ON THE PREPARATION OF LIBRARY DATA FOR AN IMPLEMENTATION OF THE METHOD OF SUBGROUPS IN WIMS–AECL

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ABSTRACT

The subgroups method of calculating self-shielded resonance cross sections, and the start of an implementation of it for WIMS–AECL, are described in a companion paper [1] published in these proceedings. The current, ongoing development follows closely the earlier works of Nikolaev et al. [2], Gregory [3] and Roth [4]. A new program called SGFIT processes ENDF/B-based nuclear data for nuclides exhibiting cross-section resonances, and it generates subgroup parameters consistent with an existing WIMS–AECL energy-group structure. Design aspects of SGFIT are described in this work. Some details of sample calculations made for ^{91}Zr are presented.

1 INTRODUCTION

The WIMS–AECL computer program [5] is used to model neutron transport in CANDU®-reactor lattices for design, safety analysis, and operation. The WIMS–AECL computer program works with two-dimensional regions, which are assigned macroscopic cross sections, $\Sigma_g = \sum_j n_j \sigma_{j,g}$. The initial concentration, n_j, of nuclide j in the material that occupies the region is defined by the user, and microscopic, multigroup cross sections, $\sigma_{j,g}$, and other nuclide-dependent nuclear data are read from a library constructed some time in advance of making WIMS–AECL simulations [6]. Spatially varying neutron-flux solutions, found by WIMS–AECL, are used to generate cell-averaged cross sections. These cross sections, which are output by WIMS–AECL to an interface file, are fed to diffusion-theory codes, such as RFSP [7], to obtain global reactor-power distributions.

The current resonance treatments in WIMS–AECL are based on equivalence theory [8]. The WIMS–AECL computer code takes into account fuel temperature and other lattice-cell properties in deriving effective shielded microscopic cross sections for the nuclides of fuel materials that display cross-section resonances. In a conventional manner, groupwise resonance integrals, evalulated using NJOY [9] on a predefined grid of temperature and dilution parameter, are stored in a library for later use by WIMS–AECL. At run-time, resonance integrals are interpolated from the tables using an effective fuel temperature and a dilution parameter evaluated by the lattice-cell transport code.

The subgroups method, and the start of an implementation of it for WIMS–AECL, are described in a companion paper [1] published in these proceedings. The current, ongoing development follows closely the earlier works of Nikolaev et al. [2], Gregory [3] and Roth [4]. The companion paper presents some preliminary results that consist of shielded ^{91}Zr cross sections calculated by Chen's implementation of the method of subgroups. Presented in the same paper for comparison are

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shielded cross sections derived by Chen from output of MCNP [10], an industry-standard computer code that employs the more physically rigorous continuous-energy Monte-Carlo method.

New sorts of library data are needed by the new subgroups method. So-called subgroups weights and cross sections are used to represent, in a condensed manner, the distribution of reaction cross sections in each of many energy groups. Nikolaev et al. [11] describe the various conditions and constraints that a set of subgroups parameters should satisfy. A new program, called SGFIT, processes pointwise ENDF/B nuclear data and generates subgroups parameters that satisfy the Nikolaev criteria.

Section 2–A of this paper reviews some of Nikolaev's earlier work. Section 2–B describes a numerical recipe based on his methods. The same section introduces the new SGFIT program, which makes use of the CFSQP optimization software system [12] in deriving subgroup weights and cross sections from ENDF/B nuclear data. Section 3 describes an SGFIT case study in which subgroup parameters were obtained for ^{91}Zr in one WIMS–AECL energy group, $g = 31$. Section 4 summarizes some of the important results and experience gained to date.

