

Innovations in the Analysis Code SAMMY

N. M. LARSON¹

Oak Ridge National Laboratory, P. O. Box 2008, Oak Ridge, TN 37831 USA

The complexity and sophistication of modern experimental techniques require that similarly complex and sophisticated analysis procedures be used to interpret and understand experimental data. One tool which is often used in the analysis of neutron (and other projectile) time-of-flight data is the computer code SAMMY. An overview of the capabilities of this code is presented here, with emphasis on recent enhancements and improvements.

KEYWORDS: *evaluation, analysis, covariance, resonance region*

I. Introduction

Three basic requirements must be met by any program designed for analysis of neutron-induced cross section data. First, the formalism used for calculation of the cross sections should enable the user to calculate *accurate* values of all types of theoretical cross sections, including total, partial, energy-differential, energy- and angle-differential, and integral cross sections. Second, mathematical methods must be available for accurately estimating all important experimental effects (e.g., Doppler broadening) which cause the measured cross section to differ from the true cross section. Finally, the fitting procedure (e.g., Bayes' method or Least Squares) must, in the process of determining a set of parameter values which reproduce the experimental data, properly account for all experimental uncertainties (both statistical and systematic), and provide a realistic output parameter covariance matrix.

Sections II, III, and IV of this paper are devoted to the treatment of the three basic requirements in the SAMMY code¹⁾, and other features are described in Section V. In Section VI, SAMMY's capabilities in the unresolved-resonance region are described. Finally, a brief discussion of future extensions of the code is given in Section VII.

II. Calculation of the Cross Section

1. R-Matrix Theory

Multi-channel, multilevel R-matrix theory²⁾ provides a phenomenological, unitary, analytic, and mathematically rigorous description for theoretical cross sections in the resolved-resonance region. The Reich-Moore approximation to the R-matrix theory is the method of choice for analysis codes, as it appears to be generally applicable.³⁾

For historical reasons and for comparison with early evaluations, SAMMY offers options to use either the single-level or the multilevel Breit Wigner (BW) approximation instead of Reich Moore. Use of BW is discouraged for new analyses, as it is often not an adequate representation.

2. Charged Particle Entrance and Exit Channels

Although SAMMY was initially designed for evaluation of neutron data, recently the capabilities of the code have been expanded to include charged particle data. Coulomb penetrabilities, shift factors, and phase shifts can now be generated for either entrance or exit channels. Rutherford

scattering can be calculated for angle-differential elastic cross sections with incident charged particles.

Another paper at this conference, entitled "R-Matrix Evaluation of ¹⁶O Neutron Cross Sections up to 6.3 MeV," reports on the first evaluation⁴⁾ using the charged-particle capability of SAMMY. This evaluation includes the (*n,α*) channel, which opens at 2.36 MeV.

Preliminary work is underway using SAMMY for analyses of several measurements with *incident* charged particles: ¹⁷F(*p,p*)¹⁷F at ORNL⁵⁾; ¹³C(*α,n*)¹⁶O and ¹⁷O(*α,n*)²⁰Ne at Cadarach⁶⁾; and ¹³C(*α,α*)¹³C at Karlsruhe⁷⁾.

3. Angle-Differential Reaction Cross Sections

It is now possible for SAMMY to calculate angular distributions for reaction products as well as for elastic scattering. Legendre coefficients for the reaction cross sections can be written in formats compatible with the evaluated nuclear data files.

4. Integral Data

Certain types of energy-integrated (integral) data may be included in the SAMMY analysis process. These include: (1) thermal values for capture, absorption, or fission (which, strictly speaking, are not integral data but are nevertheless included here); (2) Maxwellian average at thermal energy (*E* = 0.0253 eV); (3) Westcott's *g*-factor; (4) resonance integral; (5) average integral; (6) Watt spectrum average; (7) K1; (8) alpha; (9) NJOY's alpha; and (10) thermal eta integral. Exact definitions of all these quantities are given in the SAMMY manual.¹⁾

III. Description of Experimental Conditions

For an analysis to be correct, it is crucial to include accurate mathematical descriptions of those experimental conditions which cause the measured cross section to be different from the true cross section. Misunderstanding of, for example, the resolution function for a measurement can lead to incorrect values for resonance parameters, and hence to an inaccurate representation of the cross section. As measurements improve over time, the analysis codes must also improve to keep pace with the experiments.

1. Doppler Broadening

Doppler broadening is caused by motion of the target nuclei (because the sample is not at zero temperature).

