac{\partial \log L(s)}{\partial s(b)} \right|_s = -s(b) \sum_{d=1}^{D} R(b, d) + s(b) \sum_{d=1}^{D} \frac{m^*(d)R(b, d)}{\sum_{b'=1}^{B} s(b')R(b', d)} = 0 \]  \hspace{1cm} (3-14)

Eq.3-14 can be rewritten for an iteration scheme that converges to a maximum likelihood:
\[ s^{g+1}(b) = \frac{s^g(b)}{\sum_{d=1}^{D} R(b, d)} \sum_{d=1}^{D} \frac{m^*(d)R(b, d)}{\sum_{b'}^{B} s^g(b')R(b', d)} \]  

(3-15)

In the transition from Eq. 3-14 to Eq. 3-15, the term \( Q(s, s^g) = \sum_{b'}^{B} s^g(b')R(b', d) \) is referred to as the expectation step, and the process to estimate \( s^{g+1}(b) \) is referred to as the maximization step.

**Direct Inverse Method & Gaussian Mixture Method (DIM-GMM)**

**Finite Mixture Model (FMM)**

Finite mixture model (FMM) is a methodology to analyze data which is characterized by a random distribution, using statistical modeling [32]. It has been around one century since the biometrician Karl Person used mixture models for analysis of a data which is mixed of two different normal probability density functions. The enormous computational loads in fitting the mixture model have made it difficult to be applied to a problem with a large number of variables (high degree of freedom), even though the FMMs have huge advantages of modeling the complex mixture distribution. However, with the advent of faster computer technology, FMMs have been applied to numerous fields, which are involved in the computational pattern recognition, biology, engineering, marketing, and so on [66, 67, 68].

The FMMs are used to identify unobserved heterogeneity in the data, or to cluster underlying groups in the data. To this end, finite mixture models assume that observed data are a mixture of random distributions, and each distribution is characterized by the probability density function with its own parameters. A model of the observed data (probability density function) is mathematically defined as

\[ p(Y|\psi) = \sum_{k=1}^{K} a_k g_k (Y|\theta_k) \]  

(3-16)
where \( Y = (y_1, ... y_N) \) denotes a random data set of size N, and \( g_k(Y|\psi) \) indicates the probability density function of \( k^{th} \) component characterized with parameters of a vector \( \psi \). The parameter \( a_k \) is the \( k^{th} \) mixing coefficient or the \( k^{th} \) mixing weight whose physical meaning is probability that observation comes from the \( k^{th} \) component. It has the following features:

\[
0 \leq a_k \leq 1 \quad (k = 1, ..., K)
\]

\[
\sum_{k=1}^{K} a_k = 1 \quad (3-17)
\]

In the specified vector space \( \Omega \), the quantity \( \psi \) containing all the unknown parameters can be defined as

\[
\psi = \{ a_1, ..., a_{k-1}, \Theta_1, ..., \Theta_k \}, \quad \psi \in \Omega \quad (3-18)
\]

In short, Eq. 3-16 implies that the observed data can be expressed as a mixture of the probability density distributions with different parameters on the assumption that the observed data is distributed at random.

Once the probability density model is constructed for the observed data, the next step is to find unobservable parameters in order to infer which cluster the observed data originated from. One advantage of FMMs is that they can model the appreciably complicated distributions using the simple equation Eq. 3-16. However, it is still an open issue to estimate parameters in the fitting of the FMM to the observed data. Several methods have been introduced for parameter estimation: minimum-distance methods [69], maximum likelihood [70, 71], Bayesian approaches [72], and so on. In fact, the explicit methodology for parameter estimation in the FMM does not exist, but the EM method has been known as an effective and straightforward algorithm for parameter estimation in the FMM [32].
Gaussian Mixture Model and Parameter Estimation through the EM

The Gaussian mixture model is a specified case of finite mixture model (FMM), where the observed data distribution is a mixture of Gaussian distributions. Figure 3-2a depicts the observed spectrum which is represented as the probability density function, \( p(Y|\psi) \) in the mixture model. This mixture distribution can be deconvolved into three Gaussian peaks of different characteristics, variance, mean, and peak amplitude by taking advantage of the GMM if the observed spectrum originates from a convolution of the three Gaussian distributions Figure 3-2b.

The GMM starts with the assumption that the observed spectrum is independent and identically distributed, i.e., \( Y = \{ y_1, y_2, ..., y_N \} \) where \( N \) is the sample size and its components are characterized by the Gaussian distribution. Then, each Gaussian distribution is given as

\[
g(y|\Theta_k) = g(y|\mu_k, \sigma_k^2) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left\{ -\frac{1}{2\sigma_k^2} (y_i - \mu_k)^2 \right\}
\]

where \( \mu_k \) and \( \sigma_k^2 \) are mean and variance of the \( k \)th component respectively.

In order to evaluate GMM’s estimators, \( a_k, \mu_k, \) and \( \sigma_k \), the EM is applied to the GMM. The log-likelihood should be determined by the corresponding probability density function:

\[
\log L(\psi|Y) = \log \prod_{i=1}^{N} p(y_i|\psi) = \log \prod_{i=1}^{N} \sum_{k=1}^{K} a_k g(y_i|\Theta_k)
\]

\[
= \sum_{i=1}^{N} \log \left( \sum_{k=1}^{K} a_k g(y_i|\Theta_k) \right)
\]

Eq. 3-20 denotes the incomplete data log likelihood. The estimation of the parameter is mathematically a challenge for this incomplete log likelihood function because the equation includes a sum of the log function. Therefore, it would be a better idea to take advantage of the
complete log likelihood for the parameter estimation which is mathematically tractable. The complete data set for the GMM can be given as

\[ Z = \{ Y, H \} = \{ (y_1, h_1), (y_2, h_2), \ldots, (y_N, h_N) \} \quad (3-21) \]

where \( Z \) is the complete data set consisting of the observed data set \( Y=\{y_1, y_2, \ldots, y_N\} \) and the unobserved data set \( H=\{h_1, h_2, \ldots, h_N\} \), which is called hidden data or missing data. In the GMM, the hidden data \( (h_i) \) is the component identity of the observable data \( (y_i) \): that is, it tells which component is linked with the observed data. The complete data log likelihood is written as

\[
\log L(\psi|Z) = \log p(Y, H|\psi)
\]

\[
= \log \prod_{i=1}^{N} p(y_i, h_i|\psi) = \log \sum_{i=1}^{N} p(y_i, h_i|\psi)
\]

where \( \psi = (a, \Theta) = (a, \mu, \sigma) \).

With introduction of the additional information, the hidden data \( H \), the estimator calculation will be mathematically more tractable. Then, the E step of the EM method is given as

\[
Q(\psi, \psi^g) = E[\log L(\psi|Y, H) | Y, \psi^g]
\]

\[
= \sum_{i=1}^{N} \sum_{h_i=1}^{K} p(h_i|y_i, \psi^g) \log p(y_i, h_i|\psi)
\]

where

\[
p(h_i|y_i, \psi^g) = \frac{a_k^g g(y_i|\Theta_k^g)}{p(y_i|\psi^g)} = \frac{a_k^g g(y_i|\Theta_k^g)}{\sum_{k=1}^{K} a_k^g g(y_i|\Theta_k^g)}
\]

Note that Eq. 3-24 is derived from Bayesian’s rule.

If Eq. 3-23 is developed into the simpler equation, then

\[
Q(\psi, \psi^g) = E[\log L(\psi|Y, H) | Y, \psi^g]
\]

(3-25)
Because each parameter is independent from each other, we can maximize Eq. 3-25 by differentiating it with respect to an individual parameter.

\[
\psi = \arg \max_{\psi \in \Omega} Q(\psi | \psi^g)
\]  
(3-26)

\[
\frac{\partial Q(\psi | \psi^g)}{\partial a_k} \bigg|_{a_k} = 0
\]  
(3-27)

\[
\frac{\partial Q(\psi | \psi^g)}{\partial \mu_k} \bigg|_{\mu_k} = 0
\]  
(3-28)

\[
\frac{\partial Q(\psi | \psi^g)}{\partial \sigma_k} \bigg|_{\sigma_k} = 0
\]  
(3-29)

From the above maximization process, the new estimators are obtained as follows:

\[
a_k^{g+1} = \frac{1}{N} \sum_{i=1}^{N} p(k|y_i, \mu_k^g, \sigma_k^g)
\]  
(3-30)

\[
\mu_k^{g+1} = \frac{\sum_{i=1}^{N} y_i p(k|y_i, \mu_k^g, \sigma_k^g)}{\sum_{i=1}^{N} p(k|y_i, \mu_k^g, \sigma_k^g)}
\]  
(3-31)

\[
\sigma_k^{g+1} = \sqrt{\frac{\sum_{i=1}^{N} p(k|y_i, \mu_k^g, \sigma_k^g)(y_i - \mu_k^{g+1})^2}{\sum_{i=1}^{N} p(k|y_i, \mu_k^g, \sigma_k^g)}}
\]  
(3-32)

where the hidden value \(h_i\) is replaced by \(k\).

The new estimator calculation begins with guess of the initial parameters and is repeated until it converges to the expected tolerance.
Concept of the New DIM-GMM

The DIM-GMM algorithm consists of two steps, the direct inverse of the detector response function, and the peak separation of the Gaussian mixture method. The most straightforward and the easiest way to solve the inverse problem is to calculate the inverse of the response function matrix. However, the detector response matrix is ill-posed as previously mentioned several times.

Some algorithms reach the approximate solution by grouping the ill-posed response matrix into several matrices which provide stable solution and then by estimating the solution using an iterative scheme. Van-Cittert Algorithm [73], and gold deconvolution [74] are those examples. This method, however, has intrinsic limit due to the fact that the decomposition of the response function matrix is performed only in terms of mathematics without taking into account the physical situation. Thus, it may cause artificial effect.

