

Data Analysis and Evaluation with SAMMY

Luiz C. Leal

Oak Ridge National Laboratory
Oak Ridge, TN 37831-6370, USA
E-mail: leallc@ornl.gov

Various steps are required prior to the use of SAMMY¹ to search for resonance parameters that best represent the experimental data. This lecture will focus on the common practice utilized to perform data evaluation, in particular, the evaluation procedure used for data analysis in the resolved-energy region using the reduced R-matrix formalism i.e., the Reich-Moore approximation.² A similar approach can be used for data analysis and evaluation in other energy regions. The first step in the evaluation process consists of defining the energy range for which the evaluation will be carried out and making sure that all possible open reaction channels (i.e., inelastic channel, charged particle channels, etc.) are identified.

When using SAMMY for data evaluation, a minimum of three input files are required to initiate the evaluation. These files are (1) an *inp* file which contains the experimental conditions including flight-path length, temperature, sample thickness, resolution parameters, resonance spin information, etc. This file will be referred to as the *.inp* file (2) a file that has the initial estimation of the resonance parameters, which will be referred to as the *.par* file and (3) a file containing the data to be evaluated, referred to as the *.dat* file. Experience has shown that the success of completing an evaluation is highly dependent on how well these files are prepared, primarily the *.inp* and *.par* files.

To illustrate how to perform an evaluation using SAMMY, an example using the total cross section for ²³⁵U will be presented. Table 1 shows the general information for this isotope.

Table 1. General Information for ²³⁵U.

A	235
Z	92
Target Spin and Parity*, <i>I^P</i>	7/2 ⁻
Nuclear Radius	9.6 fm

*Note: neutron spin and parity: 1/2⁺

The description of the experimental conditions for which the total cross section measurements were performed for ²³⁵U is given in Table 2. The information given in Table 1 and Table 2 is very important for constructing the *.inp* file for SAMMY.

Table 2: Information on Total cross section Measurements for ^{235}U .

Measurements Descriptions	
Material	^{235}U
Data type:	Total Cross Section
Laboratory:	ORNL
Experimentalist:	J. Harvey et al.
Run Number:	10409
Date of Experiment:	7/7/1986

Experimental Conditions	
Flight Path Length \pm Dispersion (m)	80.394 ± 0.022
Neutron Overlap Filter	0.60 cm P.B. 150 mg/cm ² ^{10}B
Permanent Background Sample	(Not applicable)
Sample for the Determination of Background	(Not applicable)
Linac Burst Width (ns)	20
Repetition Rate (sec ⁻¹)	347
Power (kW)	13
Moderator	(Not applicable)
Moderator Thickness	(not applicable)
Detector Type	Glass scintillator

Table 2: (continued).

Time-of-Flight Analyzer	
Energy Range (eV)	Channel Width (ns)
$E < 13.8$	512
$13.8 < E < 35.3$	128
$35.3 < E < 114.3$	64
$114.3 < E < 408.0$	32
$408.0 < E < 1325.0$	16
$1325.0 < E < 9380.0$	8
$9380.0 < E < 4$	2

Sample Characteristics	
Weight (grams)	(Not needed)
Thickness (atom/barn)	0.03294
Isotopic Composition	99.6 % enriched ^{235}U
Sample Composition (Impurities, etc)	^{151}Ta , ^{234}U , ^{236}U , ^{238}U
Size (cm)	1.47-cm diameter 0.69 cm thick
Temperature (K)	Liquid Nitrogen (77 K)

1. Preparation of the *.inp* file:

There exist several “command statements” which indicate to SAMMY the type of actions that should be taken. For instance, a statement like “BROADENING IS NOT WANTED” indicates that no broadening, including temperature or resolution, will be calculated. Users should include the statements that best fit their problems. Much of the content included in the *.inp* file is obtained from the information given in Table 1 and Table 2. In the following, we show how this information is adapted to SAMMY.