¹Tel +1-865-574-4659 E-mail: LarsonNM@ornl.gov

Somewhat surprisingly, the free-gas model (FGM) provides an adequate description of Doppler broadening for most experimental data. During the early years of evaluation of neutron data, the high-energy Gaussian approximation (HEGA) to the free-gas model was used extensively. SAMMY has options for both FGM and HEGA, but use of HEGA is discouraged: the FGM model is more accurate, can be used at low energy, and requires no greater expenditure of computer resources than HEGA does.

For some measurements, solid-state effects are visible in the experimental data and hence must be included in the analysis. For this reason, a crystal-lattice model for Doppler broadening will soon be available in SAMMY.

2. Resolution Broadening

Resolution broadening is the result of, for example, the finite sizes of the neutron-producing target and of the detectors, and the non-negligible burst width and time-channel width. Unlike Doppler broadening, for which the mathematical descriptions apply universally to all experiments, the description of resolution broadening changes from machine to machine and experiment to experiment. For example, the burst width at the Oak Ridge Electron Linear Accelerator is well approximated by a square function of time, while at the Gelina facility the burst width has a long exponential tail.

Consequently, several different types of resolution-broadening functions are available within SAMMY :

(1) A simple Gaussian whose energy-dependent width is related to the burst width, the time-channel width, and the target and detector sizes. An exponential tail can be used along with the Gaussian.

(2) The Oak Ridge Resolution (ORR) function, which is formed by convolution of (a) the neutron burst (a square function in time), (b) the channel width (also a square function in time), (c) the neutron source (either the water moderator or the tantalum target, modeled with combinations of exponentials and Gaussians), and (d) the detector (modeled with exponential functions).

(3) The Rensselaer Polytechnic Institute (RPI) resolution function, formed by the convolution of (a) the neutron burst (a Gaussian in time), (b) the channel width (square function in time), and (c) the neutron source plus detector. This last term is modeled as a Chi-squared term plus several exponentials, with parameter values being energy-dependent.

An option to include as many exponential terms as desired has recently been added to SAMMY's RPI resolution function. Another recent addition is the option to center (or not) the resolution function directly over the energy at which the broadened cross section is being calculated; this option permits modeling of highly asymmetric and centroid-displacing resolution functions.

It is expected that a form of the RPI resolution function will eventually be found to be suitable for use with data taken at the time-of-flight facility at Gelina, Belgium.

(4) A recent addition to SAMMY's repertoire of resolution functions is the User-Defined Resolution (UDR) function, for which the user describes numerically the components of the

resolution function at specified energies, on a time-of-flight grid. For energies between those specified, SAMMY uses linear interpolation. Between positions in the time-of-flight grid, SAMMY assumes the function is linear. (This option is similar to, but implemented differently from, the resolution function used in REFIT.⁸⁾)

Compared with either the ORR or the RPI resolution functions (for which the analytic functions are convoluted analytically to the extent possible), the UDR is less efficient, less accurate, and more costly in terms of computation time. Nevertheless, the UDR should prove useful, because the development time for a "new" resolution function is shorter than for a new analytic resolution function.

3. Multiple Scattering Corrections

For measurements of capture and other partial cross sections, significant distortion of the true cross section occurs during the measurement process. A nucleus deep inside the sample may lie "in the shadow" of other nuclei, and hence see only a portion of the original neutron flux. This effect, designated self shielding, is easily and accurately calculated.

Sometimes a neutron will be first scattered by one nucleus (during which process it gives up part of its energy to that nucleus) and subsequently interact with another nucleus. Computation of this single-scattering effect requires a six-fold integration over the location and velocity of the scattered neutron; nevertheless for simplified geometry it can be calculated rapidly and accurately. (The required geometry is a cylindrical or rectangular sample centered perpendicular to the neutron beam.)

The multiple-scattering correction is far more complicated, as each additional scattering prior to capture requires another six-fold embedded integration, which would be prohibitively expensive to calculate exactly. Instead, crude approximations are employed to decouple the integrations. The methodology currently in SAMMY was borrowed from M. C. Moxon⁸⁾ (though the programming was developed independently) and may be explained as follows: Assume that after two scatterings, memory is lost of the history of the neutrons moving through the sample; that is, neutrons are taken to be uniformly distributed throughout the sample. Likewise, the directions of motion of the neutrons are uniformly distributed. Only the energy of the neutrons is remembered. With these simplifying assumptions, it is possible to calculate a reasonable estimation for the multiple-scattering correction (more precisely, for the double-, triple-, etc., scattering correction).