By contrast, the direct inverse method decomposes the response function matrix into two matrices corresponding to physical characteristics: the detector response function matrix ($\hat{R}$) without the energy broadening and the response function matrix ($B$) with energy broadening as shown at Eq. 2-6. Physically, the matrix $\hat{R}$ is involved in any effect which produces distortion of the source data, and the matrix $B$ is the detector energy resolution resulting from statistical uncertainty of the collection of visible photons in the detector and photoelectrons generated in the photo-multiplier tube (PMT).

From the mathematical point of view, the response function matrix $\hat{R}$ is well-posed even though the energy broadening matrix $B$ is still ill-posed. If the inverse of $\hat{R}$ is performed on both side of Eq. 2-6, then

$$\hat{R}^{-1} \cdot \{ M = (\hat{R} \cdot B) \cdot S + \varepsilon \} \quad (3-33)$$
\[ \hat{R}^{-1} \cdot (M - \varepsilon) = (B \cdot S) = \hat{S} \] (3-34)

\( \hat{S} \) is still subject to the energy broadening effect, but all other effects are removed except for the photo peaks of interest. As a result, Compton backgrounds and x-ray escape peaks are all eliminated, and the original data intensity of the source is recovered in Figure 3-3. This is due to properties of the response function which includes all the physical information regarding the distortion of the original source information. The reconstructed source data \( \hat{S} \) can be treated just as a mixture of the Gaussian peaks corresponding to the energy broadening. This assumption is reasonable as long as the measured data is large enough to form the Gaussian distribution.

In the second step, the reproduced spectrum is deconvolved again using the GMM (Figure 3-3), in which Eq. 3-30 to Eq. 3-32 are used to estimate three different parameters, \( a_k, \mu_k, \) and \( \sigma_k \). In this spectral application, we can benefit from the fact that the energy resolution is given by the experimental results. In other words, the number of unknowns can be reduced. The reduction in the number of unknowns diminishes the number of parameter estimations. This means it saves time taken for the parameter estimation, and reduces error propagation of the parameter estimation. As a result, it leads to a large decrease in conversion time and enhancement of the parameter estimation accuracy.

In order to apply this advantage to the parameter estimation, estimation equations Eq. 3-31 and Eq. 3-32 should be redefined. The full width half maximum (FWHM) is obtained from the experiment over all energies.

\[ FWHM = a + b \sqrt{\mu_k^g + c\mu_k^{g^2}} \] (3-35)

where \( a, b, \) and \( c \) are the user defined coefficients which are determined from the experiment. The detector resolution is related to the FWHM and the standard deviation as follows:
\[ \text{Resolution} = \frac{\text{FWHM}}{\mu_k^g} = \frac{2.35 \sigma_k^g}{\mu_k^g} \]  

(3-36)

From Eq. 3-36 the detector resolution is decided over all energies. Then, dependency between the mean energy and the standard deviation is rewritten as

\[ \sigma_k^g = \frac{\text{Resolution}}{2.35 \mu_k^g} \]  

(3-37)

Therefore, the Gaussian distribution is redefined as

\[ g(y|\Theta_k) = g(y|\mu_k) = \frac{1}{\sqrt{2\pi \sigma_k^2}} \exp \left\{ - \frac{1}{2 \sigma_k^2} \sum_{i=1}^{N} (y_i - \mu_k)^2 \right\} 
= \frac{1}{\sqrt{2\pi} \frac{\text{Resolution}}{2.35 \mu_k}} \exp \left\{ - \frac{1}{2 \left( \frac{\text{Resolution}}{2.35 \mu_k} \right)^2} \sum_{i=1}^{N} (y_i - \mu_k)^2 \right\} \]  

(3-38)

If we rewrite Eq. 3-25 using the above Gaussian distribution, and maximize it with respect to \( \mu_k \), then we obtain

\[ \mu_k^{g+1} = \frac{- \sum_{i=1}^{N} x_i p + \sqrt{\left( \sum_{i=1}^{N} x_i p \right)^2 + 4 R^2 \sum_{i=1}^{N} p \sum_{i=1}^{N} x_i^2 p}}{2 R \mu_k^g \sum_{i=1}^{N} p} \]  

(3-39)

where \( p = p_k(k|x_i, \mu_k^g) \)
Figure 3-1. How statistical methods define source data and measured data and how MLE and EM estimate parameters given a source data.
Figure 3-2. Spectra before and after it is deconvolved: a) Spectrum which is mixed with the Gaussian distribution. b) Components of the spectrum after it is deconvolved.
Figure 3-3. Descriptions of how the DIM-GMM works. The complex sample spectrum is deconvolved by the DIM and becomes the mixture of the Gaussian peak in the upper figure. In the lower figure, the preprocessed spectrum is separated by the GMM algorithm.
CHAPTER 4  
RESULTS

Two types of sample spectra were generated by MCNP5 simulations and experiments. They were employed for demonstrating performance of deconvolution algorithms, the MLEM algorithm [APPENDIX E], the DIM, and the DIM-GMM [APPENDIX F]. The detection system for demonstration was composed of a BGO detector of 2x2 inch crystal size and a source. The detector and the source were positioned 15 cm away from each other. Three sources, $^{54}$Mn, $^{22}$Na, and $^{137}$Cs, with activity of 1.0 $\mu$Ci were considered. The sources used in the experiment were encapsulated in the plastic-sealed disk of 2 cm diameter. The encapsulated source contains a small spot in epoxy in the center of the hole. The actual area of the spot is not well defined, but can be 2–4 mm in diameter depending on how the liquid wicks during pipetting. However, the source was treated as a point source in the MCNP5 since the source area is small. In the experiment, the BGO detector was connected with the standard NIMs (Nuclear Instrumentation Modules) [41], and the data was collected for each sample for 180 minutes which is regarded as to be enough time to achieve good statistics. The collected data was normalized by the total number of photons emitted from a radioactive source for a given time in order to compare the deconvolution effect of the MCNP5 prediction and the experimentally obtained spectrum.

Three different sources were considered: source 1 is $^{54}$Mn which includes one gamma line (834.8 keV), source 2 is $^{22}$Na which consists of two gamma lines (511 keV and 1274.5 keV), and source 3 is mixed with three sources $^{54}$Mn, $^{22}$Na, and $^{137}$Cs, which emit one x-ray (32.2 keV) and four gamma lines (511 keV, 661.6 keV, 834.8 keV and 1274.5 keV).

Spectra 1, 2 and 3 were generated orderly from each source using the MCNP5 simulation, and spectra 4, 5, and 6 were produced from the experiment over the same sources as shown in Figures 4-1 to 4-3, and Figures 4-7, 4-8, and 4-10 respectively. Through deconvolution of these
spectra, three most important performances of deconvolution methods were examined separately: i) recovery of the original source intensity, ii) peak searching (source identification), and iii) peak separation.

For deconvolutions of spectra 1 and 2 (or spectra 4 and 5 in the experiment) which have one single photopeak and two separated photopeaks, respectively, the MLEM and the DIM were employed in order to verify their ability of the source intensity recovery and the peak searching. Note that the accuracy of the DIM-GMM strongly depends on the recovery ability of the DIM for the source intensity. The DIM-GMM was not performed since peaks of these spectra were not closely packed so as to require for the peak separation. Accordingly, peak separation ability of the deconvolution methods used was not discussed on spectra 1 and 2.

Spectrum 3 (or spectrum 6 in the experiment) is of a rather complicated shape which includes the overlapped peak. The DIM is inappropriate for deconvolution of that spectrum due to its limit of peak separation. Therefore, in order to use the high ability of the DIM in the source intensity restoration for deconvolution of spectrum 3, one more step, the GMM (Gaussian mixture model), was introduced which is able to separate the overlapped peaks. The deconvolution effects were assessed by comparison of two methods, the MLEM and the DIM-GMM.

**Deconvolution of the Sample Spectrum Obtained from the MCNP Simulation**

**Comparison of the Deconvolution Effect of the MLEM and the DIM (sources 1 and 2)**

As depicted in Figures 4-1 and 4-2, the Compton backgrounds were remarkably removed by both algorithms, the DIM and the MLEM. This means that the two algorithms improve the signal to noise ratio. In terms of ability to recover the source intensity, both methods recovered the radiation strength of the MCNP5-simulated sample spectra within 1 % of the true value for spectrum 1. Unfolding of spectrum 2 shows the similar results as that of spectrum 1 even if a
slight increase of the relative error was observed. Table 4-1 compares true and estimated values by deconvolution.

Regarding the detector resolution, the MLEM method shows even a better energy resolution than the actual BGO detector. For example, the resolution of the BGO detector used is 11.6 % at 834.8 keV, while the MLEM leads to a significant reduction in resolution up to 2.3 % at 834.8 keV of spectrum 1. The DIM does not exhibit any discrepancy of the resolution between before and after the simulation. This inefficiency of the DIM in improvement of the energy resolution was anticipated because of its intrinsic problem that the spectrum contains the energy broadening after deconvolution. However, such a drawback is not an issue for the convolved spectrum consisting of separated peaks since the DIM successfully removes background effects such as Compton scattering, which distorted the original source spectrum, and the source intensity can be calculated by the simple integration of a peak area in Figures 4-1 and 4-2.

Comparison of the Deconvolution Effect of the MLEM and the DIM-GMM (source 3)

Over the complex spectrum 3 resulting from source 3 of more gamma lines, the deconvolution ability of the MLEM method declines compared to the case of spectra 1 and 2. A couple of small noise peaks which were not found in deconvolving spectra 1 and 2 are observed around the low energy region (~100 keV) of the reconstructed spectrum in Figure 4-3. Table 4-2 indicates the relative errors of the reconstructed source intensity considerably increase for the all peaks. The best source restoration of spectrum 3 (7.7 % relative error) occurs at the peak of 1274.5 keV which is positioned away from the overlapped peaks. It implies that the deconvolution of the MLEM method works better on the separable photopeaks than the closely packed photopeaks. There is no large variation in energy broadening for the deconvolved spectrum 3. The energy resolution, however, becomes a little bit lower than in the deconvolution of spectra 1 and 2 (2.3 % at 834.8 keV for the deconvolved spectrum 1, but 2.5 % at 834 keV for
the deconvolved spectrum 3). The MLEM method shows a good performance on the peak searching. It identifies all the peaks within 1~2 keV.

