A Computer Code for Synthetic Gamma-ray Spectra Generation

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Abstract. "GammaGen" is a Windows computer software, developed to simulate gamma ray spectra obtained from detectors such as NaI(Tl) or Ge. The detector efficiency, resolution and peak to Compton dependence are used to generate synthetic pulse height spectra for a specific detector. The spectra can be displayed in several modes: as energy lines, gaussians, with or without smoothed rectangular Compton continuum. All spectra can be exported to formats required by commercial spectra analyzing programs, including Excel format. The purposes for developing the program are to predict the detectors response when monitoring a nuclear reactor accident site, to check operational limits and performances of commercial spectrum unfolding programs and to develop a training tool for spectrometry laboratory workers.

KEYWORDS: gamma; spectra; code; simulation.

1. Introduction

The "GammaGen" is a Windows software, developed at the Nuclear Research Center Negev (NRCN) to generate synthetic gamma ray spectra obtained with detectors such as NaI(Tl) scintillation detectors or solid state Ge detectors. The spectrum for a chosen radio-nuclide is generated according to its activity, its photo-peak energy and yield (taken from a data library). The detector efficiency and resolution, and the peak to Compton dependence are also used to generate a complex pulse height spectrum for a specific detector and counting geometry, which are chosen by the user. The spectra can be displayed in several modes: as energy lines of the photo-peaks, as gaussians of each photo-peak, or as sum of all gaussians. A smoothed rectangular Compton continuum can be included, as a choice. The resulting spectra for different radio-nuclides mixtures are displayed for visual analysis together with peaks and radio-nuclides data. All spectra can be exported to formats required by commercial spectra analyzing programs and to Excel format.

There are several purposes for developing of the program:
– to generate synthetic spectra for predicting the detectors response in case of monitoring a nuclear reactor accident site.
– to check operational limits and performances of commercial spectrum unfolding programs.
– to develop a training tool for spectrometry laboratory workers.

Several synthetic spectra were generated for NaI(Tl) and Ge detectors. An example of a NaI(Tl) response is presented, which shows the complexity of analysis of fission products spectra expected for a reactor accident case, and the usefulness of the "GammaGen" program as an additional analysis tool. A different gamma spectrum for mono energetic radio-nuclides obtained from a Ge detector was generated in order to check the performance of a commercial spectrum unfolding tool employed at NRCN, the "InterWinner" program [1]. The developed program was found to be a helpful tool for checking the analysis quality for gamma ray detectors and for performing visual inspection of components of complicated spectra.

2. The method

The operation of the program is based on two separate libraries of radio-nuclides. One library is a general one, based on the Radecay program [2], containing radio-isotopes practically encountered in a radiation protection laboratory. This library is used for analyzing an arbitrary radio-nuclide mixture. The second library contains most of the gamma emitting fission products with a half life longer than 1 minute. The libraries contain all needed physical data (gamma energies and yields).

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2.1 Arbitrary radio-nuclides mixtures

Any mixture can be chosen by manual selection from the general radio-nuclides library list displayed on the screen. The radio-nuclides and their activity can be selected at will, to represent the chosen actual radio-nuclides mixture. The activity default value of each radio-nuclide is 1 Bq. The detector type (NaI(Tl) or Ge) and the display method (energy lines, gaussians or full spectra) are also to be chosen. The resulting pulse height spectrum and its components are displayed on the computer screen.

2.2 Fission products spectra

One of the purposes of the program is to predict the spectra which will be obtained in a detector monitoring the fission products after a nuclear reactor accident. Such spectra are complicated and include about hundred radio-nuclides, each emitting mostly several photon energies. The composition of the fission products inventory depends on the operational parameters of the reactor (reactor power, operation time and cooling time). The spectrum of the gamma rays reaching a detector which monitors the accident site is dependent also on the distance from the source. The detector type and geometry must be selected for calculation of the detector response, as well as the distance between the detector and the source. If the detector is shielded by lead, the shield thickness must also be given.

3. Program operation

First, the library must be chosen (general library or fission products library). The main menu options of the program for the fission products library are shown in Fig. 1A. On the left side are given the input parameters defining the reactor operational details and the detector definition. The fission products are presented on the screen with selection boxes. For the nuclear accident case, 7 groups of radio-nuclides were defined, based on the data in the literature [3]. For each group there is a different specific release probability. Different combinations of the 7 groups can be chosen by marking the boxes on the right side of the screen.