1.a. Doppler and Resolution Broadening Information

Most contemporary neutron cross-section measurements in the resolved resonance energy region are done by the time-of-flight (TOF) technique. Pulses of neutrons are collimated on a flight path, and the time intervals between the neutron pulse and the events at the detector at the end of the flight path are recorded. The neutron energy can be obtained from the time of flight t_n and the effective flight path length L by the relation

$$E_n = \mu^2 \frac{L^2}{t_n^2} \text{ where } \mu = 72.3 \text{ eV}^{1/2} \mu\text{sec/m.}$$

The energy resolution in a TOF experiment can be obtained as

$$\left(\frac{\Delta E}{E} \right)^2 = 2 \left[\left(\frac{\Delta t_n}{t_n} \right)^2 + \left(\frac{\Delta L}{L} \right)^2 \right]$$

where Δt_n is the flight-time uncertainty and ΔL is the flight-path uncertainty. Details on the calculation of the resolution functions are found in SAMMY user manual (IV-A-2). The resolution in the TOF Δt_n can be expressed as

$$\Delta t_n^2 = \sum_i \Delta t_i^2$$

where Δt_i represents the different contributions to the time uncertainty Δt_n mainly due to:

Δt_{cw} , the TOF analyzer width;

Δt_{bw} , the width of the neutron burst; and

Δt_{ed} , the instability of the electronic device (jitter), etc.

If the contributions are considered as square distributions then the full width at half-maximum (FWHM) of the equivalent Gaussian distribution is given by

$$\Delta t_G = 0.67978 \Delta t_n, \text{ where}$$

Δt_G is the parameter entered in the input file for SAMMY.

The uncertainty in the flight-path length is the combination of the uncertainty due to the neutron moderator (if any) ΔL_m and the uncertainty due to the detector ΔL_d , so the total flight-path resolution parameter is

$$\Delta L^2 = \Delta L_m^2 + \Delta L_d^2; \quad \Delta L \text{ is the input parameter to SAMMY.}$$

The experimental resolution is calculated in SAMMY using information from the *.inp* file in "CARD SET 5" according to the information given in Table 2. The first parameter in "CARD SET 5" is the sample temperature which (according to Table 2) is 77 K. The flight path length is 80.02 m and the dispersion on the flight-path is 0.022 m. No information was given in Table 2 regarding the exponential resolution (asymmetry on the resolution function). The next parameter in "CARD SET 5" indicates to SAMMY that the resolution due to the experimental devices is a Gaussian resolution function representing the burst width. Since the burst width indicated in Table 2 refers to a rectangular function, a conversion to a Gaussian width (multiplication by a factor of 0.67978) is needed. When a negative sign is assigned to the burst width, this indicates to SAMMY that the information on the channel widths is given in the following cards, "CARD SET 6", in units of μs . The remaining parameters in "CARD SET 5" may be used as needed. The information concerning channel radius and sample thickness is given in "CARD SET 7".

1.b Spin and parity

The usual quantum mechanics algebra for determination of the spin and parity of the compound nucleus $n+^{235}\text{U}$ is given as follows:

$$s = I \oplus i, \text{ where } |I \oplus i| = s \oplus |I \oplus i|;$$

$$J = l \oplus s, \text{ where } |l \oplus s| = J \oplus |l \oplus s|; \text{ and}$$

$$(J \oplus l) \oplus s = (J \oplus l) \oplus s;$$

where i is the neutron spin, I is the target nucleus spin, s is the spin of the compound nucleus, l is the relative neutron-nucleus angular momentum and J is the total angular momentum of the compound nucleus. From the information given in Table 1 and the previous equations, the spin groups for the compound nucleus $n+^{235}\text{U}$ are obtained as given in Table 3.

Table 3. Spin and Parity of the Compound Nucleus

$I p_0$	l	s	$J p$				Spectroscopic Notation	
7/2 ⁻	0	3	3-				s	
		4	4-					
	1	3	2+	3+	4+		p	
		4	3+	4+	5+			
	2	3	1-	2-	3-	4-	5-	d
		4	2-	3-	4-	5-	6-	

Users are advised to include the statement "USE NEW SPIN GROUP FORMAT" in the *.inp* file and use the option alternative to "CARD SET 10" to enter the information given in Table 3.

