

## X.C. SAMAMR: ADD, MIX, OR RECOVER VARIABLES

Because the fitting procedure in SAMMY is Bayes' method (Section IV) rather than ordinary least squares, SAMMY may be used for general evaluation purposes, that is, for determining a set of parameters that simultaneously describe a large number of different types of experimental data taken at different times and/or at different laboratories.

Performing such evaluations with SAMMY originally required sequential analyses of the various data sets,\* with the output parameter and covariance matrix from the first analyses used as input to the second, output from the second used as input to the third, and so forth. If none of the broadening parameters are varied during the analyses, and if no data-reduction parameters are included, this procedure poses no undue difficulty; the analyst simply changes the values of the thickness and/or of the broadening parameters in the INPut file to correspond to the data currently being analyzed. However, when any of the broadening parameters are varied, and/or when normalization or background is included in the analysis, the PARAmeter and COVariance files must also correspond to the current data set. The code SAMAMR performs the appropriate modifications to the PARAmeter and COVariance files.

For example, data may come from two or more samples of different thicknesses and at different temperatures. The initial PARAmeter file is set up to include thickness and temperature appropriate for the first sample; thickness and temperature for the other samples are simply omitted. After the analysis of the first data set, code SAMAMR is used to incorporate the second thickness (as yet uncorrelated to any other parameters) and to "mothball" the correlated but now-to-be-unused first thickness; a second run of SAMAMR introduces the new temperature parameter and mothballs the old. The resulting PARAmeter file can then be used as input for the SAMMY analysis of the second data set. If, for a subsequent SAMMY run, one of the "UNUSED" parameters must be used again, SAMAMR will interchange the current BROADening parameter with the appropriate UNUSED parameter.

To illustrate, suppose three data sets are available, taken from three samples at two different temperatures:

Data Set 1: Sample 1 (thickness  $n_1$ , Temperature  $T_1$ )

Data Set 2: Sample 2 (thickness  $n_2$ , Temperature  $T_2$ )

Data Set 3: Sample 3 (thickness  $n_3$ , Temperature  $T_1$ )

The sequence of commands required to properly analyze these data is shown in Table X C.1. The input PARAmeter file (t007a.par) is listed in Table X C.2. Output PARAmeter files are listed in Tables X C.3 through X C.12. (Data and analysis are courtesy of F. G. Perey [FP84].) Note that values (and covariances) of the unused parameters are updated in each SAMMY run, even though the data have no direct effect on those parameters. Rather, the effect

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\* This is still the "standard mode" of operation for SAMMY. However, it is also now possible to simultaneously analyze more than one data set (Section IV.E.1), so long as none of the data-specific parameters are varied. The uncertainties on the data-specific parameters can, however, be included in the data covariance matrix, via the PUP option as described in Section IV.D.2.

is indirect, via the parameter covariance matrix. Note also that values (and uncertainties) are never changed in a SAMAMR run. Complete listings of all INPUT, PARAMETER, DATA, and LPT files for this example are given in Test Case tr007, which is available along with the SAMMY FORTRAN from the Radiation Safety Information Computational Center [RSICC].

SAMAMR was designed to be run interactively (though a command file can of course be created, once the user is sufficiently familiar with the input). The code will prompt the user with questions about the type of operation to be performed, the parameters involved, and values for any new parameters.

Type of operation. The first question asked by SAMAMR is “Do you want to Add, Mix, Remove, reCover, or Introduce variables?” The user will type the capitalized letter for the appropriate operation.

Add refers to (1) the removal of one parameter to the unused list and (2) the introduction of another parameter (of the same kind) into the active list. The user is asked to specify the particular parameter (from a list provided), to give the variable number for that parameter if it was varied in the run which produced this covariance file, and to give the value and uncertainty to be used for the new parameter. Mix refers to the interchange of one unused parameter with the corresponding parameter in the active variable set. The user must provide the location (variable number) within the unused parameter set.