The main menu options for the general radio-nuclides combination is given in Fig. 1B. The principle is similar to the fission products screen, except the option to determine arbitrary activity values for the chosen radio-nuclides. User-optional lists can be prepared to facilitate special applications.

For both options (fission products and arbitrary mixtures) the detector type and dimension and the geometry must be selected in the left-lowest box. In addition, the lead thickness and the source to detector distance are to be defined. According to the detector data, for each photo-peak the counting efficiency is determined by taking into consideration the detector efficiency and the absorption in the various media. The corresponding resolution is also calculated.

4. Screen output characteristics

For easy visual identification of the radio-nuclides, specific colors are applied to the various peaks displayed as energy lines or separate gaussians. The Compton continuum of the radio-nuclides mixture can be displayed in a chosen color as well. The area of each photo-peak is computed based on the radio-nuclide activity, its corresponding intensity and abundance (taken from the radio-nuclides library), and based on the detector's efficiency curve. If energy line display is chosen, the height of each energy line is presented proportional to the calculated count rate. The gaussian spectrum is displayed according to the detector resolution. Each Gaussian height is calculated to give an area corresponding to the total count rate. The Compton continuum is approximated to a rectangle by calculating the Compton edge energy and normalizing the height to obtain an area corresponding to the peak to Compton ratio function. The higher end of the Compton rectangle is smoothed by a gaussian with the appropriate resolution. Zooming functions are available for easy and detailed view of the spectra obtained. The Y axis can be chosen logarithmic or linear with selected amplification. The channel, energy and radio-nuclide data are displayed according to the cursor position in the spectrum.
Figure 1: The "GammaGen" program main screen.
(A) "Fission-Products" mode.
(B) "Gamma-Nuclides" (manual) mode.

A

Fission Products Mode

Sorted display of radio-nuclides

Group Selection

Nuclides List and Activity

Nuclides selection

Group selection Options

Detector Data

Reactor Data

B

Manual Mode

Activity units

Input Activity for selected nuclides

Selected list

Nuclides of selected list

Nuclides List

Selected list
5. Sample results

The following two examples present some circumstances, where the "GammaGen" program helps to identify deviations from true activity values and analysis problems when using NaI(Tl) detectors. The spectra were generated for the case of fission products monitoring, and show the complexity of the multiple peaks presence.

In Fig. 2 the case of one main peak (of $^{95}\text{Y}$) overlapping with other minor peaks (originated by $^{90}\text{Rb}$, $^{89}\text{Rb}$, and $^{142}\text{La}$) is given. Known activities of $^{95}\text{Y}$, $^{142}\text{La}$, $^{90}\text{Rb}$ were used to produce the simplified pulse height spectrum, based on gaussians only. Each radio-isotope is characterized by a specific color. The resulting total spectrum is displayed in black color. The display shows also the energy lines, positioned at the appropriate energy, with a height relative to the calculated count rate. The gaussian corresponding to a specific energy line has the same color, and its area is relative to the specific count rate. The arrows for a specific isotope point to the corresponding energy lines. When analyzing the originated pulse height spectrum and ignoring the contribution of the smaller peaks, which mostly remain undetected in regular analysis, an error of about 30% is induced when evaluating the activity of $^{95}\text{Y}$. A similar error is obtained when performing manual analysis and subtracting background by the trapeze method.

**Figure 2:** Gaussians NaI(Tl) spectrum detail for $^{95}\text{Y}$ case.

**Figure 3:** Gaussians NaI(Tl) spectrum detail for $^{88}\text{Kr} + ^{142}\text{La}$ case.
In Fig. 3 the case of two radio-isotopes with very close energies, undistinguishable by the unfolding procedures, is given. The color definition is as described above. $^{88}$Kr and $^{142}$La produce a sum-gaussian with the same resolution and location as any one contributor. This is the case also for $^{138}$Cs. When analyzing the resulting sum-spectrum (black line), there is no indication (neither from the energy nor from the resolution values) that the peak contains several contributions. The "GammaGen" program may help to analyze the contribution of the various radio-nuclides and their influence on the resulting spectra.

