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PROGRAM SIGNAL

(Version 74-1)

Dermott E. Cullen

January 1974

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PROGRAM SIGMA1

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I. Purpose

Program SIGNAL is designed to Doppler broaden and/or thin tabulated pointwise cross sections in the ENDF/B BCD format.¹ The broadening is performed from an initial (not necessarily 0°K) temperature to up to 100 final temperatures.

II. Method

The ENDF/B BCD format is used for both input and output. Each section of File 3 data is assumed to be a linear-linear table of pointwise cross section vs energy. Using this assumption and a Maxwellian distribution for the medium it is possible to exactly Doppler broaden the cross section.²

Specifically if the nuclei in a medium have a Maxwellian distribution with an effective temperature³ T_{eff} °K, then the cross section for any reaction at T_{eff} may be related to the cross section for the same reaction at any lower temperature T_1 by the expression:⁴

$$\sigma(E, T_{\text{eff}}) = \frac{1}{E} \sqrt{\frac{\alpha}{4\pi}} \int_0^{\infty} \sqrt{E'} \sigma(E', T_1) \left\{ e^{-\alpha(\sqrt{E'} - \sqrt{E})^2} - e^{-\alpha(\sqrt{E'} + \sqrt{E})^2} \right\} dE'; \alpha = \frac{M}{m K_B \Delta T} ; \Delta T = T_{\text{eff}} - T_1 \quad (1)$$

m, M are the masses of the neutron and the target nucleus and K_B is Boltzmann's constant.

Upon changing variables to $y^2 = \alpha E$; $x^2 = \alpha E'$ Eq. (1) can be put into the form:

$$\sigma(y, T_{\text{eff}}) = \frac{1}{y^2} \sqrt{\frac{1}{\pi}} \int_0^{\infty} x^2 \sigma(x, T_1) \left\{ e^{-(x-y)^2} - e^{-(x+y)^2} \right\} dx \quad (2)$$

when the cross section $\sigma(x, T_1)$ is given as a linear-linear function of E' (i.e.,

$$\sigma(E', T_1) = A_k + B_k E' : E' \in [E_k, E_{k+1}] \rightarrow \sigma(x, T_1) = A_k + C_k x^2 : x \in [x_k, x_{k+1}])$$

Eq. (2) takes the form:

$$\sigma(y, T_{\text{eff}}) = \frac{1}{y^2} \sqrt{\frac{1}{\pi}} \sum_k \int_{x_k}^{x_{k+1}} [A_k x^2 + C_k x^4] \left\{ e^{-(x-y)^2} - e^{-(x+y)^2} \right\} dx \quad (3)$$

This expression can be exactly defined in terms of the family of functions:

$$I^n(a, b) = \sqrt{\frac{1}{\pi}} \int_a^b z^n e^{-z^2} dz = F^n(a) - F^n(b) = \sqrt{\frac{1}{\pi}} \int_a^\infty z^n e^{-z^2} dz - \sqrt{\frac{1}{\pi}} \int_b^\infty z^n e^{-z^2} dz : n=0, 1, 2, 3, 4 \quad (4)$$

These functions are:

$$F^0(a) = \frac{1}{2} \text{ERFC}(a)$$

$$F^1(a) = \frac{1}{2\sqrt{\pi}} e^{-a^2}$$

$$F^n(a) = \frac{1}{2} \left\{ (n-1) F^{n-2}(a) + \frac{a^{n-1}}{\sqrt{\pi}} e^{-a^2} \right\} \quad (5)$$

however care must be exercised in applying the algorithm to eliminate round-off problems and to minimize execution time.

Round-off problems can occur when the cross section is represented in the form: $A_k + B_k E$, because the point cross section at any given E may be a small difference between two large terms. This problem can be eliminated by representing the cross section in the form: $\sigma_k + B_k (E - E_k)$.

In general, the execution time of the proposed algorithm would be an N^2 function of the number of points used to represent a given reaction. Since the number of points may be 5,000 - 30,000⁵ this dependency would lead to an unacceptably long execution time. However the strong e^{-z^2} dependence of the $F^n(z)$ functions may be used to truncate the sum over k in Eq. (3) to those intervals centered about y . Examination of existing evaluated data⁶ and application of the proposed algorithm to a wide variety of materials indicates that the summation over intervals need only be extended to intervals in which $|x-y| \leq 4$ (e.g.: $F^0(4) = 1.3701E-8$; $F^4(4) = 3.9490E-6$).

If the temperature difference between the original cross section as read and the requested final temperature is not positive Doppler broadening will not be performed. In this case the program may be used to only thin the data.

In addition to Doppler broadening, the program thins the ENDF/B data at the original temperature and/or thins the resulting data after Doppler broadening.