On the other hand, the DIM-GMM exhibits a better performance for unfolding of the spectrum 3 than the MLEM as shown at Table 4-2. The reconstructed source intensity is in a good agreement with the true value, within 1.3 % of the relative error. Those values are similar to what were obtained in deconvolution of spectra 1 and 2 which are the relatively simpler spectra.

It is important to note that, as shown in Figures 4-5 and 4-6, the DIM-GMM did not produce noise peaks which were found in the low energy regions in the MLEM deconvolution approach. Each full energy peak position coincides with the characteristic energy of the sources with uncertainties of ~1 keV.

**Deconvolution of the sample spectrum obtained from experiments**

**Comparison of the Deconvolution Effect of the MLEM and the DIM (sources 1 and 2)**

Unlike the case of the MCNP5-simulated sample spectrum, the experimentally generated sample spectra show undesired peaks in the low energy region in Figures 4-7a and 4-8a. This discrepancy arises from the backscattering effect which was not considered in the response function generation. A backscattering peak remains in both folded spectra after the deconvolving process and several small spurious peaks are observed in the spectra deconvolved by the MLEM (Figures 4-7b and 4-8b).

The recovery of the source intensity of the measured sample spectrum significantly deteriorates compared to the deconvolution of the MCNP5-simulated sample spectrum. Especially, the spectrum 5 of two photopeaks exhibits the worse performance than spectrum 4 of one single photopeak. As shown in Table 4-3, this undesirable effect is much higher on the photopeak closer to the energy region of backscatter regardless of the deconvolution algorithm
used. For example, the relative error of the recovered source intensity for spectrum 5 increases to ~30% at the gamma line 551 keV. The magnitude of relative error is almost twice as high as that of the gamma line 1274.5 keV.

The two main reasons for a large relative error is inconsistency of the measured sample data and the MCNP5-simulated sample data, and the backscatter effect. As shown in Figure 4-9, two peaks (551 keV and 1274.5 keV) of the measured spectrum for the $^{22}$Na source are slightly larger than those of the MCNP5-simulated spectrum while the measured spectrum for the $^{54}$Mn source is in a good agreement with the MCNP5-simulation spectrum. One of the reasons that the experimental result is higher than expectation, might be related to uncertainty of the activity of the source (1±20% $\mu$Ci). Consequently, this discrepancy was reflected on the deconvolved spectrum during the deconvolution process.

The other reason is the backscatter effect. Even though the backscatter effect does not directly influence the deconvolution of the measured photopeak, it is apparently attributed to the poor recovery of photopeaks of interest. For the 834.8 keV peak of Mn-54 source and the 1274.5 keV of the $^{22}$Na source, backscatter does not contribute to the intensity of those peaks. However, backscatter has a significant effect on the intensity of 551 keV of the $^{22}$Na source. In other words, the measured 551 keV peak of the $^{22}$Na source contains contribution resulting from backscatter before deconvolution. Therefore, that increment due to backscatter is transferred to the intensity of the recovered 551 keV through the deconvolution process. Table 4-3 supports this theory. The relative error of the deconvolved 551 keV peak positioned around the backscatter energy region is two times higher than that of the deconvolved 1274.5 keV peak whose measured sample spectrum does not include the backscatter effect even though two peaks originate from the same source, $^{22}$Na.
Because of this reason, it is important to treat the backscatter effect in generation of the response function. The deconvolution ability of the MLEM and the DIM is not directly associated with the backscatter effect, but they cannot recover the true intensity of the measured spectrum when the measured spectrum includes multi peaks: that is, when the full energy peaks of the measure spectrum are located around the backscatter energy region. Therefore, in order to prevent worsening the recovery performance of the measured spectrum due to the backscatter, the response function is required to be constructed by considering the backscatter effect.

Consequently, backscatter was not removed by both of two deconvolution methods, and the MLEM created the unpredicted spurious peaks in the low energy as illustrated in Figures 4-8b and 4-9b. The deconvolved photopeaks of $^{22}$Na produced a large relative error in the peak intensity since the measured photopeak was intrinsically contaminated by backscatter. On the other hands the recovery of $^{54}$Mn in which the intensity of the photopeak is not involved in backscatter shows a good agreement between the deconvolved peak intensity and the expected true value.

**Comparison of the Deconvolution Effect of the MLEM and the DIM-GMM (source 3)**

In deconvolving spectrum 6, the MLEM produces several unexpected peaks around the backscatter energy region, which were not found in the spectrum deconvolved from the MCNP5-simulated sample spectrum. Those spurious peaks increases both in size, and in number compared to deconvolution of spectra 1 and 2 in Figure 4-11. It implies that the unfolded spectrum may develop into the more unpredictable form if the original source consists of more complex gamma lines.

It is worth nothing that the MLEM is not able to resolve the backscatter effect, and makes some undesired spurious peaks, but nevertheless its source intensity recovery over the
experimentally generated sample spectrum does not show a large discrepancy compared to the MCNP5-simulated sample spectrum (Tables 4-2 and 4-4).

As the first process of the DIM-GMM, the DIM was performed for recovery of the source intensity of spectrum 6. The recovered spectrum was obtained in Figure 4-12. However, the GMM failed to separate the recovered spectrum by the DIM. This is due to the fundamental principle of the GMM which is based on the assumption that the spectrum should be a mixture of the Gaussian peak.

The deconvolved spectrum obtained from the first process is convoluted with five Gaussian-shape peaks except for backscatter whose shape cannot be defined. Therefore, the GMM was expected to be able to separate at least the Gaussian-shape peaks within the relative error similar to that of the MLE. The outcome, however, was not good. It indicates the GMM is very sensitive to the peak shape.
Table 4-1. Comparison of deconvolution results of the MLEM and the DIM over the sample spectra which are obtained from MCNP5-simulations for two different sources, source 1 ($^{54}$Mn) and source 2 ($^{22}$Na) respectively

<table>
<thead>
<tr>
<th>MCNP5 Simulated</th>
<th>Source 1 ($^{54}$Mn)</th>
<th>Source 2 ($^{22}$Na)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak area (peak strength) of deconvoluted spectrum</td>
<td>834.8 (keV)</td>
<td>511 (keV)</td>
</tr>
<tr>
<td>True value</td>
<td>0.999</td>
<td>0.643</td>
</tr>
<tr>
<td>DIM</td>
<td>0.997 (0.2 %)*</td>
<td>0.642 (0.2 %)</td>
</tr>
<tr>
<td>MLEM</td>
<td>0.994 (0.5 %)</td>
<td>0.641 (0.3 %)</td>
</tr>
</tbody>
</table>

*Figures in the parenthesis indicate the relative error of the reconstructed source peak.

Table 4-2. Comparison of deconvolution results of the MLEM and the DIM-GMM over the sample spectra which are obtained from MCNP5-simulations for a source mixing with $^{54}$Mn, $^{22}$Na, and $^{137}$Cs (Source 3)

<table>
<thead>
<tr>
<th>MCNP5 Simulated</th>
<th>Peak area (peak strength) of deconvoluted spectrum (Source 3)</th>
<th>Peak position</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak area</td>
<td>511</td>
<td>661.6</td>
</tr>
<tr>
<td>True value</td>
<td>0.396</td>
<td>0.274</td>
</tr>
<tr>
<td>MLEM</td>
<td>0.451 (13.9%)*</td>
<td>0.304 (11.1%)</td>
</tr>
<tr>
<td>DIM &amp; GMM</td>
<td>0.396 (0.1%)</td>
<td>0.278 (1.3%)</td>
</tr>
</tbody>
</table>

*Figures in the parenthesis indicate the relative error of the reconstructed source peak.
Table 4-3. Comparison of deconvolution results of the MLEM and the DIM over the sample spectra which are obtained from experiments for two different sources, source 1 (\textsuperscript{54}Mn) and source 2 (\textsuperscript{22}Na) respectively

<table>
<thead>
<tr>
<th>Experimentally obtained</th>
<th>Source 1 (\textsuperscript{54}Mn)</th>
<th>Source 2 (\textsuperscript{22}Na)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peak area (peak strength) of deconvoluted spectrum</td>
<td>834.8 (keV)</td>
<td>511 (keV)</td>
</tr>
<tr>
<td>True value</td>
<td>0.999</td>
<td>0.643</td>
</tr>
<tr>
<td>DIM</td>
<td>1.015 (1.6 %)*</td>
<td>0.841 (30.8 %)</td>
</tr>
<tr>
<td>MLEM</td>
<td>1.009 (1.0 %)</td>
<td>0.833 (29.5 %)</td>
</tr>
</tbody>
</table>

*Figures in the parenthesis indicate the relative error of the reconstructed source peak.

