AIM

Association for Information and Image Management

1100 Wayne Avenue, Suite 1100
Silver Spring, Maryland 20910
301/587-8202

Centimeter

Inches

MANUFACTURED TO AIM STANDARDS
BY APPLIED IMAGE, INC.

1 of 1

Conf-940748--30

PNL-SA-23879

SYNTH: A SPECTRUM SYNTHESIZER

W. K. Hensley
H. S. Miley
R. M. Savard

A. D. McKinnon
M. E. Panisko

July 1994

Presented at the
Institute of Nuclear Materials Management
35th Annual Conference
July 17-20, 1994
Naples, Florida

Prepared for
the U.S. Department of Energy
under Contract DE-AC06-76RLO 1830

Pacific Northwest Laboratory
Richland, Washington 99352

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

SYNTH: A Spectrum Synthesizer

W.K. Hensley, A.D. McKinnon, H.S. Miley, M.E. Panisko, and R.M. Savard,
Pacific Northwest Laboratory
Battelle Blvd., Richland, WA 99352

Abstract

A computer code has been written at the Pacific Northwest Laboratory (PNL)⁽¹⁾ to synthesize the results of typical gamma-ray spectroscopy experiments. The code, dubbed SYNTH [1], allows a user to specify physical characteristics of a gamma-ray source, the quantity of the nuclides producing the radiation, the source-to-detector distance and the type and thickness of absorbers, the size and composition of the detector (Ge or NaI), and the electronic set up used to gather the data.

In the process of specifying the parameters needed to synthesize a spectrum, several interesting intermediate results are produced, including a photopeak transmission function vs energy, a detector efficiency curve, and a weighted list of gamma and x rays produced from a set of nuclides. All of these intermediate results are available for graphical inspection and for printing.

SYNTH runs on personal computers. It is menu driven and can be customized to user specifications. SYNTH contains robust support for coaxial germanium detectors and some support for sodium iodide detectors. SYNTH is not a finished product. A number of additional developments are planned. However, the existing code has been compared carefully to spectra obtained from National Institute for Standards and Technology (NIST) certified standards with very favorable results. Examples of the use of SYNTH and several spectral results will be presented.

I. INTRODUCTION

A gamma-ray spectroscopy experiment involves at least several components. The radiation source, absorbers, detectors, and electronics each have predictable behavior, and gamma-ray spectroscopists usually take these into account in the design or data reduction of an experiment.

Several of these steps are, at best, tedious. Others are usually considered impossible without either a significant Monte Carlo calculation or ancillary measurement.

The development of SYNTH began in 1982 with a FORTRAN code written to generate the Compton continuum associated with an arbitrary gamma-ray energy. To do this, the theoretical Compton spectral shape was parameterized, and a photo peak with the appropriate peak-to-Compton ratio and detector resolution was applied to the result. This code was primarily written as an exercise, since simulating most realistic gamma-ray spectra requires many, possibly hundreds, of gamma-ray energies with proper relative weighting and several detector parameters. The work required to perform the simulation exceeded the simulation itself. However, a subsequent, unrelated development solved these problems.

Independent of this effort, the Erdtmann-Soyka gamma-ray library was obtained on magnetic media for the purpose of creating a gamma-ray spectroscopy database able to identify isotopes. This was, in fact, achieved. The database software was expanded to provide other functions, including the generation of gamma-ray output tables in a format suitable for creating automated analysis libraries.

The first recognizable version of SYNTH was created by tailoring the output of the database software to the needed input format for the code creating the Compton spectrum. Since then a number of improvements have been made, such as transferring the code to the PC and subsequently developing a graphical user interface (GUI) built around Microsoft Windows™. Still, SYNTH is primarily a code designed to compute a complete gamma-ray spectrum from a nuclide specification.

II. SOFTWARE DESIGN

A. General Structure

SYNTH is actually a set of mini-applications written in Visual Basic™. Each of the code segments, activated by a mouse click on the main screen (see Figure 1), guides the computer through the parameter-specification process that precedes the generation of an output spectrum. The parameters are grouped in a natural way for a gamma-ray spectroscopist. For instance, all the parameters related to the detector specification are together. This grouping makes it convenient for SYNTH to immediately display traditionally-computed information, such as a transmission curve or a detector-efficiency curve.

In addition, frequently used parameters can be saved or even loaded as the user's default parameters, speeding future SYNTH sessions.

The use of a visual, Windows™-compatible compiler allowed the authors to automatically have support for most printers and to have unprecedented ease in producing a GUI. To port the existing code to the Windows™ environment, about 6,000 lines of the Compton spectrum generator were translated into BASIC (the overall size of the code is now

approximately 10,000 lines). In addition, the original database code was overhauled to communicate with the BASIC code segments via simple ASCII input and output files. The output of the database code is valuable in its own right as an input for true Monte Carlo codes.