Monte-Carlo simulations are being used to test the validity of both the approximations and the implementations for the single- and double-plus-scattering corrections.⁹⁾ Preliminary results of this study indicate that SAMMY's single-scattering correction is quite accurate. The shape of the double-plus-scattering correction is generally correct, though the relative magnitude varies somewhat from case to case. One probable outcome of this study is to introduce into SAMMY an option for a multiplicative factor for the double-plus scattering.

4. Normalization and Background Corrections

Normalization and background corrections are generally considered to be part of the data-reduction process (that is to say, the process of converting from measured “counts per time channel” to “cross section per energy”). Nevertheless evaluators often find a need to include these in the data analysis process: New information may determine that the original data reduction was incorrect; there may be discrepancies between measurements; or the evaluator may wish to include normalization and background uncertainties directly in the analysis process. Hence SAMMY provides options for a constant normalization and for several varieties of energy-dependent backgrounds.

5. Multiple Nuclides

Because the sample often contains either multiple isotopes of one element, chemical compounds, contaminants, or a combination of all of these, SAMMY includes provisions for analysis of multiple nuclides.

VI. Fitting Procedure

The fitting procedure used by SAMMY is Bayes’ method, which may be viewed as a form of generalized least squares. The derivation of Bayes’ method starts from Bayes’ theorem relating prior and posterior probability density functions (pdf) for the varied parameters. Three additional assumptions are made: (1) The prior joint probability function is a joint normal. (2) The likelihood function (pdf for the data) is a joint normal. (3) The cross section is a linear function of the parameters. Clearly none of the three assumptions is exactly valid, but each is approximately valid under the proper conditions.

One derivation of the least-squares equations makes use of the same three assumptions, plus an additional restriction: Prior knowledge is non-existent. More precisely, the uncertainty on the initial values of the parameters is infinite. [As a practical example, if the initial estimate for the energy of resonance is 138.6 keV, least squares assumes that value is $138.6 \pm \infty$. Bayes’ method assumes 138.6 ± 20.0 , a small-enough value to ensure that this resonance will not interchange position with a neighboring resonance.]

One practical consequence of the use of Bayes’ method (rather than conventional least squares) is that individual measurements may be analyzed sequentially, using output parameter values and covariance matrix from one analysis as input to another. The final set of parameter values is then valid for all included measurements (subject, always, to the validity of the assumptions, in particular to validity of the linearity assumption).

Both Bayes’ method and the least squares equations explicitly include the data covariance matrix. The large size of this matrix ($N \times N$, where N is the number of data points) makes this difficult to include in the computations; hence it is often taken to be diagonal. Such an inaccurate description of the data covariance matrix can, however, lead to erroneous results. Better techniques are therefore necessary. Options are discussed below for treating the systematic (off-diagonal) data uncertainties without actually generating and inverting the large data covariance matrix.

1. Varied Data Reduction Parameters

The parameters used in the corrections for experimental conditions (see Section III of this paper) may be included in the fitting procedure (i.e., “varied”) along with the R-matrix parameters. This includes, for example, normalization, background parameters, nuclide abundances, Doppler temperature, parameters of the resolution function.

For those parameters whose values and uncertainties are determined by the experimentalist (e.g. normalization), the input to SAMMY should include the measured value (call it a) and uncertainty (Δa). In practice, the experimentalist will normalize his data (reduce his data from “counts” to “cross section”) by dividing by a . The analyst will then specify in the SAMMY input that the normalization is $1 \pm \Delta a/a$; the data covariance matrix is taken to be diagonal, including only statistical uncertainties. Results thus obtained are mathematically equivalent to those which would be obtained by generating the full off-diagonal data covariance matrix resulting from the data-reduction process, and not varying the normalization in the analysis process. Computationally, including the normalization uncertainty in the analysis process is the preferred technique, since it is numerically more stable and does not require generation and inversion of large matrices. This technique has the added benefit of refining the value of the parameter during the analysis process.

2. Implicit Data Covariance Matrices

Nevertheless it may be preferable to include the full data covariance matrix rather than treat the data-reduction parameters as variables during the analysis. This is the case when there are many experimental data sets to be included in the evaluation; a normalization, for example, applies to only one of the data sets.

For this purpose, SAMMY can employ a mathematical technique denoted “implicit data covariance.” The formulae for the full off-diagonal data covariance matrix (dcm) are inverted mathematically, without actually generating the full dcm. The arrays which constitute the inverted dcm are dimensioned much smaller than the full dcm. Details are given in the SAMMY manual.¹⁾

V. Other SAMMY features

In addition to satisfying the three requirements described in the introduction, to be truly useful an analysis program should also include pre- and post-processing. Pre-processors provide aid in preparing input for particular cases. Post-processors generate output in appropriate formats for publication or for archiving in evaluated nuclear data files, or calculate statistical properties or other quantities of interest for specific applications.