The operations Remove, reCover, and Introduce are used to reorganize the attenuation or normalization-and-background parameters when the analysis involves both angle-differential data (such as the elastic angular distribution scattering data) and other data that are integrated over angle (such as transmission). The operation Remove moves normalization-and-background parameters for all angles, or attenuation parameters for all angles, from the active variable set to the unused variable set. The operation reCover performs the inverse, moving parameters from the unused to the active set. Introduce allows the introduction of new parameter values and uncertainties when switching from analysis of angle-integrated data to analysis of angular distribution data.

Type of parameter. The types of parameters to be treated by SAMAMR are different, depending on the operation to be performed.

For both Add and Mix, only one parameter is treated at a time; the example shown in Table X C.1 therefore requires two runs of SAMAMR between each run of SAMMY. The parameters that can be treated are taken from the following list, in which is also given the card set and line number from the PARAMETER file (see Table VI B.1):

(Broadening parameters)

TEMP , THICK, DEL-L, DEL-G, DEL-E (card set 4, line 3)

(Normalization and background parameters)

NORML, BACKA, BACKB, BACKC,  
BACKD, BACKF (card set 6, line 2)

## (ORR resolution parameters)

BURST	(card set 9, line 2)
WATR0, WATR1, WATR2	(card set 9, line 3)
TANTA	(card set 9, line 3)
X1, X2, X3, X0	(card set 9, line 4)
WWW, ALPHA	(card set 9, line 6)
D, F, G	(card set 9, line 8)
DELTA	(card set 9, line 8)
CHANN	(card set 9, line 10)

## (Miscellaneous parameters, with alternative names in square brackets)

DELTA, DELT2 [DELL1, DELL0]	(card set 11, line 2)
NU [ETA]	(card set 11, line 3)
ATTNI, ATTNO [FINIT, FINI2]	(card set 11, line 4)
TZERO, LZERO	(card set 11, line 6)
SIABN	(card set 11, line 7)
SITEM, SITHC [SELF1]	(card set 11, line 8)
EFFIC, FISEF [EFCAP, EFFIS]	(card set 11, line 9)
DELTE, DELE0, DELE2 [DELE1, DELE0, DELE2]	(card set 11, line 10)
CONCR, CONTR	(card set 11, line 11)

## (RPI/GELINA/nTOF resolution function parameters)

BURST	(card set 14, line 2)
TAU	(card set 14, line 3)
LAMBD	(card set 14, line 5)
A1	(card set 14, line 7)
EXPON	(card set 14, line 9)
CHANN	(card set 14, line 11)

In addition to giving the parameter name, as given in the above list, the user will sometimes also need to specify which parameter of this type is to be used. The name is given in the first five columns (be sure to leave blanks if the name is fewer than five characters), and an integer number is then given. For the RPI resolution parameters, the second, third, etc., variables on the line (in the PARAmeter file) are specified by “2”, “3”, etc., in the SAMAMR input. See test case tr087 for examples of this.

For the operations Remove, reCover, and Introduce, only the parameters ATTEN and ALLNB may be specified. When ATTEN is specified, all attenuation parameters (both incident and outgoing, from card set 11, line 4 of the PARAmeter file) are involved. When ALLNB is specified, all normalization and background parameters are involved (see card set 6, line 2). Again, only one type can be treated during one run of SAMAMR.

When the operation Introduce is used, attenuation or normalization/background parameters are assumed to be given in a separate file in the same format as used in the PARAmeter file (either with or without the “MISCEllaneous parameters” or “NORMAlization and background” header lines of card sets 11 and 6; however, if they are included, the first five

characters must be either all caps or all lowercase). SAMMY will ask for the file name instead of the parameter values. Test case tr036 shows examples of the use of this feature.

An additional restriction for operations Remove, reCover, and Introduce stems from the connection between the attenuation parameters and the number of angles: SAMAMR assumes that removal of attenuation parameters implies changing from angular-distribution data to angle-integrated data, and that recovery or introduction of attenuation parameters implies the reverse change. Removal of attenuation parameters, therefore, must be accomplished *after* removal of normalization and background parameters, and recovery or introduction of attenuation parameters must be accomplished *prior to* recovery or introduction of normalization and background parameters.

Test cases tr007, tr032, tr036, tr079, and tr087 all have examples of the use of program SAMAMR.