B. Source Specification

Source specification has been grouped into two parts. The first part specifies the physical dimensions and composition of the source (disk shapes and point sources are presently supported). For finite sources, the bulk composition and thickness of the source determine the self absorption. The material specification of the source can include an admixture of elements and a user-selected density. The sample geometry model and the algorithms for computing the self-attenuation factors were first derived by Gunnink and Niday [2] for use in the GAMMANAL series of codes, and implemented in the SYNTH code with minimal modification. An example of the sample properties screen is shown in Figure 2. Finally, the source-to-detector distance is specified in this code segment.

Figure 1. SYNTH main screen

Figure 2. The sample properties screen for an aluminum disk source

The second part of the source specification selects the radioisotopes contained in the sample. The Erdtmann-Soyka gamma-ray library [3] has been incorporated in a relational database (Microsoft Access™), as have certain other data (e.g., parent-daughter branching ratios for selected nuclei and stable isotopes and their thermal and resonance neutron-capture cross sections) that were not included in the original compilation.

The user may specify the element (Z) from either an alphabetic list or a representation of the periodic table and the atomic mass (A) and state (ground or metastable) from a text box. As isotopes are added to a list, the quantity of the isotope is specified in one of several units. The completed isotope list may be subjected to decay, and daughter products may be automatically added to the list based on the specified decay time. Bateman equations are used to calculate the quantities of daughter products, and thus complex decay chains may be modeled. A sample of the radioisotope selection screen is shown in Figure 3.

After the user indicates that the list is complete, SYNTH creates an ASCII file with the specified isotope list and initiates the process to search the gamma-ray database and produce a weighted, sorted list of gamma-ray energies. Besides the subsequent use in SYNTH, this list has proved useful in itself. The code that searches the database also reports all isotopes contributing to the spectrum and the number of contributing gamma rays.

Figure 3. An example of the radionuclide specification screen

C. Absorber Specification

The absorber code originally restricted absorber choices to eight specific compounds and elements. Though these materials spanned the range of electron densities, initial feedback from users indicated that a more robust absorber model was desirable. The current version of SYNTH retains all the original selections and allows up to nine additional regions in which any element may be specified as an absorber. Each element selected is initially offered at a default density, but the density may be adjusted to any desired value. This capability allows almost any absorber material to be simulated.

It should be noted that the absorber portion of SYNTH sets up a simple photopeak-attenuation model using

$$t_E = e^{-\mu_E x}$$

where μ_E is the mass attenuation function for an individual material at a given energy E and x is the absorber thickness. The composite transmission function, T_E , is then computed as

$$T_E = \prod t_E$$

A graph of T_E as a function of energy is displayed during the absorber selection process, and is quite useful in itself. An example of the absorber screen is shown in Figure 4. The display has an extra feature that allows the user to interrogate the graph

with the mouse to extract numerical values, if needed. At the present time, no attempt is made to convert attenuated photopeak intensity into increased activity in the Compton continuum.

Figure 4. Example of the main screen for defining absorbers

D. Detector Specification

The detector-specification portion of the code presently uses a combination of hard-coded efficiency curves for sodium iodide detectors, and general algorithms for germanium diodes. Though only two sodium iodide sizes are currently supported, we are in the process of developing an algorithmic model based on the results of Monte-Carlo-derived response functions for sodium iodide crystals ranging in size from 1 in. x 0.5 in. up to 10 in. x 10 in. A complete range of coaxial germanium detector sizes is supported, from about 20% to 100% relative efficiency (compared to a 3 in. x 3 in. sodium iodide crystal at 1332 keV). Specifically, the germanium intrinsic detector efficiency, $\epsilon(E)$, is computed from fundamental detector parameters such as diameter, length, and relative efficiency using an algorithm developed by Gunnink and Prindle. [4]. An absolute efficiency is then obtained by applying geometry factors to the computed intrinsic efficiency. The detector geometry model was also developed as part of the GAMMANAL code series by Gunnink and Niday [2] and was

implemented in the SYNTH code with minimal changes.

A graph of the absolute detector efficiency as a function of energy is displayed during the parameter selection process, and it also allows the user to interrogate the graph with the mouse to extract numerical values. An example of the screen used to define detector parameters is shown in Figure 5.

Figure 5. Example of the screen used to define the detector

Other relevant detector parameters are also entered here and are used to correct the detector efficiency. For instance, the detector dead-layer thickness for germanium detectors can be specified, which allows the user to evaluate the difference between an N-type (no external dead layer) and a P-type (0.5 to 1.0 mm external dead layer) detector. The effect of the end-cap material is also included. Stainless steel, aluminum, and beryllium end caps can be selected.

The detector specification segment has found uses in planning detector purchases and in selecting existing detectors for a given experiment.

E. Electronics Simulation

The electronics code segment allows the user to configure the output data to mimic the hardware choices one might make in the laboratory. The hardware choices include the zero, the gain, and a non-linearity term of the output-energy calibration. In addition, the acquisition time and the number of

data channels are also selected at this point. A sample is shown in Figure 6.

Figure 6. Counting parameter definition screen

F. Spectrum Generation

The final code segment in the SYNTH main screen generates the actual output spectrum. The algorithm begins by adding the full-energy peak to the spectrum. The form of the peak is a gaussian with a single-exponential tailing function.