The thinning algorithm treats the cross section as a function $f(x)$ and forms a function $f^*(x)$ such that $f^*(x)$ contains the minimum number of originally tabulated values and yet guarantees that at all of the original tabulated values of $f(x)$ that $f^*(x)$ is within a given fraction of $f(x)$: $|f(x) - f^*(x)| \leq \epsilon |f(x)|$. The algorithm as implemented will eliminate all points between x_j and x_k as long as at all[†] intermediate points:

[†] The all here is important since it corrects an error in the ENDF/B utility routine CROP⁷ which eliminates intermediate points one after another without checking previously eliminated intermediate points.

$$|f(x_\ell) - f^*(x_\ell)| \leq \epsilon |f(x_\ell)| \quad (6)$$

Where x_ℓ is any original tabulated point between x_j and x_k and $f^*(x_\ell)$ is obtained by interpolation between $f(x_j)$ and $f(x_k)$. The algorithm will keep the point x_k if: (1) interpolation from x_j to x_k allows all intermediate points to pass the above test, (2) interpolation from x_j to x_{k+1} causes any one or more intermediate points to fail the test.

If the thinning criteria for the original section and/or the Doppler broadened section is not positive thinning will not be performed. In this case the program may be used to guarantee that the Doppler broadened cross sections are at all of the same energies as the original data.

In order to avoid placing an upper limit on the number of points for an ENDF/B cross section the data are handled in pages of 1002 points each. Three pages of original cross sections and energies as well as a single page of Doppler broadened cross sections are core resident. In general the program will produce Doppler Broadened cross sections at the energies corresponding to the middle page of original data (the preceding and following pages are used in the Doppler broadening algorithm). The Doppler broadened data are then thinned and output. The second and third pages are then shifted forward in core one page and a new third page is read in. The program continues this loop of shifting and broadening the middle page until all the data have been broadened.

III. Limitations and Assumptions

The data are assumed to be in the ENDF/B format and no checks are performed to verify this. Each cross section (i.e. section of File 3) is assumed to be

a linear -linear function of energy vs pointwise cross section for both broadening and thinning.

The C1 field on the TAB1 record is used to determine the original temperature (on input) and to indicate the final temperature (on output). The exception to this rule is when $L2 \neq 0$ (intermediate state data) the C1 field contains a Q value. In this case the original temperature is assumed to be the same as the original temperature of the total cross section (on input) and the Q value is undisturbed on output (in this case temperature cannot be indicated in the section).

In the case of extremely high temperatures (e.g. 10^6 Kelvin) the algorithm to Doppler-broaden the middle page of data may extend to the beginning of the first page or to the end of the last page. In these cases the cross section is continued as constant beyond the limit of the core resident pages and a warning message is printed. The program will always broaden to the difference between the original and final temperatures.³

When the program is used to broaden to more than one final temperature, the original cross sections are used as the starting point for each temperature (i.e. the data are not bootstrapped from one temperature to another) to avoid accumulation of error due to thinning. Each section of Doppler broadened cross sections is written on output as a separate ENDF/B section (as opposed to writing it in the ENDF/B temperature dependent format). This is to allow the data at different temperatures to contain the minimum number of points. Due to the paging system there is no limit to the size of any section. In general all sections of file 3 data will be broadened except for $\bar{\mu}$, ξ and γ (mt = 251-253). However all sections will be thinned. In the unresolved energy region where the tabulated data are averaged cross section vs energy

(as opposed to pointwise cross sections) the broadening algorithm as outlined will yield the correct infinitely dilute broadened cross section. The program is limited to 100 final temperatures and 100 materials.

IV. Requirements

The program is written entirely in Fortran-IV and has been implemented on the CDC-6600/7600 and IBM-360. The program requires the following units: input, output, the original data, the broadened data and two scratch files (6 files). The core requirements on the CDC-7600 is 20 K₁₀. The time required to Doppler broaden U-238 (ENDF/B-III MAT 1158) from 0 °K to 293 °K was 45 seconds of CDC-7600 time.

V. Input

<u>Card</u>	<u>Cols.</u>	<u>Format</u>	<u>Description</u>
1	1-11	E11.4	Original fractional thinning criteria
	12-22	E11.4	Broadened fractional thinning criteria
	23-33	I11	Selection criteria (0=MAT, 0#ZA)
2-N	1-11	I11	Material number (MAT) or ZA (see: selection criteria above) (up to 100 cards followed by a blank or zero card)
(N+1)-M	1-11	E11.4	Temperature to broaden to (°K) (up to 100 cards followed by a blank or zero card)

Example

Using 0.5% thinning criteria for both original and broadened data and selecting U-235 and U-238 by ZA (instead of MAT) and broadening them to 0° (keep original data with broadened data), 293°, 1000° and 2000 °K, the following input cards should be used:

Card	Cols.	11	22	33
1	0.005	0.005		1
2		92235		
3		92238		
4	(Blank)			
5	0.0			
6	293.0			
7	1000.0			
8	2000.0			
9	(Blank)			

Note: Since the list of temperatures is terminated by a blank or zero card, if requested the original data at 0°K must be the first temperature requested (the list of temperatures can be terminated only after the first card).

The data will be output in the order in which they are encountered on the original file (usually MAT ordered) and temperatures will be in the order of the input cards (usually increasing temperature).

VI. Output

In addition to the broadened and/or thinned data in the ENDF/B format the program will also print a single line for each section output. Each of these lines will contain the ZA and MAT, the final temperature, the number of points after input thinning and the final number of points as output.

Figure 1 illustrates the effect of applying the proposed algorithm to the elastic cross section of U^{238} (ENDF/B-III MAT 1158). The representation of the broadened cross section required only 1/3 the number points of the 0°K cross section.

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Fig. J

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