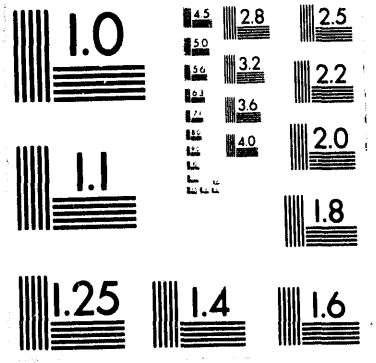
1.0
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DISCLAIMER

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SYNTH: A SPECTRUM SYNTHESIZER

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SYNTH: A Spectrum Synthesizer

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Abstract

A computer code has been written at the Pacific Northwest Laboratory (PNL) 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 presence of absorbers, the type and size of the detector, 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 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 data base 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 mostly written in Visual Basic™. Each of the code segments, activated by a mouse click on the main screen (see fig. 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,

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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 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 supported). The 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. Finally, the source to detector distance is specified in this code segment.

The second part of the source specification selects isotopes. The Erdtmann-Soyka gamma ray library [2] has been incorporated electronically, as have certain other data (parent-daughter branching ratios for selected nuclei, 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.

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

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.

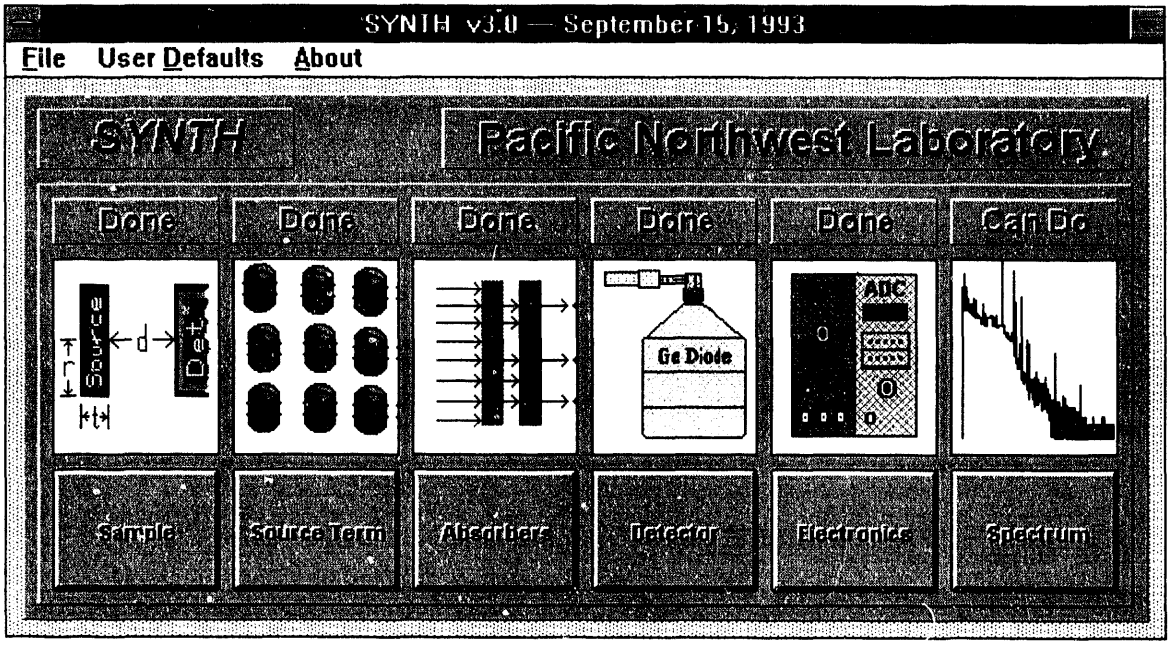

Fig. 1 SYNTH main screen

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 $\mu_{(E)}$ 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 computed as

$$T_{(E)} = \Pi\, t_{(E)}$$

A graph of $T_{(E)}$ as a function of energy is displayed during the absorber selection process, and is quite useful in itself. The display has an extra feature that allows the user to interrogate the graph with the mouse to extract numerical values, if needed.

D. Detector Specification

The detector-specification code uses algorithms produced by R. Gunnink et al. [3], obtained from the literature and from private communication. Though only two sodium iodide sizes are currently supported, a complete range of coaxial germanium detector sizes is supported, from about 20% to 100% relative efficiency (compared to a 3in. x 3in. sodium iodide crystal at 1332 keV). Specifically, the germanium intrinsic detector efficiency, ε(E), is computed by an algorithm using detector diameter, length, and relative efficiency. The absolute efficiency is then obtained by applying geometry factors to the computed intrinsic efficiency.