Table 4-4. Comparison of deconvolution results of the MLEM and the DIM-GMM over the sample spectra which are obtained from experiments for a source mixing with \textsuperscript{54}Mn, \textsuperscript{22}Na, and \textsuperscript{137}Cs (Source 3)

<table>
<thead>
<tr>
<th>Experimentally obtained</th>
<th>Peak area (peak strength) of deconvoluted spectrum (Source 3)</th>
<th>Peak position</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Peak area</td>
<td>Peak position</td>
</tr>
<tr>
<td>511</td>
<td>661.6</td>
<td>834.8</td>
</tr>
<tr>
<td>True value</td>
<td>0.396</td>
<td>0.274</td>
</tr>
<tr>
<td>MLEM</td>
<td>0.442</td>
<td>0.252</td>
</tr>
<tr>
<td>(11.7 %)</td>
<td>(8.0 %)*</td>
<td>(1.4 %)</td>
</tr>
<tr>
<td>DIM &amp; GMM</td>
<td>N/A</td>
<td>N/A</td>
</tr>
</tbody>
</table>

*Figures in the parenthesis indicate the relative error of the reconstructed source peak.
Figure 4-1. Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the MCNP5-simulated sample spectrum on source set 1, $^{54}$Mn

Figure 4-2. Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the MCNP5-simulated sample spectrum on source set 2, $^{22}$Na
Spectrum 3
MCNP5-simulated spectrum
Source 3: (Mn-54, Cs-137, Na-22)
(\(\gamma = 511, 661.6, 834.8, 1274.5\) keV)

Figure 4-3. The MCNP5-simulated sample spectrum for a mixture of \(^{54}\)Mn, \(^{22}\)Na, \(^{137}\)Cs on source set 3

Deconvoluted spectrum by the MLEM

Figure 4-4. Unfolding spectrum of source set 3 for the MCNP5-simulated sample spectrum by the MLEM algorithm
Figure 4-5. Unfolding spectrum of the MCNP5-simulated sample by the DIM on source set 3

Figure 4-6. The GMM separates the unfolding spectrum obtained by the DIM at Figure 4-5
Figure 4-7. Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the experimentally generated spectrum on source set 1, $^{54}$Mn

Figure 4-8. Comparison of unfolding ability of two algorithms (the MLEM and the DIM) for the experimentally generated spectrum on source set 2, $^{22}$Na
Figure 4-9. Comparison of the MCNP5 and measured sample spectra for $^{22}$Na and $^{54}$Mn sources: Two spectra are in a good agreement for $^{54}$Mn but the measured sample spectrum is a little bit larger than the MCNP5 simulated sample spectra for $^{22}$Na. Especially, this phenomenon is larger for 551 keV peak due to backscatter.
Figure 4-10. Experimentally generated sample spectrum for a mixture of $^{54}$Mn, $^{22}$Na, $^{137}$Cs on source set 3

Figure 4-11. Unfolding spectrum of source set 3 for the experimentally generated sample spectrum by the MLEM algorithm

Figure 4-12. Unfolding spectrum of the experimentally generated sample spectrum by the DIM on source set 3
CHAPTER 5
DISCUSSION

The in-depth study for deconvolution of the low energy gamma spectrum (< 5 MeV) has been presented on the basis of the following three steps:

- A profound understanding of the detector sensitivity: the measured spectrum reflects physical features of a detector as well as information of the incident gamma rays. The simulation code should implement such a detailed physical phenomenon. It is a very fundamental task for the spectral deconvolution. The MCNP5 code was verified for its feasibility of the spectral analysis.

- Construction of the detector response function for modeling: all the deconvolution algorithms depend on the response function. Therefore, generation of the correct detector response function is the crucial factor to regulate performance of the deconvolution methods. Regarding the response function, another important factor is to accumulate various detector response functions because the detector response function varies according to detection system conditions such as the incident gamma energy and geometry as well as the detector crystal property. However, it takes a lot of time and effort to construct the response function corresponding to all the detection environments. To overcome this difficulty, the most effective technique is to generate the response functions for several selected detection conditions, and then obtain other responses via interpolation.

- Development of the deconvolution tool: due to the intrinsic ill-posedness of deconvolution problems, there is no deconvolution method which is able to extract the exact solution. Therefore, the deconvolution technique inevitably looks for the approximate solution. The main issue is how to generate a stable and unique solution. The statistical method for
deconvolution treats this problem efficiently in spite of its slow convergence. The MLEM method and the newly developed method “DIM-GMM” have been discussed.

**Response Function**

The response function plays a key role in deconvolution of the gamma spectrum. Therefore, many researches have been performed on construction of the response function over years. The experimental methods and the semi-empirical methods, which were most widely used, have experimental difficulties and inefficiency of use, but they have advantage in that the response function can be generated without a deep understanding of the complicated physics in the detector since these methods employ the interpolation and the analytic function for generation of the response function on the basis of the mono-energetic photon spectrum obtained from experiments.

By contrast, the Monte-Carlo simulated method such as the MCNP5 obviates those problems that two methods encounter. In order to reproduce the true response, the MCNP5 should be able to simulate all physical features of the photon interaction in the detector. MCNP5 does not give a detailed description on some physics such as the exponential tail and flat continuum due to imperfection of the crystal or electron leakages [43], asymmetry of the full energy peaks due to the non-linearity of the detector response [75], and other effects (dead time, temperature sensitivity, etc) [76]. Moreover, energy resolution, one of the biggest characteristics on the detector, is not treated in the MCNP5.

Nevertheless, the MCNP5 prediction was in a good agreement with the experimental results as shown in Figures 2-13 to 2-18. Such a result can be explained by two facts: first, minor features of the detector response mentioned above have a relatively small effect on peak intensity and peak position of interest. Secondly, the energy broadening is constructed using the
experimental data. In other words, the energy broadening effect is determined by the experiment rather than the MCNP5 simulation, and the response features, which are not simulated, are offset by the energy broadening effect. This is why the simulation results have shown a good agreement with the experimental results even if the MCNP5 did not model some physical features of a detector.

It is worth noting that only one issue, i.e. loss of a count due to the dead time, is not still accounted for. As shown in Figure 2-16, the peak amplitude is slightly higher in the MCNP5 simulation of $^{60}$Co source than the experimental result unlike other modeling of $^{137}$Cs source where the experimental result is in a good agreement with the MCNP5 simulation. This discrepancy is regarded as coming from a loss of a signal due to the sum peak of 1173.2 keV and 1332.5 keV which is not treated in MCNP5 simulation.

The MCNP5-based simulation exhibits a good performance for generation of the response function. However, it does not guarantee that the desirable solution can be obtained when the response function is applied to the spectral deconvolution. This is because the MCNP5 generated response function is an approximate value even though it is very similar to the true response function. Note that even a small discrepancy can lead to unphysical results in the deconvolution process because the response function matrix is ill-posed.

In the current study, two deconvolution algorithms, MLEM and DIM-GMM, reproduced the source intensity within a low relative error of the true value in Tables 4-1 to 4-4. Failure of the GMM to separate the overlapped peaks in the experimentally obtained source spectrum is not due to the response function, but to the mechanism of the GMM. The unexpected spurious peaks were also found in the deconvolved spectra (Figures 4-7b, 4-8b and 4-11), which was deconvolved by the MLEM. It is unclear whether those peaks are associated with inaccuracy of
the MCNP5 generated response function or the deconvolution methodology applied. Regarding that the DIM did not produce the spurious peaks in the folded spectrum (Figure 4-12), the spurious peaks seem to be related to the MLEM rather than the inaccuracy of the MCNP5 generated response function.

There are some factors that the MCNP5 simulation did not treat in producing the response function: the minor physical effects in the detector, background radiation, and backscatter. The former hardly makes an impact on the spectral deconvolution. However, the effect of backscatter becomes fairly obvious in the low energy region. Backscatter will not have a direct effect on the spectral deconvolution, but could distort the intensity of the full energy peaks around the backscattering energy region in the measurement. As a result, it causes the poor recovery of the measured spectrum. Therefore, without proper treatment of backscatter in the generation of the response function matrix, it could be a very serious problem in deconvolving the measured spectrum. This adverse effect was already witnessed in the MELM and the GMM. Therefore, it is more significant in two methods to develop the response function algorithm which can deal with Compton backscatter rather than to try to construct an accurate response function.

**Deconvolution Methods**

The MLEM exhibits a very good deconvolution ability for the MCNP5 simulated spectra 1 and 2 which do not include backscatter and overlapped peaks. When the MLEM was performed on the MCNP5 simulated spectrum 3 which include the overlapped peaks, it was very effective in peak searching and peak separation, but it presented a relatively poor result for the recovery of the source intensity. And also, several spurious peaks were observed around in the low energy region.

The DIM-GMM is combined of advantages of two algorithms, the DIM (Direct Inverse Method) and the GMM (Gaussian Mixture Method): the DIM provides a simple and effective
way to recover the source intensity, and the GMM a resolving power to separate the overlapped peaks. The DIM-GMM decomposes the response function matrix into two other matrices, one of which is well-posed. The well-posed matrix can be directly solved by the simple inverse method. Therefore, the biggest advantage of the DIM is that its solution is not artificially distorted but physically understandable unlike a solution of the MLEM which may cause the spurious peaks. The DIM eliminates all phenomena occurring in a detector except for the photoelectric absorption, such as Compton scattering, x-ray escape, and single and double escape peaks which attribute to the spectrum backgrounds. And then, it recovers information about photons including backscatter before entering the detector. As described at section 4-3-2 (Figure 4-11), the DIM can remove the backgrounds mentioned above from even a complicated spectrum which is convolved of backscatter and overlapped spectra.

Its drawback is that it is not able to resolve the energy broadened spectrum. In the DIM-GMM, this problem is solved using the GMM which is a technique to separate the overlapped spectrum on the assumption that the unfolded spectrum is convolved with Gaussian peaks. This method is very effective to resolve a spectrum of a mix of Gaussian peaks. The most significant issue of the GMM is how to improve the slow convergence due to the computational complexity, and how to determine the initial guessing with regard to the local maximum. Especially, determination of the initial value may be a critical problem when there are many peaks to be separated. For that reason, the initial value guessing should be carefully treated in deconvolution of a spectrum of a mixture of unknown sources.

As discussed in Chapter 4, the DIM-GMM gave an excellent accuracy of the spectral deconvolution (the relative error of the true value is less than 1 %) when the spectrum which was processed by the DIM was a mix of Gaussian peaks, i.e., it does not contain backscatter.
However, it had a difficulty dealing with the backscatter effect. Previously mentioned, the backscatter effect may contribute to the intensity of the photopeak in the measured spectrum. Such a phenomenon inevitably brings about the inaccuracy of the recovered peaks in the deconvolution process. Accordingly, for a successful deconvolution, the response function should be generated considering backscatter.
CHAPTER 6
CONCLUSION

All the general procedures necessary for extracting information from the measured gamma spectrum of a BGO detector and point-line radioisotope sources have been discussed with regard to the MCNP modeling and different deconvolution methods.