In the next example a check of the analysis results of the commercial "InterWinner" unfolding program for a Ge spectrum is presented. In this case, less overlapping problems than for the NaI(Tl) detector are expected. For this check, a synthetic spectrum was produced by summing the individual spectra of 23 radio-nuclides, which are characterized by a single photo-peak emission over 100 keV. The case of single photo-peaks emission is the most difficult, as there is no additional information to assist the unfolding process if overlapping occurs. The list of these 23 radio-isotopes can be seen in the displayed screen in Fig 1B (the marked radio-isotopes). The activity of all radio-isotopes is given as 1 Bq. Also for this case, only the gaussian photo-peak presentation was chosen. The resulting pulse height spectrum was prepared in the format required by the "InterWinner" software.

The "InterWinner" program was applied to analyze the obtained complex pulse height spectrum. The results for three energy regions are presented. Fig. 4A presents the pulse height spectrum obtained by the "GammaGen" program for the energy range 100 keV – 180 keV. The isotopes, the corresponding gamma energies and the relative contributions to the peaks in this region (the yields), based on the input data, are marked in the figure. The color definitions are as described above. Fig. 4B shows the result of the "InterWinner" analysis in the 100 keV – 180 keV range. It can be seen, that in the case of several radio-nuclides at close energy values, only one radio-nuclide is marked in the analysis resulting spectrum. The omitted radio-nuclides are marked in red in Fig. 4A. At $\sim$129.5 keV, only $^{105m}$Rh is given in the analysis spectrum (see Fig. 4B), although $^{191}$Os has a similar intensity (see Fig. 4A). At $\sim$159 keV $^{47}$Sc is shown, but not $^{123m}$Te, although it has a higher intensity. $^{131m}$Xe appears as a small gaussian at the lower part of the $^{139}$Ce peak (at $\sim$164 KeV), but it is not identified as an additional radio-isotope in Fig 4B. However, in the summary of the analysis results by the "InterWinner" program, an alert is given on the program inability to discriminate between several overlapping peaks, as seen in Fig. 7. Warnings are given on the $^{47}$Sc and $^{123m}$Te pair (case 1) and the $^{105m}$Rh and $^{191}$Os pair (case 2), but not on $^{131m}$Xe.

Fig. 5A and 5B present the results for the energy region 270 keV – 290 keV. Two radio-nuclides overlap at $\sim$276 keV : $^{81}$Kr and $^{133m}$Ba. Also in this case the overlapping causes a warning on unresolved peaks (case 3, see Fig. 7). Fig. 6A and 6B present the results for the energy region 380 keV – 400 keV. Three radio-nuclides have overlapping peaks in this region: $^{113m}$In, $^{187}$Zr and $^{87m}$Sr. The "InterWinner" program identifies these three radio-nuclides, but another un-identified gaussian is added, probably to improve the fitting (see Fig. 6B). This addition does not change the results qualitatively, but influences the quantitative analysis, as seen further.

The quantitative results of the "InterWinner" analysis were compared to the given activities for the 23 single photo-peak radio-nuclides (1 Bq for each radio-isotope), which composed the analyzed complex spectrum. The results are summarized in Table 1. The activities overestimated by more than $\sim$10% are marked in red, and the activities underestimated by more than $\sim$10% are marked in blue. It can be seen that for about half of these radio-isotopes the evaluated activities were within a range of about 10%. There are strong deviations, associated with the cases mentioned above (see notations 1-3 for the specific cases mentioned above, in Fig. 7, Fig. 8 and Table 1). A graphical presentation of the differences between the expected and the evaluated activities by the "InterWinner" program is presented in Fig. 8. These deviations occur, as without any additional energy peak to help identify the isotope, the whole activity is attributed to either isotope contributing to the same peak. This problem is not solely an unfolding problem, but an experimental problem as well.
Figure 4: Gaussian Ge spectrum for the mixture of 23 single photo-peak radio-nuclides in the energy range 100 keV - 180 keV.

(A) "GammaGen" spectrum.                         (B) "InterWinner" unfolding results.