The Reich-Moore formalism, which is appropriate to treat the interference effects in the fission channels, will be used to analyze ^{235}U . Although several fission channels can be used, two fission channels give a reasonable description of the interference effects and, therefore, the total number of opened channels will be three: one neutron channel and two fission channels.

The input file *.inp* for the ^{235}U is shown in Table 4. It should be noted that the spin data included are those for s-wave ($l=0$) and p-wave ($l=1$) totaling eight spin group numbers. These spin group numbers will match the corresponding resonance levels given in the *.par* file. For instance, a resonance with spin group number one corresponds to a s-wave with total angular momentum $J=3$.

Table 4. Input for SAMMY, the *.inp* file

```

92-U-235 total cross section data (Harvey et al. 1986)
  U235      235.
use new spin group format
csisrs
chi squared is wanted
generate plot file a
use free gas model of

  77.00      80.394      .022      .0      -.0136
    1.0      7
    13.8      0.512      35.3      0.128      114.3      0.064      408.0      0.032
    1325.0      0.016      9380.0      0.008      100000.0      0.002
  9.6      .03294
total cross section
-3.5      0.      0      1
1      1      2      -3.      1.      -3.5      U235      S3- (s=3)
  1      1      0      0      -3.      0.      0.000
  2      0      0      0      -3.      0.      0.000
  3      0      0      0      -3.      0.      0.000
2      1      2      -4.      1.      -3.5      U235      S4- (s=4)
  1      1      0      0      -4.      0.      0.000
  2      0      0      0      -4.      0.      0.000
  3      0      0      0      -4.      0.      0.000
3      1      2      2.      1.      -3.5      U235      P2+ (s=3)
  1      1      0      1      -3.      0.      0.000
  2      0      0      1      -3.      0.      0.000
  3      0      0      1      -3.      0.      0.000
4      1      2      3.      1.      -3.5      U235      P3+ (s=3)
  1      1      0      1      -3.      0.      0.000
  2      0      0      1      -3.      0.      0.000
  3      0      0      1      -3.      0.      0.000
5      1      2      4.      1.      -3.5      U235      P4+ (s=3)
  1      1      0      1      -3.      0.      0.000
  2      0      0      1      -3.      0.      0.000
  3      0      0      1      -3.      0.      0.000
6      1      2      3.      1.      -3.5      U235      P3+ (s=4)
  1      1      0      1      -4.      0.      0.000
  2      0      0      1      -4.      0.      0.000
  3      0      0      1      -4.      0.      0.000
7      1      2      4.      1.      -3.5      U235      P4+ (s=4)
  1      1      0      1      -4.      0.      0.000
  2      0      0      1      -4.      0.      0.000
  3      0      0      1      -4.      0.      0.000
8      1      2      5.      1.      -3.5      U235      P5+ (s=4)
  1      1      0      1      -4.      0.      0.000
  2      0      0      1      -4.      0.      0.000
  3      0      0      1      -4.      0.      0.000

```

2. Preparation of the *.dat* file

Selection of experimental data for neutron-nucleus interaction for use in a resonance evaluation can often be done by consulting one or more nuclear data banks. Nuclear data banks, such as the Brookhaven National Nuclear Data Center, the data bank of the Nuclear Energy Agency, and the data bank of the International Atomic Energy Agency, contain a variety of data which originate from contributions of several laboratories around the world. The data are available in the data bank on the Cross-Section Information Standard Retrieval System (CSISRS)³ in the EXFOR files (EXchange FORmat). Additional information can be obtained also in the Computer Index of Neutron Data (CINDA).⁴ Part of the information provided in Table 2 was obtained from the EXFOR file of which a portion is shown in Table 5. As can be seen in Table 5 the descriptions are not complete, since details such as the TOF analyzer have not been furnished. The evaluator should consult the published reference, or, if possible, get in touch with the experimentalist and inquire about information on the experimental conditions. The run number (in this particular case 10409) is used to identify the experiment. It should be noted that the data in Table 5 are energy (in decreasing order), cross section and the absolute cross section error.