2 NIKOLAEV'S APPROACH AND ITS IMPLEMENTATION IN SGFIT

2–A The Approach of Nikolaev Revisited

Nikolaev et al. list a series of conditions that must be satisfied by a set of subgroup parameters in order that they reflect the same dependence of various self-shielding factors on the dilution parameter σ_0 as when the neutron-flux density in a homogeneous medium is assumed to be of the Bondarenko form. Using the notation $\langle f(u)\rangle_g$ to represent the group lethargy average $\int_{\Delta u_g} f(u)du/\Delta u_g$, we have [11]:[a,b]

$$\left\langle \frac{1}{\sigma_t(u)+\sigma_0} \right\rangle_g \approx \sum_{i=1}^{I} \frac{w_{gi}}{\sigma_{t,gi}+\sigma_0}; \tag{1}$$

$$\left\langle \frac{1}{(\sigma_t(u)+\sigma_0)^2} \right\rangle_g \approx \sum_{i=1}^{I} \frac{w_{gi}}{(\sigma_{t,gi}+\sigma_0)^2}; \tag{2}$$

$$\left\langle \frac{\sigma_x(u)}{\sigma_t(u)+\sigma_0} \right\rangle_g \approx \sum_{i=1}^{I} \frac{w_{gi}\sigma_{x,gi}}{\sigma_{t,gi}+\sigma_0}; \tag{3}$$

$$\langle \sigma_t(u)\rangle_g \approx \sum_{i=1}^{I} w_{gi}\sigma_{t,gi}; \quad \text{and} \tag{4}$$

$$\langle \sigma_x(u)\rangle_g \approx \sum_{i=1}^{I} w_{gi}\sigma_{x,gi}, \tag{5}$$

where x represents capture, fission and any other neutron-induced nuclear reactions. Separate instances of the expressions involving $\sigma_x(u)$ would apply to each sort of reaction. The approximation

[a] The nomenclature for the subgroup weights, w_{gi}, and for the subgroup cross sections, $\sigma_{t,gi}$ and $\sigma_{x,gi}$, is the same as in the companion paper [1] with only one minor exception: only nuclides displaying cross-section resonances are relevant in the current context, and so the superscripts r used in Reference 1 are omitted here. The symbol $\sigma_t(u)$ has its usual meaning: it represents a microscopic total cross section functionally dependent on neutron lethargy, u.

[b] Here, the subgroup weights and cross sections are based on Lebesgue measure within a *lethargy* domain, not energy, as has been assumed throughout Reference 1.

signs are used because small, finite values of I are implied in the practical application of these equations to be outlined in Section 2–B. With the usual Lebesgue-integral convergence criteria in effect, the left- and right-hand sides of Equations (1) through (5) tend towards equality in a limit-at-infinity sense.

Nikolaev's approach is, in essence, to raise the status of these conditions from *necessary* to *sufficient* for the purpose of determining the subgroups weights and cross sections. In the context of this numerical approximation, I is not infinite. In fact, the use of 3 to 8 subgroups is typical; I is not even very large in any usual sense. Exact agreement of the left- and right-hand sides of Equations (1) through (5) is not sought. Instead, agreement is enforced approximately in a least-squares manner for a suitable range of values of dilution parameter σ_0 selected to cover a preselected, and somewhat problem-domain-dependent, range of values.

2–B A Numerical Recipe for Generating Subgroup Parameters Based on the Methods of Nikolaev

A new program, called SGFIT, reads as input pointwise ENDF/B-based nuclear data Doppler-broadened by the BROADR module of NJOY [9], and it generates subgroups parameters that best satisfy, in a least-squares sense, the aforementioned Nikolaev criteria cast in a slightly different form. The SGFIT program seeks to eliminate the following set of residuals:[c]

$$g_1(\sigma_0) = \frac{\langle \sigma_t(u)/(\sigma_t(u)+\sigma_0) \rangle_g}{\langle 1/(\sigma_t(u)+\sigma_0) \rangle_g} - \frac{\sum_i \frac{w_{gi}\sigma_{t,gi}}{\sigma_{t,gi}+\sigma_0}}{\sum_i \frac{w_{gi}}{\sigma_{t,gi}+\sigma_0}}; \tag{6}$$