The MCNP5 code was employed to study the detector sensitivity. The code embodies the typical characteristics of the BGO detector except for backscatter which was not treated in this simulation. Even though we partially treated the exponential tail on the low energy side of the full energy peak which is a very interesting topic in many literatures, the simulation results are in good agreement with the experimental results. The modeling of the BGO detector exhibits a reasonable spectrum variation corresponding to four physical changes of the detector, i.e., crystal size, detector-to-source distance, window thickness and detector-source angle. The energy resolution was semi-empirically calculated through the analytical function since the MCNP5 does not present the transport of visible photons which are the main cause of the energy broadening. The artificially-added energy broadening effect shows a good correspondence with the experimental result. The energy broadening function of Eq. 2-7 was used to implement the energy broadening effect in the MCNP5 simulated spectrum. Coefficients of the energy broadening function was determined using three gamma energies, 81 keV, 661.2 keV, and 1274.5 keV coming from 81 keV, $^{133}$Ba, $^{137}$Cs, and $^{22}$Na respectively. However, for the exact estimation of the coefficients, more gamma ray sources should be selected in the gamma spectrum analysis which spans the wide energy range because there is no guarantee that the coefficients will fit the entire region [77]. Actually, in the energy region below the 50 keV a slight discrepancy was observed between the simulation result and the experimental result.
The detector response matrix was constructed which has a 1500 x 1500 dimension. Each matrix element corresponds to 1 keV. In fact, 1500 response functions are required for generating the 1500 x 1500 response function matrix. It would be an unimaginably tedious and laborious job. Thus, most of the response functions were produced using a linear numerical interpolation from 21 selected response functions. This is a very effective method to build many response functions.

The MLEM method exhibits a very good unfolding ability for the MCNP5 simulated spectra. The energy resolution is remarkably improved from ~14 % to 2 %. In the experimentally measured spectra, some artificial peaks were observed in the Compton backscattering region. The measured spectrum which was convolved with a variety of backgrounds reduces the detector resolution compared to the MCNP5 simulated spectrum. However, the overall performance of the MLEM is satisfactory.

The new deconvolution algorithm, so called the DIM-GMM, was developed, which combines advantages of the DIM and the GMM. The DIM-GMM was carried out with a series of two methods. First, the DIM filtered out the Compton background effectively and recovered the full energy peak of the source. It did not, however, exhibit good performance in unfolding of the measured spectrum for closely spaced full energy peaks due to the low resolution of the BGO detector. If the DIM is applied to a detector of high resolution such as the HPGe detector, it could yield a better result. Therefore, one more process is required for resolving the spectra obtained from the DIM. The overlapping peaks were unfolded using the GMM after deconvolution of the DIM.

The deconvolving power of the DIM-GMM is superior to the MLEM method for the MCNP5 simulated sample spectrum. However, it failed to separate peaks from the
experimentally measured sample spectrum because backscatter was not treated in constructing the response function. The reason that the DIM & GMM brought about the worse outcome for the experimentally measured sample spectrum than the MLEM is that the GMM is based on the assumption that the sample spectrum consist of many Gaussian peaks: that is, backscatter is not a Gaussian form of a peak.

The present study has demonstrated that the MCNP5 code is a very good tool to model characteristics of the BGO detector and to build the detector response function even though it did not model some detailed features of the BGO detector. The small discrepancy of the MCNP5 calculated response function from the true one did not make a noticeable impact on the spectral deconvolution. On the contrary, two deconvolution methods show that treatment of backscatter in the response function is more significant rather than accuracy of the calculated response function. The need for treatment of backscatter in the response function does not arise from a problem of the deconvolution method, but from distortion on the measured photopeak intensity due to backscatter.

The deconvolution result has proved that the MLEM and the DIM & GMM are very useful in deconvolution of the MCNP5 simulated spectrum which does not contain backscatter. The DIM-GMM gives a better performance. Such a result is due to the powerful recovery ability of the source information of the DIM, and the effective peak separation ability of the GMM. Of course, the backscatter effect should be well treated for the desirable deconvolution of the experimental data because it seriously degrades performance of the spectral deconvolution. Then, the DIM-GMM will provide a strong tool for unfolding of the spectrum.

In order to enhance the deconvolution ability of the DIM-GMM in various applications, more in-depth studies are required in the future with regards to its drawbacks already shown in
this research. First, development of an algorithm should be carried out, which is able to treat backscatter in construction of the detector response function. Secondly, the peak separating ability of the IDM-GMM should be studied for more complicated situations in which the measured spectrum includes more gamma peaks or overlapped peaks. Thirdly, an application method of the DIM-GMM to multi-sources or bulk source should be investigated because the gamma source is not a point source in real spectral applications such as NDA (Non-Destructive Analysis). Lastly, it is worth applying the DIM to the measured gamma spectrum obtained by the HPGe detector. The current study has shown that the DIM successfully recovers information of the original source except for energy broadening which is created by the BGO detector. Therefore, if the DIM is applied to the HPGe detector-measured spectrum whose energy resolution is very low, it could provide a simple and powerful tool for spectral deconvolution without using complicated algorithms.
APPENDIX A
MCNP CODE FOR THE BGO DETECTOR MODELING

In this Appendix, we provide sample MCNP5 input files for the $^{137}$Co placed at 5 cm away from a BGO detector of size 3"x3".

******************************************************************************

MODEL: 3.0"(diameter) X 3.0"(length) - Case 3
c
c MODELING OF THE BGO DETECTOR
c
c ---------------------- CELL CARDS ----------------------
1 1 -7.13 4 -5 -11 imp:e=1 imp:p=1 $ CRYSTAL
2 0 (3 -4 -12):(4 -5 11 -12) imp:e=1 imp:p=1 $ Between CRYSTAL AND WINDOW
3 2 -2.7 (2 -3 -13):(3 -5 12 -13) imp:e=1 imp:p=1 $ DETECTOR WINDOW
4 0 1 -2 -13 imp:e=1 imp:p=1 $ SRC CELL (ISOTROPIC DISK SRC)
5 0 -1: 5: 13 imp:e=0 imp:p=0 $ REST OF THE UNIVERSE

c ---------------------- SURFACE CARDS ----------------------
1 px -15.1 $ PLANE DELIMITING THE SOURCE REGION
2 px 0.0 $ PLANE DELIMITING THE FRONT OF THE DETECTOR
3 px 0.05 $ PLANE DELIMITING THE INSIDE OF THE DETECTOR WINDOW
4 px 0.25 $ PLANE DELIMITING THE FRONT OF THE CRYSTAL
5 px 7.87 $ PLANE DELIMITING THE BACK OF THE CRYSTAL
11 cx 3.81 $ RADIUS OF THE CRYSTAL (3.0" DIAMETER)
12 cx 4.01 $ RADIUS OF THE INSIDE OF THE DETECTOR WINDOW
13 cx 4.06 $ RADIUS OF THE DETECTOR

c ---------------------- DATA CARDS ----------------------
c SIMPLE GEOMETRY - MCNP5 CALCULATES THE VOLUMES
mode p e $ PHOTON/ELECTRON MODE
c
c ---------------------- SOURCE CARDS ----------------------
sdef erg=d1 pos -2.0 0 0 axs= 1 0 0 rad=d2 par 2 $ ISOTROPIC DISK SRC Co-60
si1 1 1.1732 1.3325
sp1 1.0 1.0
c
si2 0 0.15 $ Co-60 source radius
sp2 -21 1
c
c ---------------------- TALLY CARDS ----------------------
f4:p 1
fc4 Crystal total flux
f8:p 1
fc8 Pulse height in crystal volume (cell 1)
e8 0.0 1.0E-05 1.0E-04
0.001 0.002 0.003 0.004 0.005 0.006 0.007 0.008 0.009 0.01
0.011 0.012 0.013 0.014 0.015 0.016 0.017 0.018 0.019 0.02
0.021 0.022 0.023 0.024 0.025 0.026 0.027 0.028 0.029 0.03
0.031 0.032 0.033 0.034 0.035 0.036 0.037 0.038 0.039 0.04
0.041 0.042 0.043 0.044 0.045 0.046 0.047 0.048 0.049 0.05
0.051 0.052 0.053 0.054 0.055 0.056 0.057 0.058 0.059 0.06
0.061 0.062 0.063 0.064 0.065 0.066 0.067 0.068 0.069 0.07
0.071 0.072 0.073 0.074 0.075 0.076 0.077 0.078 0.079 0.08
0.081 0.082 0.083 0.084 0.085 0.086 0.087 0.088 0.089 0.09
0.091 0.092 0.093 0.094 0.095 0.096 0.097 0.098 0.099 0.1

c
0.101 0.102 0.103 0.104 0.105 0.106 0.107 0.108 0.109 0.11
0.111 0.112 0.113 0.114 0.115 0.116 0.117 0.118 0.119 0.12
0.121 0.122 0.123 0.124 0.125 0.126 0.127 0.128 0.129 0.13
0.131 0.132 0.133 0.134 0.135 0.136 0.137 0.138 0.139 0.14
0.141 0.142 0.143 0.144 0.145 0.146 0.147 0.148 0.149 0.15
0.151 0.152 0.153 0.154 0.155 0.156 0.157 0.158 0.159 0.16
0.161 0.162 0.163 0.164 0.165 0.166 0.167 0.168 0.169 0.17
0.171 0.172 0.173 0.174 0.175 0.176 0.177 0.178 0.179 0.18
0.181 0.182 0.183 0.184 0.185 0.186 0.187 0.188 0.189 0.19
0.191 0.192 0.193 0.194 0.195 0.196 0.197 0.198 0.199 0.2