In addition to the total cross section, the evaluator will find it useful to include other data in the evaluation. For instance, if the ²³⁵U evaluation is to be performed in the energy range from few eV to 10 eV, the evaluator would very likely be looking for the following additional data: transmission data (total cross section), fission cross section, capture cross section, data which include cross section at thermal (0.0253 eV), integral values, etc. Once the evaluator has carefully selected the experimental data, the next step is to make sure that all the data are consistent. The most likely sources of inconsistency will be energy calibration, normalization, background, etc. The energy alignment of the data should be made by choosing the best resolution data (longer flight-path, low temperature measurement, low background) as the standard and aligning all other data according to the standard.

3. Preparation of the *.par* file

Perhaps the hardest task the evaluator will face is the preparation of a *.par* file. It is an interesting issue because a *.par* file is actually the goal of the evaluation; i.e., the best set of parameters that fit all the data consistently. Experience has shown that preparing a good set of initial resonance parameter values may save a substantial amount of time in completing an evaluation. The open literature (for instance, *Physics Review*, *Journal of Nuclear Science and Engineering*, etc.) is an important source which evaluators should use in looking for information on resonance parameters. Other sources are the nuclear data libraries such as ENDF, JEF, JENDL, etc., and books on resonance parameter compilations, such as the Mughabghab BNL-325 book.⁵ However, when no other information is available, the evaluator must use heuristic approaches based on observation of the experimental data. In the following, a procedure is presented to help evaluators to construct an initial set of resonance parameters. The evaluator should be aware that in the SAMMY evaluation a resonance parameterization using the Reich-Moore approach may require the following parameters: the resonance energy (E_r), neutron width (G_n), gamma width (G_γ), two channels, (G_{f1}) and (G_{f2}) describing the fission channels, and the spin of the resonance (J). These five parameters characterizing a resonance are input to SAMMY in the *.par* file. To help evaluators to construct a starting set of resonance parameters a simple tool was developed at ORNL; it is built in as an option in the plotting package RSAP⁶ based on the method developed by Mariscotti.⁷ RSAP is a computer code that plots neutron cross section data generated by SAMMY. The basic idea is to search the total cross section and extract information on maximum, peak height, areas etc. The parameters are those equivalent to the cross section representation based on the Single-Level Breit-Wigner approach. Remember that the initial set of resonance parameters is a set of numbers with the purpose of providing evaluators with an initial guess and therefore may not have any physical meaning. The initial set of resonance parameters is generated in the user-specified energy range by searching the experimental total cross section. The resonance energies are determined by searching for maxima, or peaks, in the total cross section. Once a peak is found, RSAP estimates the resonance width, height, and area of each peak and creates a set of resonance parameters in the format required for SAMMY. A downside of this approach is that resonance spin is not given, so the evaluators should assign spin to each resonance at random. Likewise, the fission widths are all assumed to be positive, so the evaluator should assign random signs to the fission widths.

To illustrate the application of the approach for determining an initial resonance set, let us consider the total cross section data given in Table 5 in the energy range from 4 eV to 20 eV. In this energy range the resonances are most likely to be due to s-wave ($l=0$). There will be only two resonance spin states, corresponding to total angular momentum $J=3$ and $J=4$, respectively. The initial set of resonance parameters in the SAMMY format of the *.par* file generated by RSAP with resonance spins and fission channels signs assigned at random is given in Table 6. The numbers in the last column in Table 6 are not the total angular momentum but rather the spin group for each resonance. In other words, the total angular momentum for $J=3$ is grouped in the spin group 1, whereas the total angular momentum for $J=4$ is grouped in the spin group 2. These spin groups match the ones provided on "CARD SET 10" of the *.inp* input. A comparison of the experimental total cross section and the calculation with SAMMY using the initial resonance parameter set is shown in Fig. 1. As can be

seen, most of the resonances are included in the set. However, there are still some resonances that are missing, as for example, in the energy regions 9 eV to 10 eV and 13 eV to 14 eV. The advice to the evaluators is to localize the resonance energy and use the widths of a resonance with a shape similar to the one in question. This exercise can be done by trial-and-error. At this point evaluators should let SAMMY search solely for the resonance energy and the neutron width to evaluate the total cross section. This procedure will improve the estimation of the neutron width. The next step is to include the fission cross section data. Evaluators are advised to fit the fission cross section data by letting SAMMY search alternatively for one fission channel at a time. After, around ten iterations, evaluators should vary both fission channels and run SAMMY until a roughly good representation of the fission cross section is obtained. At this point the one should use the total cross section and the fission cross section, respectively, in the fitting, keeping the capture width unchanged. The resonance parameters generated in this procedure address the energy region 4 eV to 20 eV. No information regarding the contribution of resonances below 4 eV and above 20 eV are given. External levels need to be included in the evaluation to account for the interference effects of these resonances.