$$g_2(\sigma_0) = \frac{\langle \sigma_c(u)/(\sigma_t(u)+\sigma_0) \rangle_g}{\langle 1/(\sigma_t(u)+\sigma_0) \rangle_g} - \frac{\sum_i \frac{w_{gi}\sigma_{c,gi}}{\sigma_{t,gi}+\sigma_0}}{\sum_i \frac{w_{gi}}{\sigma_{t,gi}+\sigma_0}}; \tag{7}$$

$$g_3(\sigma_0) = \frac{\langle 1/(\sigma_t(u)+\sigma_0) \rangle_g}{\langle 1/\sigma_t(u) \rangle_g} - \frac{\sum_i \frac{w_{gi}}{\sigma_{t,gi}+\sigma_0}}{\langle 1/\sigma_t(u) \rangle_g}; \tag{8}$$

$$g_4(\sigma_0) = \frac{\langle 1/(\sigma_t(u)+\sigma_0)^2 \rangle_g}{\left\langle 1/\left(\sigma_t(u)\right)^2 \right\rangle_g} - \frac{\sum_i \frac{w_{gi}}{(\sigma_{t,gi}+\sigma_0)^2}}{\left\langle 1/\left(\sigma_t(u)\right)^2 \right\rangle_g}; \tag{9}$$

$$s_1 = \langle \sigma_t(u) \rangle_g - \sum_i w_{gi}\sigma_{t,gi}; \quad \text{and} \tag{10}$$

$$s_2 = \langle \sigma_c(u) \rangle_g - \sum_i w_{gi}\sigma_{c,gi}. \tag{11}$$

The last two residuals, s_1 and s_2, are special cases of $g_1(\sigma_0)$ and $g_2(\sigma_0)$ in the limit of infinite dilution. The SGFIT program makes use of the CFSQP software package [12], which solves minimax optimization problems involving multiple simultaneous constraints and objective functions. The subgroup weights, w_{gi}, and cross sections, $\sigma_{t,gi}$ and $\sigma_{c,gi}$, are treated as the optimization parameters upon which the objective functions depend. The subgroup weights are individually constrained to lie in the range $[0, 1]$. It is implicit in the implementation of SGFIT that their sum is equal to 1. The individual subgroup cross sections are constrained only to lie in the range between the minimum and maximum values of the corresponding continuous functions attained on the energy interval in

[c] The first terms in the expressions for $g_i(\sigma_0)$ are very similar in nature to those used in the evaluation of shielded cross sections by the GROUPR module of NJOY [9].

question. An additional I inequality constraints are imposed: each subgroup's total cross section must be no less than the sum of explicitly represented partial cross sections.[d] That is,

$$\sigma_{t,gi} \geq \sum_{x=c,f,\ldots} \sigma_{x,gi} \qquad \text{for } i = 1, \ldots, I. \tag{12}$$

There is a one-to-one correspondence between the residual functions defined by Equations (6) through (11) and each of the objective functions passed within SGFIT as arguments to the CFSQP software routines. The objective function corresponding to the residual function $g_i(\sigma_0)$ is, within a multiplicative factor, equivalent to the weighted sum of squared residuals $\sum_j g_i^2(\sigma_{0j})$ evaluated on a user-specified set of dilution parameters $\{\sigma_{0j}\}$. In some numerical experiments involving nuclear data for ^{91}Zr, 101 values of the dilution parameter spanning the range from 50 to 5000 barns were used (see Section 3).

When fission cross sections must be modelled, the set of objective functions is expanded in an obvious manner via fission-related residuals analogous to $g_2(\sigma_0)$ and s_2, which, in their current form, represent only neutron capture.