- **Gd-153**: 103.18 KeV 22.22%
- **Eu-155**: 105.31 KeV 20.67%
- **Sc-46m**: 142.53 KeV 62.7%
- **Ce-141**: 145.44 KeV 32.5%
- **Os-191**: 129.1 KeV 25.9%
- **Rh-105m**: 129.57 KeV 20.4%
- **Ce-144**: 133.54 KeV 10.8%
- **Te-123m**: 159.0 KeV 84.1%
- **Sc-47**: 159.39 KeV 68%
- **Hg-203**: 279.1 KeV 77.3%
- **Ce-139**: 165.85 KeV 80.35%
- **Xe-131m**: 163.93 KeV 1.96%
Figure 5: Gaussian Ge spectrum for the mixture of 23 single photo-peak radio-nuclides in the energy range 270 keV - 290 keV.

(A) "GammaGen" spectrum.                         (B) "InterWinner" unfolding results.

- Ba-133m 276.1Kev 17.98%
- Kr- 81  275.9Kev 3.6%
- Hg-203  279.1Kev 77.3%
Figure 6: Gaussian Ge spectrum for the mixture of 23 single photo-peak radio-nuclides in the energy range 380keV - 400 keV.
   (A) "GammaGen" spectrum. (B) "InterWinner" unfolding results.

Figure 7: The alert messages of the "InterWinner" program for the mixture of 23 single photo-peak radio-nuclides analysis.
Table 1: The 23 radio-nuclides with single photo-peaks, their activity as evaluated by the "InterWinner" program and the differences from the expected activity (1 Bq).

<table>
<thead>
<tr>
<th>Isotope</th>
<th>Name</th>
<th>Energy [KeV]</th>
<th>Activity [Bq]</th>
<th>Stdev [%]</th>
<th>Calculated activity difference [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Gd-153</td>
<td>103.18</td>
<td>1.04E+00</td>
<td>10.8</td>
<td>3.70</td>
</tr>
<tr>
<td>2</td>
<td>Eu-155</td>
<td>105.31</td>
<td>9.92E-01</td>
<td>5.4</td>
<td>-0.78</td>
</tr>
<tr>
<td>3</td>
<td>Os-191</td>
<td>129.40</td>
<td>1.60E+00</td>
<td>20.8</td>
<td>60.20</td>
</tr>
<tr>
<td>4</td>
<td>Rh-105m</td>
<td>129.57</td>
<td>2.29E+00</td>
<td>1.3</td>
<td>129.40</td>
</tr>
<tr>
<td>5</td>
<td>Ce-144</td>
<td>133.54</td>
<td>9.77E-01</td>
<td>4.5</td>
<td>-2.27</td>
</tr>
<tr>
<td>6</td>
<td>Sc-46m</td>
<td>142.53</td>
<td>1.02E+00</td>
<td>2.9</td>
<td>2.40</td>
</tr>
<tr>
<td>7</td>
<td>Ce-141</td>
<td>145.44</td>
<td>1.00E+00</td>
<td>3.2</td>
<td>0.00</td>
</tr>
<tr>
<td>8</td>
<td>Te-123m</td>
<td>159.00</td>
<td>1.83E+00</td>
<td>2.4</td>
<td>82.70</td>
</tr>
<tr>
<td>9</td>
<td>Sc-47</td>
<td>159.39</td>
<td>2.26E+00</td>
<td>1.3</td>
<td>125.70</td>
</tr>
<tr>
<td>10</td>
<td>Xe-131m</td>
<td>163.93</td>
<td>7.82E-01</td>
<td>7.5</td>
<td>-21.78</td>
</tr>
<tr>
<td>11</td>
<td>Ce-139</td>
<td>165.85</td>
<td>1.10E+00</td>
<td>3.0</td>
<td>10.14</td>
</tr>
<tr>
<td>12</td>
<td>Fe-52</td>
<td>168.68</td>
<td>9.96E-01</td>
<td>3.0</td>
<td>-0.41</td>
</tr>
<tr>
<td>13</td>
<td>Kr-81</td>
<td>275.99</td>
<td>6.01E+00</td>
<td>0.7</td>
<td>500.90</td>
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<tr>
<td>14</td>
<td>Ba-133m</td>
<td>276.09</td>
<td>1.20E+00</td>
<td>2.5</td>
<td>20.20</td>
</tr>
<tr>
<td>15</td>
<td>Hg-203</td>
<td>279.19</td>
<td>9.47E-01</td>
<td>3.2</td>
<td>-5.27</td>
</tr>
<tr>
<td>16</td>
<td>Sr-87m</td>
<td>388.40</td>
<td>9.77E-01</td>
<td>3.1</td>
<td>-2.30</td>
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<tr>
<td>17</td>
<td>In-113m</td>
<td>391.69</td>
<td>4.03E-01</td>
<td>7.5</td>
<td>-59.68</td>
</tr>
<tr>
<td>18</td>
<td>Zr-88</td>
<td>392.90</td>
<td>1.40E+00</td>
<td>2.2</td>
<td>39.80</td>
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<tr>
<td>19</td>
<td>Y-87</td>
<td>484.70</td>
<td>1.00E+00</td>
<td>3.0</td>
<td>0.00</td>
</tr>
<tr>
<td>20</td>
<td>Pm-143</td>
<td>741.98</td>
<td>3.35E-01</td>
<td>9.0</td>
<td>-66.53</td>
</tr>
<tr>
<td>21</td>
<td>Nb-97m</td>
<td>743.36</td>
<td>1.27E+00</td>
<td>2.4</td>
<td>26.90</td>
</tr>
<tr>
<td>22</td>
<td>Na-22</td>
<td>1274.50</td>
<td>1.00E+00</td>
<td>3.0</td>
<td>0.00</td>
</tr>
<tr>
<td>23</td>
<td>Cu-64</td>
<td>1345.90</td>
<td>1.04E+00</td>
<td>32.6</td>
<td>4.20</td>
</tr>
</tbody>
</table>