c
0.201 0.202 0.203 0.204 0.205 0.206 0.207 0.208 0.209 0.21
0.211 0.212 0.213 0.214 0.215 0.216 0.217 0.218 0.219 0.22
0.221 0.222 0.223 0.224 0.225 0.226 0.227 0.228 0.229 0.23
0.231 0.232 0.233 0.234 0.235 0.236 0.237 0.238 0.239 0.24
0.241 0.242 0.243 0.244 0.245 0.246 0.247 0.248 0.249 0.25
0.251 0.252 0.253 0.254 0.255 0.256 0.257 0.258 0.259 0.26
0.261 0.262 0.263 0.264 0.265 0.266 0.267 0.268 0.269 0.27
0.271 0.272 0.273 0.274 0.275 0.276 0.277 0.278 0.279 0.28
0.281 0.282 0.283 0.284 0.285 0.286 0.287 0.288 0.289 0.29
0.291 0.292 0.293 0.294 0.295 0.296 0.297 0.298 0.299 0.3

c
0.301 0.302 0.303 0.304 0.305 0.306 0.307 0.308 0.309 0.31
0.311 0.312 0.313 0.314 0.315 0.316 0.317 0.318 0.319 0.32
0.321 0.322 0.323 0.324 0.325 0.326 0.327 0.328 0.329 0.33
0.331 0.332 0.333 0.334 0.335 0.336 0.337 0.338 0.339 0.34
0.341 0.342 0.343 0.344 0.345 0.346 0.347 0.348 0.349 0.35
0.351 0.352 0.353 0.354 0.355 0.356 0.357 0.358 0.359 0.36
0.361 0.362 0.363 0.364 0.365 0.366 0.367 0.368 0.369 0.37
0.371 0.372 0.373 0.374 0.375 0.376 0.377 0.378 0.379 0.38
0.381 0.382 0.383 0.384 0.385 0.386 0.387 0.388 0.389 0.39
0.391 0.392 0.393 0.394 0.395 0.396 0.397 0.398 0.399 0.4

c
0.401 0.402 0.403 0.404 0.405 0.406 0.407 0.408 0.409 0.41

99
0.411 0.412 0.413 0.414 0.415 0.416 0.417 0.418 0.419 0.42
0.421 0.422 0.423 0.424 0.425 0.426 0.427 0.428 0.429 0.43
0.431 0.432 0.433 0.434 0.435 0.436 0.437 0.438 0.439 0.44
0.441 0.442 0.443 0.444 0.445 0.446 0.447 0.448 0.449 0.45
0.451 0.452 0.453 0.454 0.455 0.456 0.457 0.458 0.459 0.46
0.461 0.462 0.463 0.464 0.465 0.466 0.467 0.468 0.469 0.47
0.471 0.472 0.473 0.474 0.475 0.476 0.477 0.478 0.479 0.48
0.481 0.482 0.483 0.484 0.485 0.486 0.487 0.488 0.489 0.49
0.491 0.492 0.493 0.494 0.495 0.496 0.497 0.498 0.499 0.5

0.501 0.502 0.503 0.504 0.505 0.506 0.507 0.508 0.509 0.51
0.511 0.512 0.513 0.514 0.515 0.516 0.517 0.518 0.519 0.52
0.521 0.522 0.523 0.524 0.525 0.526 0.527 0.528 0.529 0.53
0.531 0.532 0.533 0.534 0.535 0.536 0.537 0.538 0.539 0.54
0.541 0.542 0.543 0.544 0.545 0.546 0.547 0.548 0.549 0.55
0.551 0.552 0.553 0.554 0.555 0.556 0.557 0.558 0.559 0.56
0.561 0.562 0.563 0.564 0.565 0.566 0.567 0.568 0.569 0.57
0.571 0.572 0.573 0.574 0.575 0.576 0.577 0.578 0.579 0.58
0.581 0.582 0.583 0.584 0.585 0.586 0.587 0.588 0.589 0.59
0.591 0.592 0.593 0.594 0.595 0.596 0.597 0.598 0.599 0.6

0.601 0.602 0.603 0.604 0.605 0.606 0.607 0.608 0.609 0.61
0.611 0.612 0.613 0.614 0.615 0.616 0.617 0.618 0.619 0.62
0.621 0.622 0.623 0.624 0.625 0.626 0.627 0.628 0.629 0.63
0.631 0.632 0.633 0.634 0.635 0.636 0.637 0.638 0.639 0.64
0.641 0.642 0.643 0.644 0.645 0.646 0.647 0.648 0.649 0.65
0.651 0.652 0.653 0.654 0.655 0.656 0.657 0.658 0.659 0.66
0.661 0.662 0.663 0.664 0.665 0.666 0.667 0.668 0.669 0.67
0.671 0.672 0.673 0.674 0.675 0.676 0.677 0.678 0.679 0.68
0.681 0.682 0.683 0.684 0.685 0.686 0.687 0.688 0.689 0.69
0.691 0.692 0.693 0.694 0.695 0.696 0.697 0.698 0.699 0.7

0.701 0.702 0.703 0.704 0.705 0.706 0.707 0.708 0.709 0.71
0.711 0.712 0.713 0.714 0.715 0.716 0.717 0.718 0.719 0.72
0.721 0.722 0.723 0.724 0.725 0.726 0.727 0.728 0.729 0.73
0.731 0.732 0.733 0.734 0.735 0.736 0.737 0.738 0.739 0.74
0.741 0.742 0.743 0.744 0.745 0.746 0.747 0.748 0.749 0.75
0.751 0.752 0.753 0.754 0.755 0.756 0.757 0.758 0.759 0.76
0.761 0.762 0.763 0.764 0.765 0.766 0.767 0.768 0.769 0.77
0.771 0.772 0.773 0.774 0.775 0.776 0.777 0.778 0.779 0.78
0.781 0.782 0.783 0.784 0.785 0.786 0.787 0.788 0.789 0.79
0.791 0.792 0.793 0.794 0.795 0.796 0.797 0.798 0.799 0.8

0.801 0.802 0.803 0.804 0.805 0.806 0.807 0.808 0.809 0.81
0.811 0.812 0.813 0.814 0.815 0.816 0.817 0.818 0.819 0.82
0.821 0.822 0.823 0.824 0.825 0.826 0.827 0.828 0.829 0.83
1.251 1.252 1.253 1.254 1.255 1.256 1.257 1.258 1.259 1.26
1.261 1.262 1.263 1.264 1.265 1.266 1.267 1.268 1.269 1.27
1.271 1.272 1.273 1.274 1.275 1.276 1.277 1.278 1.279 1.28
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1.381 1.382 1.383 1.384 1.385 1.386 1.387 1.388 1.389 1.39
1.391 1.392 1.393 1.394 1.395 1.396 1.397 1.398 1.399 1.4
1.401 1.402 1.403 1.404 1.405 1.406 1.407 1.408 1.409 1.41
1.411 1.412 1.413 1.414 1.415 1.416 1.417 1.418 1.419 1.42
1.421 1.422 1.423 1.424 1.425 1.426 1.427 1.428 1.429 1.43
1.431 1.432 1.433 1.434 1.435 1.436 1.437 1.438 1.439 1.44
1.441 1.442 1.443 1.444 1.445 1.446 1.447 1.448 1.449 1.45
1.451 1.452 1.453 1.454 1.455 1.456 1.457 1.458 1.459 1.46
1.461 1.462 1.463 1.464 1.465 1.466 1.467 1.468 1.469 1.47
1.471 1.472 1.473 1.474 1.475 1.476 1.477 1.478 1.479 1.48
1.481 1.482 1.483 1.484 1.485 1.486 1.487 1.488 1.489 1.49
1.491 1.492 1.493 1.494 1.495 1.496 1.497 1.498 1.499 1.5

---

MATERIAL CARDS

MOST RECENT PHOTOATOMIC LIBRARY MCLIB04 IS USED

M1 = BGO CRYSTAL: Bi4-Ge3-O12

M2 = ALUMINUM HOUSING (DETECTOR WINDOW): Al

---

ENERGY CARDS

phys:p $ DEFAULT VALUES
phys:e $ DEFAULT VALUES

c --- CUTOFF CARDS

cut:p $ DEFAULT VALUE
cut:e $ DEFAULT VALUE

---

PERIPHERAL CARDS

print
prdmp 2j 115000000
APPENDIX B
C LANGUAGE CODE FOR ENERGY BROADENING EFFECT

In this Appendix, we provide a C-code for the energy broadening.

```c
#include <math.h>
#include <stdio.h>
#include <stdlib.h>

#define a 4.87125
#define b 2.87358
#define c 0.00026

main()
{
    FILE *out;
    char output[10] = "Res.txt";

    int i=0, j, k, Nfile, intx=0;
    int x=0, SourceE0, SourceE[1501]={0,}, energy, E, Eh, Eho, Eo[1501]={0,};

    float count, error;
    float peak[1501]={0.0,};
    float sum, gaus, gaus_n, Amp, P[1501]={0.0,};
    float FWHM = 0.0, s, h, s_peak;

    Nfile = 1501;

    if ((out = fopen(output, "wt")) == NULL)
    {
        fprintf(stderr, "Cannot open output file.\n");
        exit(0);
    }

    for(i=1; i < Nfile; i=i+1)
    {
        for (k=1; k<1501; k++)
        {
            SourceE[k] = k;
            P[k] = 0.0;
            peak[k] = 0.0;
        }

        for(energy=1; energy <1501; energy++)
        {
            Eo[energy] = energy;
            if (energy == i)
```
for (j=1 ; j <= (SourceE[i]) ; j++)
{
    FWHM = a + b*sqrt(Eo[j]+c*pow(Eo[j],2));
    s = FWHM/2.35;                                              // standard deviation
    E = Eo[j];
    gaus = 1;
    
    while (gaus > 0.0001)
    {
        gaus = exp(-pow(E-Eo[j],2)/(2*pow(s,2)));
        E = E + 1;
        Eho = E;
        Eh = E;
    }
    
    x=0;
    sum = 0.0;
    gaus_n = 0.0;
    Amp = 0.0;
    if (E > 1500)
        Eh = 1500;
    
    for ( x = (2*Eo[j]-E) ; x <= E; x=x+1)
    {
        Amp = peak[j]/sum;
        s_peak =0.0;
    }
    for ( x = (2*Eo[j]-Eho); x <= Eh; x=x+1)
    {
        if ( x >= 0)
        {
            intx = x;
            P[intx] = P[intx] + Amp*exp(-pow(x-Eo[j],2)/(2*pow(s,2)));
            s_peak = s_peak + Amp*exp(-pow(x-Eo[j],2)/(2*pow(s,2)));
        }
        }
    }
    fclose(out);
}
APPENDIX C

Linear interpolation of the response function

The first procedure for generating the response function determines energy intervals whose response functions are constructed using the MCNP5 simulation. In the present study, 100 keV was used as the energy interval in the range of 200 keV to 1500 keV. Then, a linear interpolation approach is used to obtain the response function for the energies in the selected energies.