3 A CASE STUDY: SUBGROUP PARAMETERS FOR ^{91}Zr

The abundance of ^{91}Zr in natural zirconium is 11.22 atom-% [13]. Owing to the size of some of its nuclear resonances, the self-shielding of ^{91}Zr is not unimportant in simulating neutron transport in CANDU-reactor pressure tubes and other structural material. Doppler-broadened cross sections of ^{91}Zr in the vicinity of its large 292.6-eV resonance are shown in Figures 1 and 2.[e] The 292.6-eV resonance falls in WIMS–AECL group $g = 31$. Four representative target functions of dilution parameter are depicted in Figure 3. Each was evaluated by algebraically manipulating various numerical energy-group integrations made using ENDF/B–VI-based ^{91}Zr nuclear data. It is to such target functions that CFSQP seeks to fit functional forms involving the subgroup parameters w_{gi}, $\sigma_{t,gi}$ and $\sigma_{c,gi}$ (see Equations (6) through (9)).

The cross-section probability distribution $P_g^u(\sigma_t)$ represents the likelihood of the event of selecting a total cross section with value *less than* σ_t if one were to do so by randomly sampling uniformly from the lethargy interval corresponding to the energy group with index g and then look up the total cross section corresponding to that value of lethargy. Where the derivative exists, the corresponding *probability density* is $p_g^u(\sigma_t) = \frac{dP_g^u}{d\sigma_t}$. Numerical evaluations of the cross-section probability densities $p_g^u(\sigma_t)$ for two different temperatures and $g = 31$ are shown in Figure 4 along with fitted subgroup weights and total cross sections corresponding to $I = 4$. Nowhere are the evaluations of $p_g^u(\sigma_t)$ used directly in SGFIT; they are displayed here only to assist the discussion. The hooklike feature of $p_g^u(\sigma_t)$ in the vicinity of 1000 to 2000 barns is due to the flattening and turnover of the total cross section at energies very near the resonance peak at 292.6 eV. The hooklike feature moves lower in cross section with increasing temperature because the peak cross section of the Doppler-broadened resonance is reduced at higher temperature.

It is evident that certain features of $p_g^u(\sigma_t)$ are retained by the subgroup weights and cross

[d] No scattering cross section is included in this sum.

[e] Cross sections are shown, and calculations were made, for ^{91}Zr at $T = 296$ K and $T = 2400$ K. The second, very high temperature for zirconium is unlikely to be used in any practical WIMS–AECL simulation. It is employed here only to illustrate the effects of Doppler broadening in this context.

sections evaluated by SGFIT even when only four subgroups are represented.[f] The four discrete cross sections appear to be fairly evenly distributed in the figure, and the weights associated with each value of $\sigma_{t,gi}$ show roughly the same overall decreasing trend with increasing cross section, as do the plots of $p_g^u(\sigma_t)$ for each of the two temperatures.

When four subgroups are used, SGFIT yields a very good fit to the target functions for each of the three temperatures listed in Table 1. Nowhere did the magnitude of any residual exceed 0.07% of its corresponding target-function value, and discrepancy magnitudes equal to 0.01% or less were more typical. This result, however, cannot be extrapolated to other nuclides, or to other energy groups, since the complexity of the target functions depends strongly on the details of cross-section variation within an energy group.

4 CONCLUSION

The methods used in SGFIT are still under investigation and development. Preliminary results obtained for ^{91}Zr are promising: attributes of the full cross-section density $p_g^u(\sigma_t)$ derived from ^{91}Zr pointwise cross sections are reflected qualitatively by the fitted subgroup weights and cross sections, and the fits to the target functions are very good despite the fact that only a small number of subgroups were used. Similar success was obtained (but is otherwise not documented here) when SGFIT was applied, in each case, to data representing ^{238}U at $T = 296$ K and $T = 600$ K in WIMS–AECL groups $g = 25$ through 47.

The calculations discussed in the companion paper [1] were based on the subgroup weights and cross sections for ^{91}Zr reported here. The ultimate utility of SGFIT, and this work, depends on the overall success of the subgroups scheme and its future, full implementation in WIMS–AECL, both of which are under continuing development.

