Appendix A.5. MODIFICATIONS AND ADDITIONS IN REVISION 5

(This page is taken from the Introduction to Revision 5 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 4 of this manual are summarized here.

(1) The ability to calculate Coulomb penetrabilities, shift factors, and phase shifts will extend the applicability of SAMMY to other types of data such as (n,α), (n,p), (p,n), (α,n). Section ~~III.H~~ {II.C.4} provides details on the Coulomb implementation in SAMMY.

(2) One change which is essentially invisible to the SAMMY user is the combination of the various segments into one large program. In addition to easing portability problems, this change has resulted in increased computation speed; SAMMY runs with Version M5 will require less CPU time than the same runs with earlier versions. Details are found in Section ~~XI~~ {XIII.C}.

(3) From the equations for Doppler broadening (~~Sect. IV.A.1 and IV.F~~ {Section III.B}), it is clear that the Doppler width is mass dependent, and therefore changes from nuclide to nuclide. Unfortunately this detail was overlooked in prior versions of SAMMY (M2a and earlier). That oversight has been corrected for Version M5. For most experimental conditions, this will be a small effect. For cases in which two nuclides, both with large abundances, have vastly different masses, the effect will be more pronounced. SAMMY users will want to be aware of this error and consider what impact it might have on their evaluations.

(4) It is now possible to calculate individual reaction types or individual fission channels. For example, one might wish to know the (n,α) cross section separately from (n,p) or (n,n`). [In prior versions of SAMMY, all "exit channels" were automatically included in the outgoing final state whenever the data was specified as inelastic, fission, or reaction.] Details on how this is accomplished are given in ~~Sect. V.L, page 98w~~ {Section II.B.1.c}.

(5) A bug was discovered (and exterminated) in the derivatives with respect to resonance parameters. This bug was found while the author was playing with artificial data, and occurred only when the penetrability was very small, that is, for low energies and non-zero angular momentum. Hence it is highly unlikely to have affected calculations relating to physical data.

(6) Errors in implementation of the RPI resolution function have been corrected, and the form of the function generalized. Preliminary values of resolution parameters suitable for use with Geel data are provided. See ~~Sect. IV.G.~~ {Section III.C.3}.

(7) Values of parameters for either the RPI resolution function or the ORR resolution function can now be given in either the INPut file or the PARameter file. If any parameter is to be varied, the PARameter file must be used.

(8) Improvements in the treatment of the unresolved-resonance region include more exact calculation of partial derivatives, normalization options for the experimental data, and increased flexibility for input of experimental data. Details are given in Section ~~V.J (page 98s)~~ {VIII }.

(9) Derivatives with respect to the matching radius (channel radius) are now generated in a self-consistent and logical manner. When the matching radius is varied but the neutron width is held fixed, the width Γ_n and not the partial-width amplitude γ_n remains unchanged. This is true also for other widths with non-unit penetrabilities (including Coulomb penetrabilities).

(10) It is now possible to utilize the ~~MPW~~ {M+W} solution for Bayes' equations in the resolved resonance region in a limited fashion. Individual SAMMY runs can generate W_i and Y_i for several data sets, and an additional SAMMY run will read those arrays, add them appropriately, and update the parameter values and covariance matrix (i.e., solve Bayes' equations via ~~MPW~~ {M+W} method). See ~~Sect. II.B.1.c (page 20c)~~ {Section IV.B.3} for more details. This scheme was initially devised for retroactively generating an approximate covariance matrix for a pre-existing set of resonance parameters {Section IV.E.2}.

(11) Bondarenko averaging is now available for the generation of multigroup cross sections; see Section V.C.2 for details.

(12) Output covariance matrices for the resonance parameters can now be provided in an abbreviated ~~"concise"~~ {"compact"} ASCII file, which the author intends to propose for adoption as an ENDF format. Details are given in Section VII.E.

(13) SAMMY can utilize ENDF File 2 (LRU=1, LRF=3, i.e. the Reich-Moore format) for input of resonance parameters (see ~~Sect. VI.G~~ {Section VI.F.3}), and can also provide output in ENDF File 2 format (see ~~Sect. VI.F~~ {Section VI.F.2}). The format change approved at the November 1999 CSEWG meeting is included; this format change permits specification of channel spin as well as resonance spin and orbital angular momentum for each resonance.

(14) Additional output files, in legible (ASCII) format, are now provided by the auxiliary programs SAMORT (~~Sect. VIII.C~~ {Section X.H}) and SAMRPT (~~Sect. VIII.M~~ {Section X.K}). These new files, with extensions PLT, are intended for use where the ORNL plotting package FORODF is replaced by another package.

(15) Auxiliary code SAMSMC can be used to generate Monte Carlo simulations of the multiple-scattering corrections to capture and/or fission yields. See ~~Sect. VIII.O page 150z.7~~ {Section X.M}.