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A PROGRAM FOR THE CALCULATION OF MAXWELL-BOLTZMANN AVERAGED CROSS SECTIONS ON THE IBM-704 COMPUTER

C. W. Nestor

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REACTOR EXPERIMENTAL ENGINEERING DIVISION

A PROGRAM FOR THE CALCULATION OF MAXWELL-BOLTZMANN AVERAGED CROSS SECTIONS ON THE IBM-704 COMPUTER

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ABSTRACT

A 704 program has been written and checked for the calculation of cross sections averaged over a Maxwell-Boltzmann flux. Up to 200 energy values and corresponding point cross sections may be used to compute average cross sections at as many values of thermal energy (kT) as may be specified. The upper limit of the integration may be either a multiple of the thermal energy or the last energy for which cross sections are available.

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INTRODUCTION

The existence of low-energy resonances and "non- $\frac{1}{v}$ " behavior in many elements of interest (e. g., U^{235}, Pu^{239}) requires the use of suitably averaged cross sections in the calculation of reactor parameters. The program described in this report provides a convenient means of calculating average cross sections for a Maxwell-Boltzmann flux, given the value of the cross section of interest at several energies in the thermal range.

METHOD

The cross section integration required in the calculation is done numercally. In order to facilitate the use of the cross section data presented in BNL 325,[1] the integration range is broken into N intervals and two assumptions are made concerning the behavior of the cross section; viz,

1. In the first interval $(0 < E < E_2)$ the cross section can be represented by

$$\sigma(E) = \sigma(E_2)\sqrt{E_2/E} \quad ; \tag{1}$$

2. In the remaining intervals $(E_i < E < E_{i+1},\ i = 2, 3 \ldots, N)$ the cross section can be represented by[2]

$$\sigma(E) = \sigma(E_i)(E/E_i)^{B_i} \tag{2}$$

---

[1] D. J. Hughes et al., Neutron Cross Sections, BNL 325, Ed. 2.

[2] This assumption implies that a log-log plot of cross section versus energy is linear in each interval. The cross section data in BNL-325 is then fitted with straight line segments for a number of intervals in the range 0.001 ev < E < 1 ev.

The average cross section for thermal energy kT and an energy range $0 < E < E_U$ is given by

$$\bar{\sigma}(kT) = \frac{\int_0^{E_U} \sigma(E)\, M(E,kT)\, dE}{\int_0^{E_U} M(E,\, kT)\, dE} \tag{3}$$

where the unnormalized Maxwell-Boltzmann flux is

$$M(E,\, kT) = E\, e^{-E/kT} \tag{4}$$

Substitution of (1) and (2) into (3) yields, after performing the integrations over the first interval and in the denominator

$$\bar{\sigma}\,(kT) = \frac{\sigma(E_2)\left[\frac{\sqrt{\pi}}{2}\sqrt{\alpha_2}\,\mathrm{Erf}\,(\sqrt{\alpha_2}) - \alpha_2\, e^{-\alpha_2}\right] + \sum_{i=2}^{L} G_i\, \sigma(E_i)}{1 - (1 + \alpha_L)\, e^{-\alpha_L}} \tag{5}$$

where

$$\alpha_i \equiv E_i/kT \tag{6}$$

$$\mathrm{Erf}(x) \equiv \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt \tag{7}$$

$$G_i \equiv \int_{\alpha_i}^{\alpha_{i+1}} \left(\frac{u}{\alpha_i}\right)^{B_i} e^{-u}\, u du, \text{ if } B_i \neq 0 \text{ (Note 1)} \tag{8}$$

$$G_i \equiv (1 + \alpha_i)\, e^{-\alpha_i} - (1 + \alpha_{i+1})\, e^{-\alpha_{i+1}}, \quad \text{if } B_i = 0 \tag{9}$$

$$B_i \equiv \frac{\ln\left[\sigma(E_{i+1})/\sigma(E_i)\right]}{\ln(E_{i+1}/E_i)} \tag{10}$$

---

1 The integration is performed numerically using a sixteen-point Gaussian quadrature subroutine programmed by M. P. Lietzke for the IBM-704.

The program is constructed to allow for up to 200 energy values E_i and corresponding cross sections to be stored for averaging. These values are read in for each element after which the averaging process is performed for as many values of kT as may be specified on successive cards. If it is possible to represent two cross sections of a given element by straight line segments over the same energy intervals, both cross sections may be averaged with one pass through the program.

For flexibility, the upper limit E_U of the integrations in (3) is taken as a multiple of the thermal energy:

$$E_U = R\ kT. \tag{11}$$

In order to allow for this, the value of R must be specified for each thermal energy for which the averaging is to be performed. The program will then find the interval j such that

$$E_j < E_U < E_{j+1},$$

and set up L, the upper limit of the sum in equation (5) accordingly. If the upper limit is to be E_{N+1}, the last energy for which cross sections are specified, the value of R should be such that

$$RkT > E_{N+1}$$

for all kT values.