ACKNOWLEDGEMENTS

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[f] See also Table 1, which lists values w_{gi}, $\sigma_{t,gi}$ and $\sigma_{c,gi}$ generated for ^{91}Zr by SGFIT at $T = 296$ K, $T = 600$ K and $T = 2400$ K.

REFERENCES

1. H.C. Chen and P.J. Laughton. The method of subgroups in the calculation of shielded cross sections for WIMS–AECL. In *Proceedings of the 1997 Nuclear Simulation Symposium*, Niagara-on-the-Lake, Ontario, 1997 September. Canadian Nuclear Society.

2. M.N. Nikolaev, A.A. Ignatov, N.V. Isaev and V.F. Eokhlov. The method of subgroups for considering the resonance structure of the cross sections in neutron calculations (part 1). *Soviet Atomic Energy*, 29(1):689–695, 1970.

3. M.V. Gregory. A correlation technique for resonance calculations. *Nuclear Science and Engineering*, 71:59–64, 1979.

4. M.J. Roth. Resonance absorption in complicated geometries. AEEW–R 921, United Kingdom Atomic Energy Authority (Atomic Energy Establishment, Winfrith), Dorchester, Dorset, England, 1974 March.

5. J.V. Donnelly. WIMS–CRNL: A User's Manual for the Chalk River Version of WIMS. Atomic Energy of Canada Limited Report, AECL–8955, 1986 January.

6. P.J. Laughton. NJOYPREP and WILMAPREP: Unix-based tools for WIMS–AECL cross-section library production. Unpublished internal report, AECL (Chalk River), 1993 May.

7. B. Rouben. Overview of current RFSP-code capabilities for CANDU core analysis. Atomic Energy of Canada Limited Report, AECL–11407, 1996 January.

8. J.V. Donnelly. Description of the resonance treatment in WIMS–AECL. Atomic Energy of Canada Limited Report, AECL–10550, 1993 May.

9. R.E. MacFarlane and D.W. Muir. *The* NJOY *Nuclear Data Processing System—Version 91.* Los Alamos National Laboratory, Los Alamos, NM, 1994 October.

10. Judith F. Briesmeister. MCNP—A general Monte Carlo N–particle transport code. Manual LA–12625, Los Alamos National Laboratory, 1993 November.

11. M.N. Nikolaev, A.A. Ignatov, N.V. Isaev and V.F. Eokhlov. The method of subgroups for considering the resonance structure of cross sections in neutron calculations (part 2). *Soviet Atomic Energy*, 30(5):528–533, 1971.

12. J.L. Zhou and A.L. Tits. An SQP algorithm for finely discretized continuous minimax problems and other minimax problems with many objective functions. *SIAM Journal on Optimization*, 6(2):461–487, 1996 May.

13. F. William Walker, Josef R. Parrington and Frank Feiner. Chart of the Nuclides (14th edition). General Electric Company, Nuclear Energy Operations, San Jose, CA, 1988 April.

Table 1: The subgroup cross sections and weights fitted by SGFIT to ^{91}Zr nuclear data Doppler-broadened by NJOY to three different material temperatures. A fit to $I = 4$ subgroups was requested in each case listed. (See Figure 4 for a graphical depiction of some of the same data.)

i	w_{gi}	$\sigma_{t,gi}$ (barns)	$\sigma_{c,gi}$ (barns)
$T = 296$ K, $g = 31$			
1	0.8918	10.27	0.227
2	0.0797	62.47	4.568
3	0.0174	490.84	49.789
4	0.0112	1984.83	204.031
$T = 600$ K, $g = 31$			
1	0.8870	10.22	0.231
2	0.0816	58.52	4.070
3	0.0181	455.36	46.196
4	0.0133	1702.30	174.876
$T = 2400$ K, $g = 31$			
1	0.6502	8.10	0.125
2	0.2982	22.34	0.967
3	0.0287	271.80	26.436
4	0.0229	1093.52	112.455