A graph of the absolute detector efficiency as a function of energy is displayed during the parameter selection process, and also allows the user to interrogate the graph with the mouse to extract numerical values.

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.

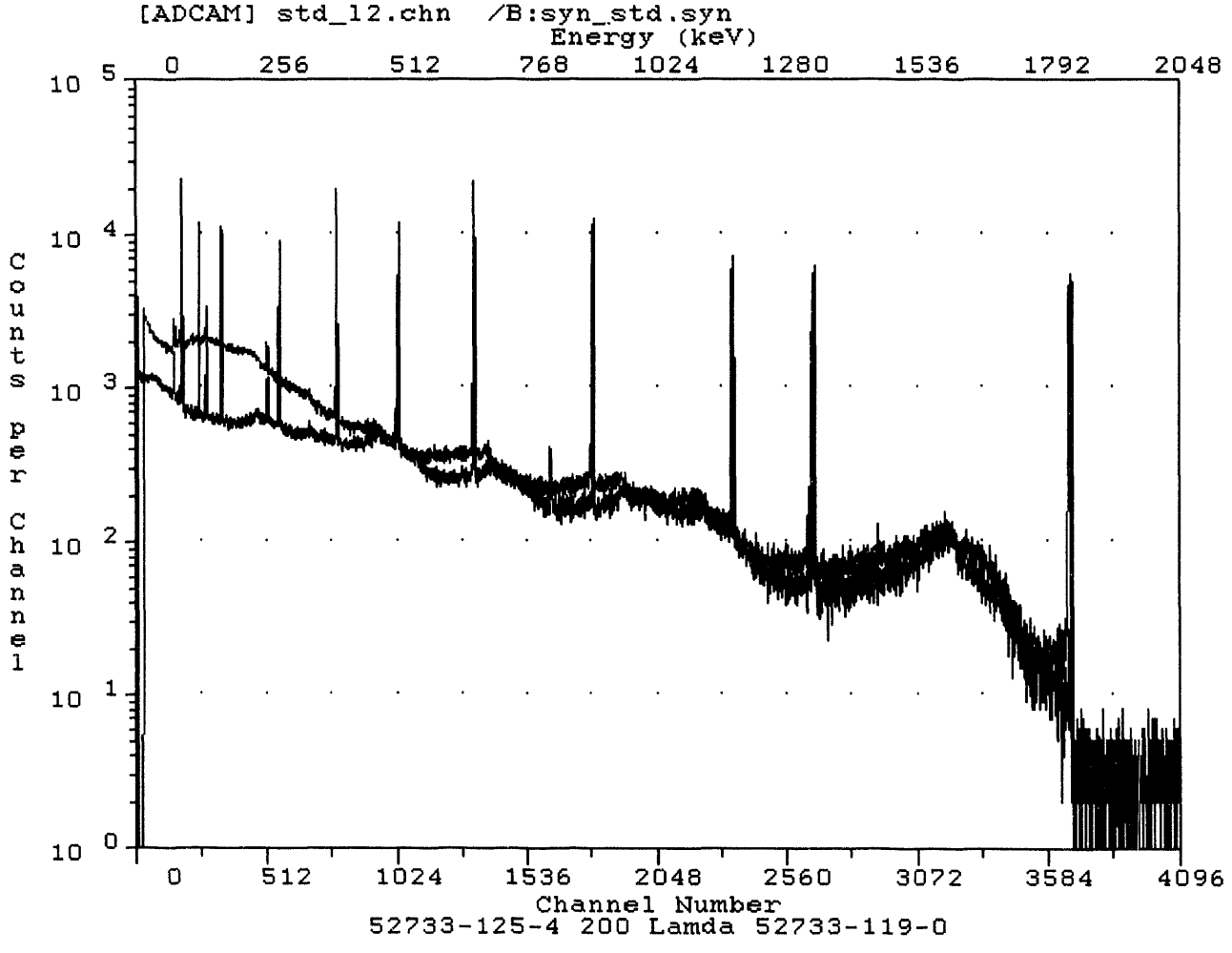

Fig. 2 A complex experimental spectrum compared to a SYNTH simulation

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.

F. Spectrum Generation

The final code segment in the SYNTH main screen simply generates the actual output spectrum. The algorithm takes the theoretical shape of a Compton spectrum and implements the effects of peak-to-Compton ratio, photopeak resolution, efficiency, and solid angle. The impact on the spectrum due to other physical effects is also included, such as multiple Compton scattering, 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 add statistical fluctuations, save the generated spectrum to disk, and add previously stored spectra. A group of display options also allows detailed examination of the output spectrum and comparison with a reference spectrum.

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 fig. 2. 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.

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

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