1. Pre-Processors

Whenever possible, SAMMY provides an interface with the evaluated nuclear data formats (ENDF). When resonance parameters are available in an ENDF File 2 Reich Moore file, these may be used as the initial input to SAMMY; part of the output from that SAMMY run will be equivalent SAMMY-style input files for use in future runs.

When no resonance parameters are available from previous work, “auxiliary” codes (designed specifically for interface with SAMMY) may be helpful in preparing input. R. O. Sayer’s RSAP code¹⁰ can be used to estimate energies and widths for peaks in experimental data. S. Y. Oh and L. C. Leal’s code SUGGEL¹¹ uses statistical methods to suggest values of spin and orbital angular momentum appropriate for particular resonances.

2. Post-Processors

At the completion of an evaluation for which the physics is compatible with the ENDF Reich-Moore format, SAMMY can provide output in that format. This is not always possible because, while SAMMY permits the full generality of the Reich-Moore R-matrix approximation, the ENDF format allows at most one elastic and two fission channels, does not permit charged-particle channels, and has other limitations.

Values for multi-group cross sections, using Bondarenko or plain energy-averaging, can be calculated in SAMMY; covariance matrices for the multigroup cross sections are also calculated.

For nuclear astrophysics applications, stellar (Maxwellian) averages can be calculated as a function of temperature.

VI. Unresolved Resonance Region (URR)

For energies just above the resolved resonance region, the intrinsic resonance width is larger than the spacing between resonances, so that individual resonances cannot be resolved. Averaging techniques must therefore be employed. The methods used in SAMMY are essentially those of F. H. Fröhner’s FITACS code,¹² in which Hauser-Feshbach theory is used for the average total cross section, and Moldauer’s prescription for the partial cross sections. Extensions made for SAMMY’s URR treatment include the ability to use as many experimental data sets as may be available, and an option for energy-dependent normalization for each data set.

VII. Future Extensions to SAMMY

Implementation of a crystal-lattice model for Doppler broadening, extensions to existing resolution functions, and improvements in the as-yet-untried user-defined resolution function are underway.

Modernization of the FORTRAN coding is an on-going process, with the goal of increasing the efficiency and legibility. New, less-cumbersome, input formats are under development.

High on the author’s wish list is restructuring of the entire code to permit truly simultaneous analysis of all available data. With the restructuring, improvements in input will also occur: (a) All R-matrix information (channel definitions, quantum numbers, resonance parameters, etc.) for one compound nucleus will be stored together in a single file. (b) Because the nuclear information will be organized around the compound nucleus (rather than incident particle plus target nucleus, as is now the case), it will be possible to analyze together reciprocal reactions going to the same compound nucleus (e.g., $n+^{16}\text{O}$ and $\alpha+^{13}\text{C}$). (c) All information relevant to a particular experiment (isotopic abundances, normalization and background, resolution functions, etc.) will likewise be isolated into a separate file. (d) Redundancies and ambiguities will be eliminated.

Reorganization is a long-term goal; because it requires a major effort, it will not necessarily be accomplished soon.

Acknowledgments

The author is grateful to the many SAMMY users who offer comments both critical and favorable, suggest improvements, and assist in locating bugs in the program and in the manual. Without their input, the code would be a poor shadow of its current self.

Research sponsored by the Office of Environmental Management, U.S. Department of Energy, under contract DE-AC05-00OR227525 with UT-Battelle, LLC.

References

- 1) N. M. Larson, ORNL/TM-9179/R5, Oak Ridge National Laboratory, Oak Ridge, TN (November, 2000).
- 2) A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958).
- 3) F. H. Fröhner, JEFF Report 18, NEA/OECD (2000)
- 4) R. O. Sayer, L. C. Leal, N. M. Larson, R. R. Spencer, and R. Q. Wright, ORNL/TM-2000/212, August 2000.
- 5) Private communication, J. C. Blackmon, Oak Ridge National Laboratory, USA, 2001.
- 6) Private communication, O. Bouland & R. Babut, Cadarach, France, 2001.
- 7) Private communication, M. Heil, Karlsruhe, Germany, 2001
- 8) M. C. Moxon, NEA-0914/02, July 1989.
- 9) N. M. Larson and K. N. Volev, to be published.
- 10) R. O. Sayer, ORNL/TM-2001/15, February, 2001.
- 11) S. Y. Oh and L. C. Leal, ORNL/TM-2000/314, February 2000.
- 12) F. H. Fröhner, *Nucl. Sci. Eng.* **103**, 119 S 128 (1989).