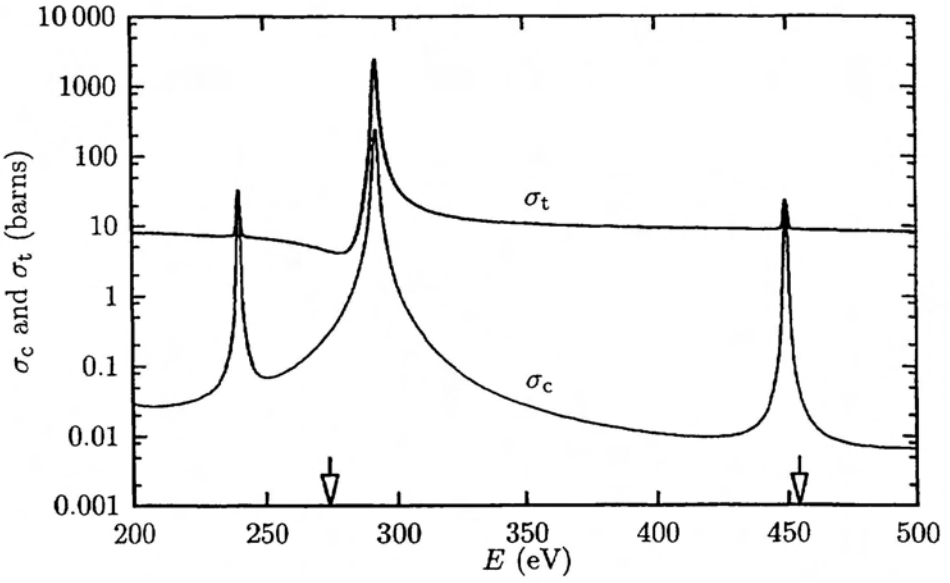

Figure 1: The Doppler-broadened capture and total cross sections of ^{91}Zr in the vicinity of its large resonance at 292.6 eV. Data are displayed for one material temperature, $T = 296$ K. The upper and lower bounds of WIMS–AECL energy group $g = 31$ are marked with arrows.

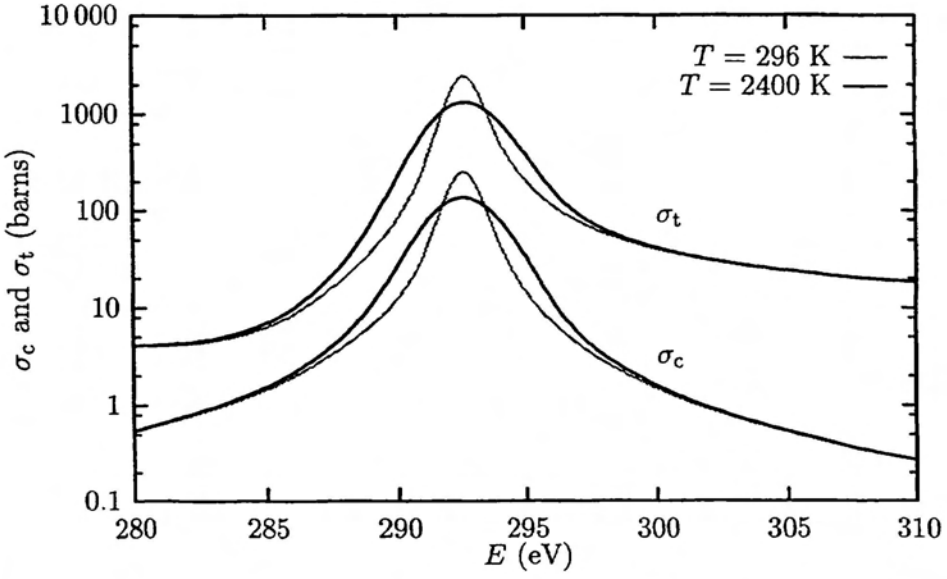

Figure 2: The Doppler-broadened capture and total cross sections of ^{91}Zr in the vicinity of its large resonance at 292.6 eV. Data are displayed for two material temperatures, $T = 296$ K and $T = 2400$ K.