Suppose that the response function of the 662 keV is obtained from the linear interpolation. Two response functions of 600 keV and 700 keV are selected as shown in Figures C-1a and C-2a. The response function of the low energy (600 keV) is scaled up and the response function of the high energy (700 keV) is scaled down. The reason for interpolating from two response functions is to estimate the average response function so as to minimize the error. For more exact interpolation, the energy scale is divided into two regions corresponding to physical characteristics of the response: Region 1 (Compton scattering region), and Region 2 (full photopeak region) as shown in Figures C-1 and C-2.

Let us start the interpolation with expanding the response function of 600 keV to that of the 662 keV. The scaling of the response function is done separately for Regions 1 and 2. The relation of the interpolated response function and the response function of the low energy is given by

\[ f_{1L-\text{int}}(E) = f_{1L} \left( \frac{E * E_{1L}}{E_{1\text{int}}} \right) \quad \text{for} \quad 0 < E < E_{1\text{int}} \quad \text{(C-1)} \]

where \( E_{1L} \) indicates the division point of the low energy in Region 1, and \( E_{1\text{int}} \) denotes the division point of the interpolated energy in this region. \( f_{1L-\text{int}}(E) \) is the interpolated response function obtained from the low energy in Region 1, and \( f_{1L} \left( \frac{E * E_{1L}}{E_{1\text{int}}} \right) \) is the response function of the low energy (600 keV) in Region 1 (Figure C-1).
The scaling of the response function in Region 2 is carried out following the same procedure as in Region 1.

\[
f^{2\text{L-int}}_L(E) = f^{2\text{L-int}}_L \left( E_{1\text{L}} + \frac{(E - E_{1\text{int}}) \times (E_{2\text{L}} - E_{1\text{L}})}{E_{2\text{int}} - E_{1\text{int}}} \right) \text{ for } E_{1\text{int}} < E < E_{2\text{int}} \quad \text{C-2)}
\]

Then, we compress the response function of the high energy (700 keV). The procedure of the scale-down of the response function is the same as that of the scale-up. Therefore, the response function of scale-up can be expressed as

\[
f^{1\text{H-int}}_H(E) = f^{1\text{H-int}}_H \left( \frac{E \times E_{1\text{H}}}{E_{1\text{int}}} \right) \text{ for } 0 < E < E_{1\text{int}} \quad \text{C-3)}
\]

\[
f^{2\text{H-int}}_H(E) = f^{2\text{H-int}}_H \left( E_{1\text{H}} + \frac{(E - E_{1\text{int}}) \times (E_{2\text{H}} - E_{1\text{H}})}{E_{2\text{int}} - E_{1\text{int}}} \right) \text{ for } E_{1\text{int}} < E < E_{2\text{int}} \quad \text{C-4)}
\]

Two response functions obtained from the interpolation is averaged over each region considering weighting factor.

\[
f_{\text{int}}^{1}(E) = \frac{(100 - k) \times f^{1\text{L-int}}_L(E) + k \times f^{1\text{H-int}}_H(E)}{100} \quad \text{C-5)}
\]

\[
f_{\text{int}}^{2}(E) = \frac{(100 - k) \times f^{2\text{L-int}}_L(E) + k \times f^{2\text{H-int}}_H(E)}{100} \quad \text{C-6)}
\]

where weighting factor is given as \( k = 662 - 600 = 62 \).
Figure C-1. Linear expansion of the response function of the low energy

Figure C-2. Linear compression of the response function of the low energy
APPENDIX D
MATLAB CODE FOR INTERPOLATION OF THE RESPONSE FUNCTION MATRIX

In this Appendix, we provide a C-code for the interpolation of the detector response matrix.

```c
#include <stdio.h>
#include <stdlib.h>
#define moC2 511

main()
{
    FILE *in1,*in2,*out[101];
    char Open1[15], Open2[15];
    int endpoint, zeroL, zeroH;
    int i=0, j=0, k=0, chn;
    float jj;
    float DL0, DL1, DL2, DH0, DH1, DH2, flux=0.0;
    float gL[1501]={0.0,}, gH[1501]={0.0,};
    int peakL0, peakL1, peakL2, peakL3, peakL4, peakL5, peakL6, peakL7;
    int peakH0, peakH1, peakH2, peakH3, peakH4, peakH5, peakH6, peakH7;
    int lpeak0, lpeak5;
    int AL, BL, AH, BH, AI, BI;
    float EL[101][1501]={0,}, EH[101][1501]={0,}, E[101][1501]={0,};
    char Oput[101][5]=
    printf (" Type the 1st Source file name:");
    scanf("%s",Open1);
    printf (" Type the 2nd Source file name:");
    scanf("%s",Open2);
    
    
    
    };
```
printf (" Type the 1st Source energy:");
scanf("%d", &peakL0);

printf (" Type the 2nd Source energy:");
scanf("%d", &peakH0);

if ((in1 = fopen(Open1, "rt")) == NULL)  
{  
    fprintf(stderr, "Cannot open input file.
");  
    exit(0);  
}

if ((in2 = fopen(Open2, "rt")) == NULL)  
{  
    fprintf(stderr, "Cannot open output file.
");  
    exit(0);  
}

for (i=0; i < 101; i++)  
{  
    if ((out[i] = fopen(Oput[i], "wt")) == NULL)  
    {  
        fprintf(stderr, "Cannot open output file.
");  
        exit(0);  
    }  
}

i = 0;

while(!feof(in1))  // (!feof(in))  
{  
    fscanf(in1, "%f %g %f\n", &DL0, &DL1, &DL2);

    if (i >= 3)  
    {  
        gL[i-2] = DL1;  
    }  
    i = i+1;  
}  //while

i=0;

while(!feof(in2))  
{  
    fscanf(in2, "%f %g %f\n", &DH0, &DH1, &DH2);

    if (i>=3)  
    {  
        
    }
gH[i-2] = DH1;
}
i = i+1;
}

zeroH = 1 + peakH0;
peakL1 = peakL0 - 75;
peakL2 = peakL0 - 77;
peakL3 = peakL0 - 87;
peakL4 = peakL0 - 90;
peakL5 = (int) (2.0*peakL0*peakL0/(moC2 + 2*peakL0) + 0.51);
peakL6 = peakL0 - 511;
peakL7 = peakL0 - 1022;

peakH1 = peakH0 - 75;
peakH2 = peakH0 - 77;
peakH3 = peakH0 - 87;
peakH4 = peakH0 - 90;
peakH5 = (int) (2.0*peakH0*peakH0/(moC2 + 2*peakH0) + 0.51);
peakH6 = peakH0 - 511;
peakH7 = peakH0 - 1022;

AL = peakL0 - 92;
BL = peakL0;
AH = peakH0 - 92;
BH = peakH0;

/*******************************************************************************/
for(k=0;k<101;k++)
{
    Ipeak0 = peakL0 + k;
    Ipeak5 = (int) (2.0*Ipeak0*Ipeak0/(moC2 + 2*Ipeak0) + 0.51);
    AI = Ipeak0 - 92;
    BI = Ipeak0;

    for(chn=1; chn <= AI; chn++)
    {
        EL[k][chn] = gL[(int)(chn*AL/AI+0.5)];
    }

    for(chn= AI; chn <= BI; chn++)
    {
        EL[k][chn] = gL[AL + (int)((chn-AI)*(peakL0-AL)/(Ipeak0-AI)+ 0.5)];
    }
}
for(chn=1; chn <= AI; chn++)
{
    EH[k][chn] = gH[(int)(chn*AH/AI + 0.5)];
}

for(chn=AI; chn <= BI; chn++)
{
    EH[k][chn] = gH[AH + (int)((chn-AI)*(peakH0-AH)/(Ipeak0-AI) +0.5) ];
}

for(chn=1; chn <= BI; chn++)
{
    E[k][chn] = ((100-k)*EL[k][chn] + k*EH[k][chn])/100;
}

for (i=0; i<101; i++)
{
    for(chn=1; chn <= BI; chn++)
    {
        fprintf( out[i], "%d %g\n", chn, E[i][chn]);
    }
}
fclose(in1);
fclose(in2);

for (i=0; i<101; i++)
{
    fclose(out[i]);
}
In this Appendix, we provide a Matlab code for the deconvolution of the measured spectrum using the MLEM algorithm.

clear all;

in1 = fopen('Rmatrix-R00','r');
in2 = fopen('RMn.txt','r');
in3 = fopen('Initial10-7.txt','r');

out1 = fopen('ML-MP-YB-Mn-result.txt','w');

e=1.0;

A1=fscanf(in1,'%g %g %g %g \n', [1500 inf]);
A2=fscanf(in2,'%d %g \n', [2 inf]);
A3=fscanf(in3,'%d %g \n', [2 inf]);

