Appendix A.4. MODIFICATIONS AND ADDITIONS IN REVISION 4

(This page is taken from the Introduction to Revision 4 of this manual, with ~~strikeouts and~~ {inserts} to clarify topics that might otherwise cause confusion.)

Modifications and improvements to SAMMY subsequent to the publication of Revision 3 of this manual are documented here. These changes fall into several categories: (1) Significant additions to the code were requested (and funded) to ensure compatibility with experimental conditions of the linac at Renssaelar Polytechnic Institute (RPI). (2) Other features were designed to facilitate interaction between differential and integral data analysis; this work was funded primarily by the Nuclear Criticality Predictability Program (NCPP). (3) Miscellaneous new features and/or new descriptions of old features. (4) Modifications that fall under the general heading of "routine maintenance." (5) Planned future modifications and improvements. Even though the features are itemized in this section under these categories, the reader is encouraged to read the entire introduction, because features developed for one purpose are often suitable for use for another.

1. RPI Options

Further options have been added for background functions. See Section ~~V.E.1, page 98g~~ {III.E.3.a}.

A resolution function has been added which was designed specifically for use with data taken at the Gaerttner LINAC at RPI, but is presumably useful for data taken on other machines as well. See Section ~~IV.G, page 92s~~ {III.C.3}. Note that this resolution function is not necessarily the "final word" for RPI data, but may be updated for the next revision of SAMMY.

The ability to analyze self-indication experiments has been implemented; composition and temperature of the transmission and capture samples need not be identical. See Section ~~III.G~~ {III.E.6}.

A truly *multiple* multiple-scattering correction has been developed for capture and fission yields, and implemented in the code; see Section ~~III.F~~ {III.D}. Detailed documentation is being prepared, to describe precisely what approximations are used for this important correction factor.

An option has been added to use *l*-dependent detector efficiencies for capture or fission yields or for self-indication experiments. See Section ~~V.K~~ {III.E.5}.

An option has been added to include paramagnetic cross section in addition to the total cross section calculated from the resonance parameters. See Section ~~V.H~~ {III.E.4}.

2. Integral/differential features

Average theoretical cross sections can now be calculated accurately, using SAMMY's auxiliary energy grid, without generating experimental corrections (Doppler and resolution

broadening, etc.) on the theoretical values. The inability to do so was a shortcoming overlooked until recently and therefore not included in earlier versions of the code. Use the command "`MAKE NO CORRECTIONS To theoretical values`" in the INPut file (see Section VI.A., Table VIA.2), and do include some broadening parameters (which will not be used, but will force SAMMY to generate and use the dense auxiliary grid).

In addition to the energy-differential (and angle-differential) data that SAMMY was designed to analyze, some types of integral data can now be fitted directly with SAMMY. These are described in Section ~~VI.I, page 130m~~ {V.B}, and in greater detail in a separate document [NL97]. (Note that two additional types of integral data have been added to SAMMY subsequent to the release of that document.)

Most experimental data have both statistical errors (for which the covariance matrix is diagonal) and systematic errors (for which the covariance matrix is decidedly off-diagonal). Often analyses include only the statistical errors, or only the diagonal portion of the systematic errors, even though this practice is known to give inaccurate results. To make it easier for SAMMY users to use the correct covariance matrix, SAMMY now contains an option to include Implicit Data Covariance (IDC) information, for which the user must provide only minimal input; see Section VI.C.3. For an application of this technique, see ref. [HD97].

In an effort to improve communication with data processing codes, and to encourage such codes to make use of covariance information for resonance parameters, SAMMY can now provide output of the resonance parameter covariance matrix in a format that may be efficient for transmittal to those codes. See Section ~~V.K (page 98u)~~ {VII.E}.

3. Miscellaneous New Features

Values for fundamental physical and mathematical constants have been sited at one location only within the code, to ensure that the exact same values are used consistently throughout the code. Default values have been modified to conform to the current ENDF standards; see ~~Appendix E, page 241~~ {Section IX}, for the Cross Section Evaluation Working Group recommendations regarding values of constants.

Test cases (both input and output) have always been available for quality control with SAMMY and can also be useful in learning to use a new feature. A table describing the various test cases has been added to this manual (see Section ~~XI.D, Table XID.1~~ {XII.B}), and many sections now include references to the appropriate test cases.