The area of the peak is computed from the intensity of the specified source term (corrected for gamma-ray branching ratios), the "counting" time, the geometry factor, the self attenuation in the source, transmission through any absorbers, and the intrinsic detector efficiency. The location of the Compton edge E_C , and backscatter peak (in KeV), is given by the relationship

$$E_C = \frac{511}{2} \cdot \frac{1}{1 + \frac{511}{2 \cdot E_{\text{gam}}}}$$

Next, the Compton continuum is added to the spectrum by taking the theoretical shape of a Compton spectrum [5], and normalizing it with a peak-to-Compton ratio appropriate for the volume

of the detector. The impact on the spectrum due to other physical effects is also included, such as multiple Compton scattering (the region between the full-energy peak and the Compton edge), single and double escape peaks (from pair production), the difference in peak shape of gamma and x rays (gaussian vs. lorentzian), the variation of resolution as a function of energy, and others.

Options exist to include statistical fluctuations, add (and normalize) a previously stored spectrum (real or synthetic), and save the generated spectrum to disk. A group of display options also allows detailed examination of the output spectrum and comparison with a reference spectrum. A sample of the "Pan / Zoom" screen is shown in Figure 7.

Figure 7. An example of the "Pan / Zoom" screen

III. TESTING

SYNTH has been tested in a number of ingenious ways. Although one of the early criteria of success adopted by the SYNTH developers has been the capability of the code to fool a trained spectroscopist, most of the tests have been simulations of actual experiments.

In one test, a complex radioisotopic standard containing ^{109}Cd , ^{57}Co , ^{139}Ce , ^{203}Hg , ^{113}Sn , ^{85}Sr , ^{137}Cs , ^{88}Y , and ^{60}Co was counted on a 22% relative-efficiency P-type germanium detector. SYNTH was

then used to simulate the results. The laboratory records that provide traceability of the source were used to specify the quantity of the isotopes on the certification date of the standard, and SYNTH decayed the source to the date of the measurement. The detector manufacturer's quality-assurance data sheet was used to specify the germanium diode parameters. No absorbers were specified other than air (the default), the detector end cap material (Al), and the germanium dead layer. The source-to-detector distance and the count time were specified, as was the system gain and zero. Almost all of the peak areas were correctly modeled to an average error of <10% as seen in Figure 8. The Compton continuum was remarkably free of deviation down to 500 keV, at which time SYNTH underestimated the experimental value by a factor of 2 or 3. This is attributed to gamma rays scattering in the lead shield of the detector, an effect that is not calculated in SYNTH's physical model.

Figure 8. A complex experimental spectrum compared to a SYNTH simulation

Other benchmarks were done with very active sources (background negligible) and without nearby scatterers, and SYNTH was shown to function at least as well or better than the example shown.

IV. CONCLUSIONS

SYNTH has proven itself to be a very valuable productivity enhancer for gamma-ray spectroscopists. It has been used, in its various incarnations, in the Nuclear Chemistry Section at

PNL for over two years. During this time, a number of applications have been found for SYNTH that were not originally intended.

Among the unintended uses of SYNTH, its use as a front-end for Monte Carlo codes is perhaps the most ironic, since SYNTH was designed to reduce the need for mundane Monte Carlo analyses. However, as is usually the case, researchers push all tools beyond their originally intended boundaries.

As an example of pushing SYNTH beyond its original intent, SYNTH was used to create a very old source of ^{238}U , ^{235}U , and ^{232}Th . The resulting spectrum had 720 gamma rays and was created in a total of 3 minutes on a 33 MHz 486 laptop, including the specification phases.

This tool, particularly when used in the field, provides much scientific support for spectroscopists.

VII. REFERENCES

- [1] *SYNTH: A Computer Code for Synthetic Gamma Ray Spectrum* (reference manual). PNL-8903, Pacific Northwest Laboratory⁽¹⁾, Richland, Washington, 1995.
- [2] Gunnink, R. and J. B. Niday. *Computerized Quantitative Analysis by Gamma ray Spectrometry, Vol. 1: Description of the GAMMANAL Program*. UCRL-51061, Lawrence Livermore National Laboratory, Livermore, CA. 1972.
- [3] G. Erdtmann, W. Soyka. *The Gamma Rays of the Nuclides*, New York, Verlag Chemie, 1979.
- [4] R. Gunnink, A.L. Prindle. *Nonconventional Methods for Accurately Calibrating Germanium Detectors*. UCRL-JC-105283, Lawrence Livermore National Laboratory, Livermore, California, 1991.
- [5] Kopecky, J., W. Ratynski and F. Warming. *Curves for the Response of a Ge(Li) Detector to Gamma Rays up to 11 Mev*, NIM, 50:333. 1967.

⁽¹⁾ Pacific Northwest Laboratory is operated by Battelle Memorial Institute for the US Department of Energy under Contract DE-AC06-76RLO 1830.

DATE

FILMED

10/7/94

END