MS =zeros(1500,2);
initS =zeros(1500,1);
convergeS =zeros(1,1500);
NewS = zeros(1500,1);
P = zeros(1500,1);
iNo = zeros(1500,1);
e = zeros(1500,1);
correction =zeros(1500,1);

for (i=1:1500)
    MS(i) = A2(2,i);
    initS(i) = A3(2,i);
end

correction = zeros(1500,1);

for b=1:1500
    for d=1:1500
        P(b) = P(b) + A1(d,b);
    end
end

ee=1.0;
eiNo=50;
while (ee > 0.0001 & eiNo < 500)
    correction = zeros(1500,1);
for (d=10:1500)
dmean =0.0;
for(b=10:1500)
dmean = dmean + initS(b)*A1(d,b);
end

if (dmean ~= 0.0)
  for (k=10:1500)
    correction(k) = correction(k) + MS(d)*A1(d,k)/dmean;
  end
end

for (k=10:1500)
  NewS(k) = (initS(k)/P(k))*correction(k);
  if k==1170
    dd = NewS(k,1);
  end
  if initS(k) > 0.0
    diff = NewS(k) - initS(k);
    if diff > 0
      e(k) = diff/initS(k);
    else
      e(k) = 0.0;
    else
      e(k) = 0.0;
    end
    initS(k) = NewS(k);
    kk = initS(k);
    iNo(k)= iNo(k)+1;
  end
  eiNo = max(iNo(1:1500));
  ee = max(e(1:1500));
end

for (i=1:1500)
  convergeS(1,i)= initS(i);
end

fprintf(out1,'%g \n', convergeS);
fclose(in1);
fclose(in2);
fclose(in3);
fclose(out1);
APPENDIX F
C LANGUAGE CODE FOR THE SPECTRAL DECONVOLUTION USING THE GMM

In this Appendix, we provide a C-code for the peak separation using the GMM.

```
#include <math.h>
#include <stdio.h>
#include <stdlib.h>
#include "Gaussian.c"

#define c1 4.87125
#define c2 2.87358
#define c3 0.00026
#define N 1500

main()
{
    FILE *in,*out, *out1;
    char Open[30],Oput[30], oput1[20];

    int x=0, NoP, i=0, j=0, K=0, m=0, flag=1, flag0=0, Sample_Int = 0;

    float Sample_X[1501] = {0.0,}, Calculated_X[1501]={0.0,}, g[1501] = {0.0,}, Error[1501]={0.0,};
    float a[7]={0.0,}, mu[7]={0.0,}, Sig[7]={0.0,}, a_NK[1501]={0.0,};
    float a_new[7]={0.0,}, mu_new[6]={0.0,}, Sig_new[7]={0.0,};
    float e1[7]={0.0,}, e2[7]={0.0,}, e3[7]={0.0,}, peak[7][1501]={0.0,}, R[1501];

    float mu_p1=0.0, mu_p2=0.0, mu_p3=0.0, mu_p4=0.0, mu_p5=0.0, sig_p1=0.0, R0;
    float t=0.0, Tolerance1, h, TSample_No = 0.0, mixing;
    float measured_x, FWHM = 0.0, sumup=0.0, a_sum =0.0;
    float a_ik = 0.0, mu_upper, mu_lower, Sig_upper, Sig_lower, Px_mu, PxSig;

    float Gaussian();

    printf ("Type the Source file name:");
    scanf("%s",Open);

    if ((in = fopen(Open, "rt")) == NULL)
    {
        fprintf(stderr, "Cannot open input file.
"));
        exit(0);
    }

    printf("\n\n Output file name1 :");
    scanf("%s",Oput);
```

printf("\n\n Output file name2 : ");
scanf("%s", out1);

printf("\n\n Put the number of peaks : ");
scanf("%d", &NoP);
K=NoP;

if ((out = fopen(Oput, "wt")) == NULL)
{
    fprintf(stderr, "\nCannot open output file.\n")
    exit(0);
}

if ((out1 = fopen(oput1, "wt")) == NULL)
{
    fprintf(stderr, "\nCannot open output file.\n")
    exit(0);
}

while(!feof(in)){
    i=i+1;
    fscanf(in,"%f \n", &measured_x);
    Sample_X[i]= measured_x;
}

h=0.0;
for (i=1; i <= N; i++){
    if (Sample_X[i] < 1e-7 ){
        h = h + 1.0;
        Sample_X[i] = .0;
    } else {
        Sample_Int = (int) 1000000*Sample_X[i];
        Sample_X[i] = (float) Sample_Int;
        TSample_No = TSample_No + Sample_X[i];
    }
}

for (m=1; m<=1500; m=m+1){
    FWHM = c1 + c2*sqrt(m + c3*pow(m,2));
    R[m] = (1/2.35)*FWHM/m;
}
while (flag ==1){
    for (i=1; i<=K; i=i+1){
        a[i] = (float) 1/K;
        FWHM = c1 + c2*sqrt(mu[i]+c3*pow(mu[i],2));
        Sig[i] = pow(FWHM/2.35,2);
    }
    m=0;
    Tolerance1 = 1.0;
    while (m<200){ //&& Tolerance1 > 0.000001){
        m = m+1;
        if ( m != 1){
            for (j=1; j<=K; j=j+1){
                a[j] = a_new[j];
            }
        }
        for (i=1; i<=K; i=i+1){
            a_new[i] = 0.0;
            for (x=1; x<=N; x=x+1){
                g[x] = Gaussian( (float) x, mu[i], Sig[i], flag0);
                sumup = 0.0;
                for (j=1; j<=K; j=j+1){
                    sumup = sumup + a[j]*Gaussian((float) x, mu[j], Sig[j], flag0);
                }
                if (sumup != 0.0){
                    a_ik = a[i]*g[x]/sumup;
                    if (Sample_X[x] != 0.0)
                        a_new[i] = a_new[i] + Sample_X[x]*a_ik;
                    else
                        a_new[i] = a_new[i] + a_ik;
                } else {
                    a_new[i] = a_new[i] + 1;
                }
            }
            a_new[i]= (1/(TSample_No))*a_new[i];
            e1[i] = abs(a_new[i]-a[i])/a[i];
    }
}
if (m != 1)
    for (j=1; j<=K; j=j+1)
        mu[j] = mu_new[j];

for (i=1; i<=K; i=i+1)
    mu_p1 = 0.0;
    mu_p2 = 0.0;
    mu_p3 = 0.0;
    for (x=1; x<=N; x=x+1)
        g[x] = Gaussian( (float) x, mu[i], Sig[i], flag0);
        sumup = 0.0;
        for (j=1; j<=K; j=j+1)
            sumup = sumup + a[i]*Gaussian( (float) x, mu[j], Sig[j], flag0);
        if (sumup != 0.0)
            Px_mu = a[i]*g[x]/sumup;
        else
            Px_mu = 0.0;
        mu_p1 = mu_p1 + Sample_X[x]*Px_mu;
        mu_p2 = mu_p2 + Sample_X[x]*x*Px_mu;
        mu_p3 = mu_p3 + Sample_X[x]*pow(x,2)*Px_mu;
    }
    for (i=1; i<=K; i=i+1)
        FWHM = c1 + c2*sqrt(mu[i] + c3*pow(mu[i],2));
        R0 = (1/2.35)*FWHM/mu[i];
        mu_p5 = pow(R0,2);
        mu_p4 = pow(mu_p2,2) + 4*mu_p1*mu_p3*mu_p5;
        mu_new[i] = (-mu_p2 + sqrt(mu_p4))/(2*mu_p1*mu_p5);
        e2[i] = abs(mu_new[i]-mu[i])/mu[i];
    }
    for (i=1; i<=K; i=i+1)
        FWHM = c1 + c2*sqrt(mu_new[i] + c3*pow(mu_new[i],2));
        sig_p1 = FWHM/2.35;
        Sig_new[i] = pow(sig_p1,2);
        e3[i] = abs(Sig_new[i]-Sig[i])/Sig[i];
        Sig[i] = Sig_new[i];
    }

117
Tolerance1 = e1[1];

for (i=1; i<=K; i=i+1){
    t = Tolerance1 - e1[i];
    if (t < 0.0)
        Tolerance1 = e1[i];
    t = Tolerance1 - e2[i];
    if (t < 0.0)
        Tolerance1 = e2[i];
    t = Tolerance1 - e3[i];
    if (t < 0.0)
        Tolerance1 = e3[i];
}

for (x=1; x<=N; x=x+1){
    for (i=1; i<=K; i=i+1){

        Calculated_X[x]= Calculated_X[x] + a[i]*Gaussian( (float) x, mu_new[i], Sig_new[i], flag0);
    }

    peak[1][x] = a[1]*Gaussian((float) x, mu_new[1], Sig_new[1], flag0);
    peak[2][x] = a[2]*Gaussian((float) x, mu_new[2], Sig_new[2], flag0);
    peak[3][x] = a[3]*Gaussian((float) x, mu_new[3], Sig_new[3], flag0);
    peak[4][x] = a[4]*Gaussian((float) x, mu_new[4], Sig_new[4], flag0);
    peak[5][x] = a[5]*Gaussian((float) x, mu_new[5], Sig_new[5], flag0);
    peak[6][x] = a[6]*Gaussian((float) x, mu_new[6], Sig_new[6], flag0);

    Error[x] = Sample_X[x] - Calculated_X[x];
}

flag = 0;
}

for (j=1; j<=1500; j=j+1){
    fprintf(out,"%d %f \n", j, Calculated_X[j]);
    fprintf(out1,"%d %f %f %f %f %f %f %f \n", j, peak[1][j], peak[2][j], peak[3][j], peak[4][j], peak[5][j], peak[6][j]);
}

fclose(in);
fclose(out);
fclose(out1);
LIST OF REFERENCES


BIOGRAPHICAL SKETCH

Jangyong Huh was born in 1967 in Seoul, South Korea to Jongwook Huh and Chundo Lee and is their only son. They did not interfere with his life unless he broke the fundamental rules and principles which are required for the human society. So, he grew up in a free atmosphere and as a result had a very open mind to the world. He began his academic career at Chung-Ang University in Seoul in 1986 where he studied physics. After finishing with a Bachelor of Physics degree in 1992, he continued his master degree for nuclear physics in the same university in 1994. Finally, he completed his doctorate in 2002.

Even though he was offered a decent job after his doctorate, he decided to further his education at the University of Florida in pursuit of his long-cherished desire to study and work in America. Such a hardly understandable decision might be due to his liberal spirit which has been built up through his life. For now, he has completed a Master of Nuclear Science degree in University of Florida in 2008 and then has been waiting for his another journey in America.