Input Preparation

The input for a particular case (1 element, several kT values) is discussed in detail in Table 1. Point value cross sections are on file for several elements.[1]

---

[1] Total cross section: O^{16}, U^{233}, U^{234}, U^{235}, U^{236}, Pu^{239}, Pu^{240}, Pu^{241}
Fission cross section: U^{233}, U^{235}, Pu^{239}, Pu^{241}.

Table 1. Input Formats

1.	Title card:	printer control character[1] in col. 1, any 71 Hollerith characters for identification in cols. 2-72.
2.	Control card:	N, the number of energy values (including zero) in cols. 2-4; N_F, the number of cross sections to be averaged (either 1 or 2) in col. 8.
3.	Point value cards:	for each $i \geq 2$, E_i in cols. 1-8, $\sigma_1(E_i)$ in cols. 9-16, and (if desired) $\sigma_2(E_i)$ in cols. 17-24.
4.	kT cards:	identical in form to point value cards, except that the value of R must be punched in cols. 25-32 for each kT value.
5.		blank to indicate end of case.

The numbers on the point value and kT cards may be in any acceptable floating point notation,[2] provided the field width is eight characters. Six blank cards should be added to the input deck after the last case to obtain the normal stop; otherwise an end of file stop will occur.

Output

A typical output is shown (for $N_F = 1$) in Table 2. KT is the thermal energy in hundredths of an electron volt; SIG1(KT) is the cross section at thermal energy; SIG1AVG is the average cross section; and F1 is the "f-factor" defined by

$$f(kT) = \frac{2}{\sqrt{\pi}} \frac{\bar{\sigma}(kT)}{\sigma(kT)}$$

[1] A 1 punch gives a new page; a 2, either a new page or the middle of the present page.

[2] Refer to p 29 of the FORTRAN Programmer's Reference Manual.

Output for $N_F = 2$ is shown in Table 3; the symbols SIG2(KT), SIG2AVG, and F_2 are the same quantities as SIG1(KT), SIG1AVG, and F1, except they refer to the second cross section.

Experience to Date

The program has been used to compute average cross sections for the elements listed in note 1, p 3 for the thermal energies shown in Tables 2 and 3. A case with 17 energy values and two cross sections (cf. Table 3) required approximately two minutes of machine time.

Operating Instructions

1. Sense switch 1 should be down if on-line output is desired; all others up.

2. Output will be written on logical tape 9, whether sense switch 1 is up or down; this should be listed on 8-1/2 x 11 paper, 1 file, program control. (The "end file" will be produced by the program.)

3. To run the program, place the program and input decks in the card reader, ready the reader and press the "clear" and "load cards" switches on the console. After the last case has been run, the machine should stop in octal location 115 with $(102)_8$ in the address portion of the storage register.

Table 2. Output for Sigma Fission Pu^{239}

KT ev x 10^2	SIG1(KT) bn/atom	SIG1AVG bn/atom	F1
2.52	737.00	679.30	1.040
3.21	640.00	626.91	1.105
4.07	576.00	605.14	1.185
4.93	530.00	646.42	1.376
5.79	500.00	740.00	1.670
6.66	485.00	815.21	1.897
7.52	470.00	872.88	2.096
8.38	462.00	918.32	2.243
9.24	461.00	951.00	2.328
10.10	460.00	972.11	2.385
10.96	465.00	983.35	2.386

Table 3. F Factors and Average Cross Sections for U^{235}*

KT	SIG1(KT)	SIG1AVG	F1	SIG2(KT)	SIG2AVG	F2
2.52	705.00	605.79	0.970	590.00	506.43	0.969
2.52	705.00	595.70	0.953	590.00	497.94	0.952
3.21	605.00	527.06	0.983	510.00	440.82	0.975
3.21	605.00	518.77	0.968	510.00	433.77	0.960
4.07	525.00	459.49	0.988	440.00	384.26	0.985
4.07	525.00	453.40	0.974	440.00	378.88	0.972
4.93	460.00	413.09	1.013	390.00	345.00	0.998
4.93	460.00	406.91	0.998	390.00	339.65	0.983
5.79	425.00	378.80	1.006	355.00	315.73	1.004
5.79	425.00	370.92	0.985	355.00	309.24	0.983
6.66	375.00	349.91	1.053	320.00	291.21	1.027
6.66	375.00	342.37	1.030	320.00	285.04	1.005
7.52	360.00	326.02	1.022	300.00	270.98	1.019
7.52	360.00	326.02	1.022	300.00	270.98	1.019
8.38	335.00	309.59	1.043	285.00	256.99	1.017
8.38	335.00	309.59	1.043	285.00	256.99	1.017
9.24	318.00	296.18	1.051	270.00	245.56	1.026
9.24	318.00	296.18	1.051	270.00	245.56	1.026
10.10	298.00	285.08	1.079	254.00	236.11	1.049
10.10	298.00	285.08	1.079	254.00	236.11	1.049
10.96	280.00	275.75	1.111	235.00	228.18	1.096
10.96	280.00	275.75	1.111	235.00	228.18	1.096

* For the same KT values, the successive values correspond to R = 5.5 and R = 40. (The actual upper limit for R = 40 was 1 ev, independent of the KT value; see discussion under Method.)

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