Figure 8: Graphical presentation of the differences between the expected and evaluated activities by the "InterWinner" program.
As seen by the results in Table 1, although $^{191}$Os is not marked in the resulting analyzed spectrum (see Fig. 4B), it appears in the results table. However, for both $^{105m}$Rh and $^{191}$Os, the calculated activities are strongly overestimated (by $\sim$60% and $\sim$130%). Similarly, the activities of the overlapping $^{123m}$Te and $^{47}$Sc are strongly overestimated, pointing to the basic problem of overlapping mono-energetic peaks, which makes the quantitative evaluation for these cases impossible. Although $^{131m}$Xe is not noted in the resulting analyzed spectrum (see Fig. 4B), it appears in Table 1, with an activity of about 20% lower than expected. For the case of $^{113m}$In + $^{88}$Zr (see Fig. 6), no additional radio-nuclide appears in Table 1, although an additional Gaussian appears in Fig. 6B. However, an overestimation of $\sim$40% for $^{88}$Zr and an underestimation of $\sim$60% for $^{113m}$In can be observed. The yield of $^{133m}$Ba is $\sim$5 times higher than the yield of $^{81}$Kr. Due to the low yield of $^{81}$Kr, its error is multiplied and a very high error of a factor of 6 is obtained (see Table 1).

6. Conclusions

The developed "GammaGen" program is a helpful tool for graphical inspection of complicated spectra, particularly for the case of the poor resolution NaI(Tl) detectors. It is especially useful for the hundreds of photo-peaks present in the case of a nuclear reactor accident, where a risk evaluation is to be made according to the fission products analysis and release fractions.

The "GammaGen" program is a useful tool for checking the performances of commercial gamma spectra analyzing software, with any combination of radio-isotopes, and without the need to perform experiments. Evaluations for problematic or short lived radio-isotopes can be performed, for which the experimental possibilities are limited or non-existent.

A simulation for the response of a Ge detector to a complex mixture of 23 single photo-peak radionuclides, was produced and analyzed by the "InterWinner" software (Eurisys/France). Significant deviations from the expected activities were obtained for overlapping single photo-peaks, which points to the experimental problem of resolving two single overlapping photo-peaks of different radioisotopes. The "GammaGen" program could be used to check the "InterWinner" response to this situation. In any case, the results of unfolding programs should be carefully checked for assuring correct analysis, in particular the special warnings. It is to be mentioned that also the selection of the Region of Interest for unfolding process may influence the results.

The "GammaGen" program can be applied as a training tool for spectrometry laboratory workers. Different synthetic radio-nuclide mixtures can be prepared without the need to use real radioactive materials.

The "GammaGen" program is still under development and additional features are intended to be added, as combining the calculated spectra with an existing measured background and adding statistical noise fluctuations.

REFERENCES

[1] "InterWinner" 4.1 software, provided by Eurisys Measures, France.