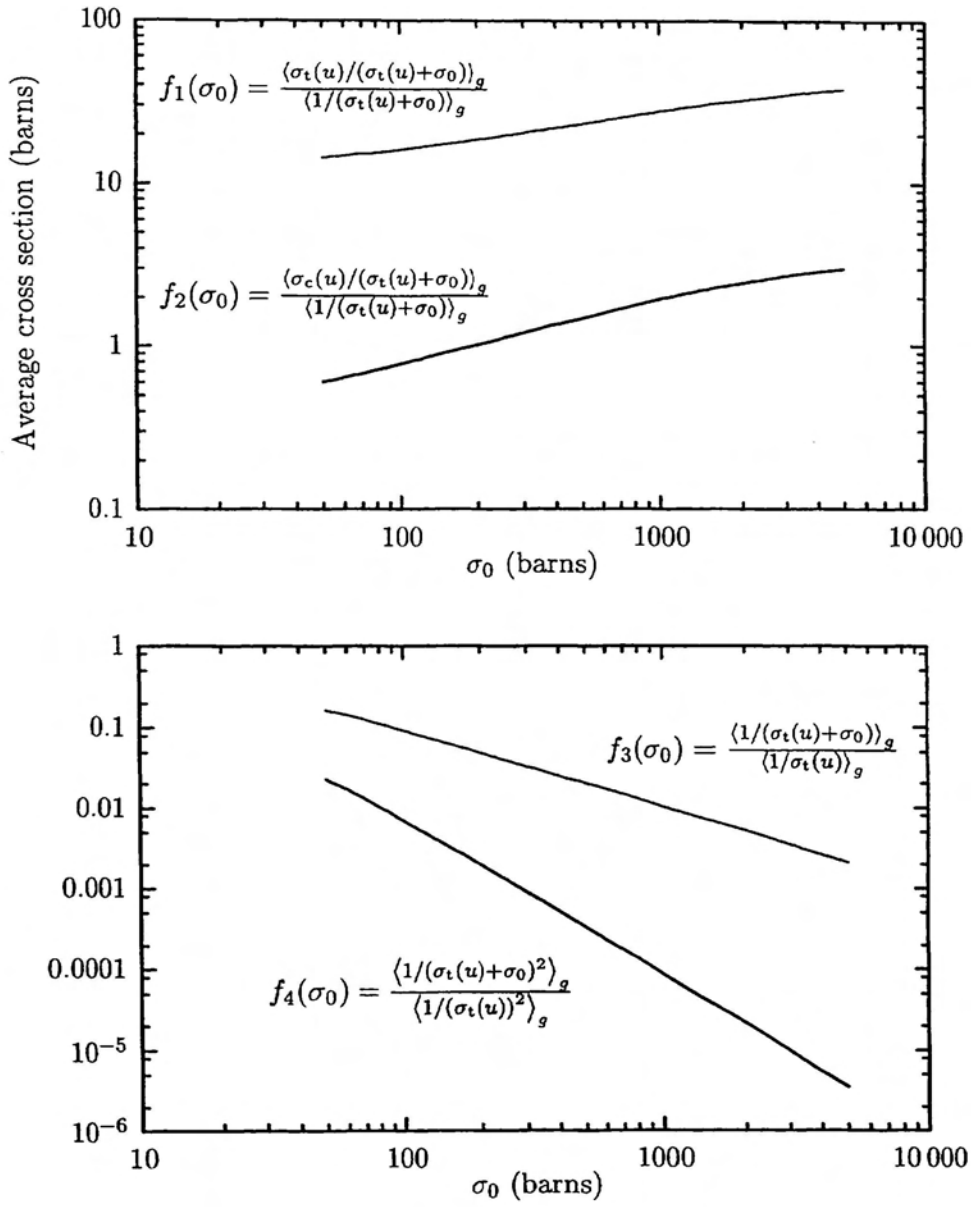

Figure 3: The four functions of dilution parameter to which expressions involving the subgroup parameters are fitted by SGFIT. The target functions $f_j(\sigma_0)$ correspond to the first terms on the right-hand side of the residual functions $g_j(\sigma_0)$ defined by Equations (6) through (9). The target functions $f_j(\sigma_0)$ are shown evaluated at $\sigma_0 = 50 \ldots 5000$ using ENDF/B–VI cross-section data for ^{91}Zr Doppler-broadened by the BROADR module of NJOY to the material temperature $T = 296$ K.