Table 6: Initial set of resonance parameters in the SAMMY format generated by RSAP in the energy range from 4 eV to 20 eV.

E_r	G_γ	G_n	G_{f1}	G_{f2}	J
4.810	3.8000E+01	4.4764E-02	2.063E+01	-2.063E+01	1 0 1 0 1
4.871	3.8000E+01	4.8218E-02	2.638E+01	-2.638E+01	1 0 1 0 2
5.164	3.8000E+01	1.9562E-02	-2.118E+02	2.118E+02	1 0 1 0 1
5.466	3.8000E+01	9.8105E-03	8.095E+00	8.095E+00	1 0 1 0 2
6.206	3.8000E+01	6.3603E-02	4.772E+01	4.772E+01	1 0 1 0 1
6.336	3.8000E+01	6.1664E-02	-4.507E+01	-4.507E+01	1 0 1 0 1
6.396	3.8000E+01	5.8226E-02	3.082E+01	3.082E+01	1 0 1 0 1
6.468	3.8000E+01	1.1635E-01	5.274E+01	5.274E+01	1 0 1 0 2
6.675	3.8000E+01	2.1521E-01	-1.014E+03	-1.014E+03	1 0 1 0 1
7.081	3.8000E+01	1.0638E-01	4.120E+01	4.120E+01	1 0 1 0 2
8.608	3.8000E+01	1.4457E-01	6.203E+01	6.203E+01	1 0 1 0 2
8.713	3.8000E+01	1.2215E-01	9.959E+01	9.959E+01	1 0 1 0 1
9.283	3.8000E+01	6.8630E-02	3.112E+01	3.112E+01	1 0 1 0 1
10.172	3.8000E+01	6.5080E-02	4.997E+01	4.997E+01	1 0 1 0 2
11.715	3.8000E+01	2.2957E-01	7.989E+01	7.989E+01	1 0 1 0 1
12.291	3.8000E+01	3.5522E-01	1.198E+02	-1.198E+02	1 0 1 0 1
12.484	3.8000E+01	3.5296E-01	1.198E+02	1.198E+02	1 0 1 0 2
12.864	3.8000E+01	2.2692E+00	2.480E+03	2.480E+03	1 0 1 0 1
13.289	3.8000E+01	2.9070E-02	6.649E+01	6.649E+01	1 0 1 0 1
13.697	3.8000E+01	1.2236E-01	6.344E+01	-6.344E+01	1 0 1 0 2
14.546	3.8000E+01	1.5165E-01	3.942E+01	3.942E+01	1 0 1 0 2
15.417	3.8000E+01	1.8825E-01	-4.541E+01	4.541E+01	1 0 1 0 2
16.075	3.8000E+01	2.6288E-01	-4.937E+01	4.937E+01	1 0 1 0 2
16.656	3.8000E+01	2.9711E-01	7.735E+01	-7.735E+01	1 0 1 0 1
18.040	3.8000E+01	3.3474E-01	7.583E+01	7.583E+01	1 0 1 0 1
18.973	3.8000E+01	4.5320E-01	9.827E+01	9.827E+01	1 0 1 0 1
19.163	3.8000E+01	5.3121E-01	-1.147E+02	1.147E+02	1 0 1 0 1
19.279	3.8000E+01	3.9626E-01	1.608E+02	1.608E+02	1 0 1 0 2
19.469	3.8000E+01	7.4532E-01	1.466E+02	-1.466E+02	1 0 1 0 1