For the *Workshop on Nuclear Reaction Data and Nuclear Reactors—Physics, Design and Safety* (held February 23 through March 27, 1998, at the International Centre for Theoretical Physics, Trieste, Italy), a series of exercises was developed as an aid in learning how to run SAMMY. These exercises are now included in the standard SAMMY package when the code is requested from the Radiation Safety Information Computational Center (RSICC) (formerly the Radiation Shielding Information Center) or other data centers. See Section ~~X.D (page 206a)~~

{XII.A} for information about these exercises. The companion lecture notes are available as [NL98a].

Generating the appropriate set of spin groups for the nuclide of interest can be a confusing task. See Section ~~VIII.I (page 150o)~~ {X.J} for guidance.

Converting from REFIT input [MM89] to SAMMY input (or vice versa) is discussed in Section ~~VIII.J (page 150w)~~ {X.B}.

Direct comparison of theoretical cross sections calculated by SAMMY with those calculated by other codes is facilitated by the use of program SAMCMP. See Section ~~VIII.K, page 150y~~ {X.E}.

SAMMY now automatically calculates average resonance widths and uncertainties thereon. These widths and uncertainties are reported in the LPT file, along with the updated resonance parameters, after data are fitted.

For guidance on the analysis of experimental data for which the sample contains more than one nuclide (multiple isotopes, chemical compounds, contaminants), see Section ~~V.D on page 98c~~ {III.E.2}.

Previously, when varying channel radii, SAMMY has implicitly assumed that reduced width amplitudes are held constant; hence the various partial widths (neutron widths, in particular) would be modified even if they were not explicitly varied. The user now has an option to override this assumption by specifying "DO NOT MODIFY UNVARied widths" in the INPut file; see Table VIA.2~~, page 114c~~.

4. Routine Maintenance

The entire code has been converted to double precision; previously, only those pieces deemed critical utilized double precision.

Output in the LPT file has been modified to (usually) fit 80 columns rather than 120; this change was driven by the current habit of viewing files on a screen rather than making hard (paper) copy of each file.

A few of the defaults have been changed:

USE 1999 ENDF-102 CONSTANT VALUES now replaces USE PRECISE VALUES OF CONSTANTS. This change ensures that SAMMY results are consistent both with ENDF conventions and with results obtained from other Reich-Moore codes such as NJOY [RM82], {PREPRO [DC04]} MULTIPOLE [RH87], and REFIT [MM89]. Internally, values for the constants are now sited in only one location in the coding, to ensure self-consistency and to facilitate future changes. See ~~Appendix E~~ {Section IX.A} for the CSEWG recommendations regarding values for

physical constants and Table {VI A1.2} ~~VIA.2 (page 114)~~ for description of how "older" values of the constants may be obtained.

The free-gas model (FGM) of Doppler broadening has been shown [NL98] to be a better choice for **all** energies, rather than the high-energy Gaussian approximation to the free-gas model. FGM is now the default option for Doppler broadening.

The "new" spin group format is more versatile and contains more information than the original format, and is now the default. Users whose INPut files do not use this format will receive error messages from SAMMY, along with suggestions about the necessary changes. [Note: The obsolete spin group format has been found to produce erroneous results when used in conjunction with angle-differential calculations (e.g., multiple-scattering corrections for capture or fission yields). Use of the obsolete spin group option is therefore not permitted in cases where it would produce errors.]

Minor bugs have been fixed; a partial list is given here:

The ASCII option for reading differential elastic scattering data now works consistently.

Integration limits for Doppler broadening have been extended somewhat to ensure more accurate results in those situations where the end of the integration region falls in the middle of a resonance. In addition, the algorithm for choosing the auxiliary grid near small resonances has been improved.

Errors in the documentation of the differential elastic cross section (Section ~~III.E~~ {II.B.1.b}) have been corrected. These errors were only in the documentation, not in the coding.

A correction has been made for programming error affecting only reaction (inelastic or fission) cross sections, in the case when there are more than two reaction channels.

5. Future Plans

Among the features planned for addition to SAMMY in the near future are: (1) More integral quantities, particularly those appropriate for intermediate energies. (2) Charge-dependent penetrabilities, to more accurately describe outgoing fission channels and to extend the capability of the code from neutron-induced reactions to charged-particle-induced reactions. {See Section II.C.4.} (3) Interface with other codes for use of covariance matrix. (4) Resolution function appropriate for use with Geel data (in collaboration with Saclay and Cadarache). {See Section III.C.3.} (5) Restructuring of the code to permit truly simultaneous analysis of any and all data sets~~; see Appendix F for details.~~