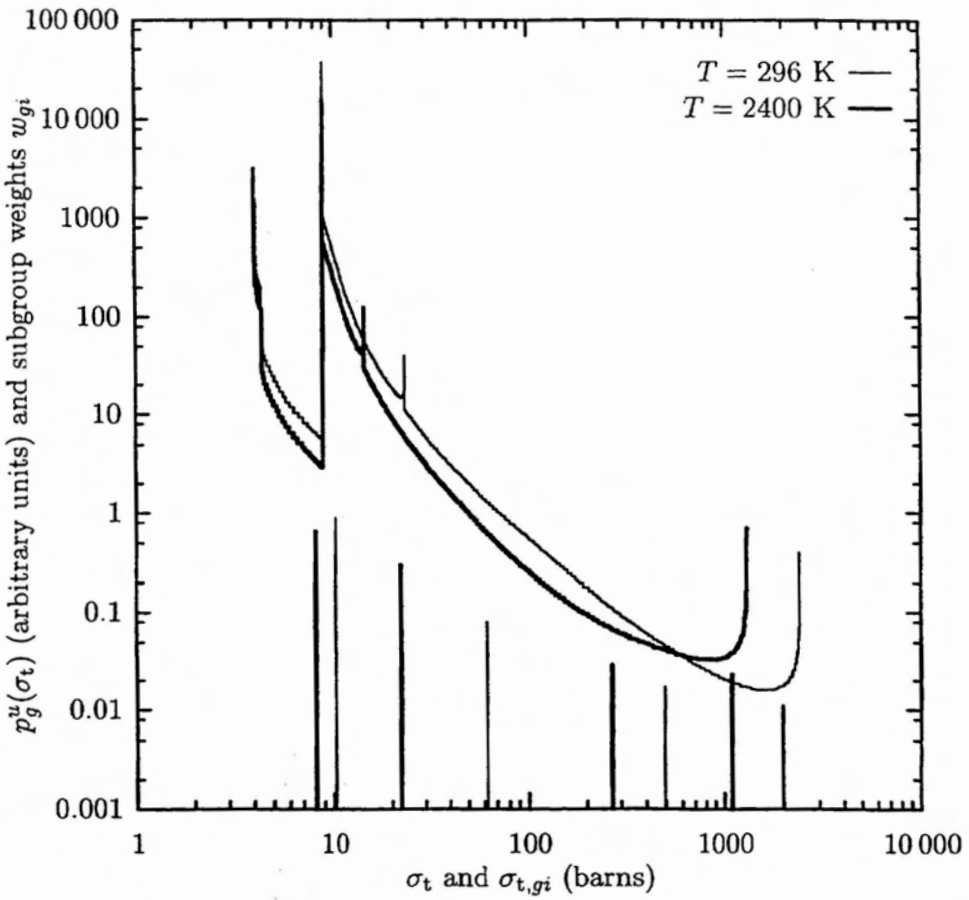

Figure 4: The lethargy-measure-based probability density, $p_g^u(\sigma_t)$, for the total cross section of ^{91}Zr in energy group $g = 31$ (275.36 to 454 eV), and the corresponding subgroup weights, w_{gi}, and total cross sections, $\sigma_{t,gi}$, returned by SGFIT when a fit to $I = 4$ subgroups is made. Data for two different material temperatures are displayed. See also Table 1.