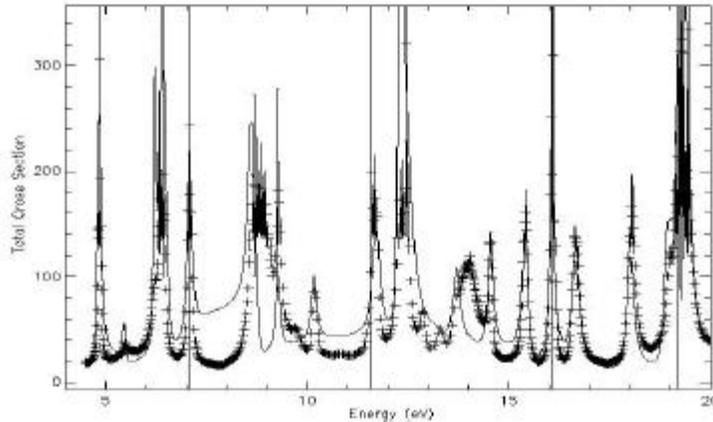


Fig. 1. Comparison of the experimental data (crosses) for the total cross section and SAMMY calculations using the initial set of resonance parameters (solid line).

3.1 External Resonance Contribution

External resonances describe the potential scattering cross section effects for the energy region where the evaluation is performed. An inaccurate representation of the external contribution may lead to problems in the SAMMY evaluation procedure, causing difficulties in the production of a set of resonance parameters which fit all the experimental data in a consistent manner. There exists an infinite number of external resonances contributing to these potential scattering effects. In practical applications, the contribution of the infinite number of levels is mocked up by a small number of resonance parameters, often called pseudo resonance parameters. There are several ways to determine the pseudo resonance parameters; in particular:

- a. A general analytical method describing the contribution of the external levels to the R-matrix in terms of average resonance parameters (strength functions, effective radius, etc.). For an explanation see the SAMMY users manual section III.A.1.a. “Logarithmic parameterization of external R-function”;
- b. A method developed by F. Fröhner⁸ where the effect of the external levels is approximated by two external resonances one below and one above the energy region where the evaluation is performed.
- c. A method introduced by H. Derrien⁹ which consists of shifting the resonances in the region where the evaluation is made into external regions below and above the resonance evaluation region.

Concluding Remarks

Analysis and evaluation of the neutron cross section using the computer code SAMMY has been presented. We have illustrated the use of SAMMY for data evaluation in the resolved energy region via the Reich-Moore approximation using the total cross section of the ^{235}U in the energy range from 4 eV to 20 eV. The details on how to construct the three basic input files to begin a SAMMY evaluation were given. In this lecture we have not covered the use of statistical analysis of the resonance parameters. A more complete description of data evaluation for ^{235}U cross section can be found on reference 10.

References:

1. N. M. Larson, Updated Users' Guide for SAMMY: Multilevel R-matrix Fits to Neutron Data Using Bayes' Equations, ORNL/TM-9179/R4, Oak Ridge National Laboratory, Oak Ridge, TN (1998).
2. C. W. Reich and M. S. Moore, Phys. Rev. **111** (1958) 929.
3. "CSISRS: Cross-Section Information Standard Retrieval System," Brookhaven National Laboratory.
4. "CINDA: The Index to Literature and Computer Files on Microscopic Neutron Data," International Atomic Energy Agency (1987).
5. S. F. Mughabghab, "Neutron Cross Sections, Neutron Resonance Parameters and Thermal Cross Sections, Vol. A: Z=61-100, Acad. Press, New York etc. (1984).
6. R. O. Sayer, RSAP-Royce's SAMMY Plotter, Version 4, Oak Ridge National Laboratory, Jan 11, 2000.
7. M. A. Mariscotti, Nucl. Inst. Methods **50**, 309 (1967).
8. F. Fröhner, "Account for External Levels in Neutron Resonance Fitting," private communication, Feb/1999.
9. H. Derrien, *J. Nucl. Sci. Technol.*, **31**, 5, 379 (1994).
10. L. C. Leal et al., "R-Matrix Analysis of ^{235}U Neutron Transmission and Cross-Section Measurements in the 0- to 2.25-keV Energy Range," *Nuc. Sci.* **131**, 230-253 (1999).