WRITTEN BY B. L. Scott*		ATOMICS INTERNATIONAL A Division of North American Aviation, Inc. TECHNICAL DATA RECORD	TDR NO. 4220	
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UNIT Theoretical Physics			SUB-ACCT. 4420	
APPROVED BY: (SUPERVISOR) <i>B. L. Scott</i>		PROGRAM Advanced SGR		TWR
OTHER		PROJECT Methods for making SGR Neutron Physics Calculations		DATE 8/5/59
				PAGE 1 OF 12

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SUBJECT:

The HEMAD Code

CONTENTS:

I	STATEMENT OF PROBLEM	PAGE 1
II	SUMMARY OF RESULTS AND RECOMMENDATIONS	PAGE
III	METHOD USED, DESCRIPTION OF EQUIPMENT, SAMPLE CALCULATIONS . . .	PAGE
IV	REFERENCES AND APPENDICES	PAGE

I STATEMENT OF PROBLEM

The Hemad code, programmed by M. N. Moore, A. Schwartz, and E. R. Cohen, has been available for some time now but has not been greatly used due to the lack of instructions for the input data. This is an undesirable situation because the only other code available for computing thermal cross sections, Sofocate, solves the Wigner-Wilkins equation as is appropriate for hydrogenous moderator. Hemad, on the other hand, solves the Wilkins equation suitable to a heavy moderator (e.g. carbon) and hence should be very useful. The purpose of this letter is to present instructions for using the Hemad code; however, for ease of reference, certain information contained in the (obsolete) NAA Program Description (HEMAD-W3-088-3), July 14, 1958, will also be given here. (Note there seem to be several Hemad decks extant. These instructions pertain to a deck available from B. L. Scott or F. L. Fillmore (W3-088) and may or may not be applicable to other decks). This code is not in finished form but appears to be usable.

The purpose of Hemad is to compute the energy spectrum of neutrons in an infinite (i.e. the buckling is zero), homogeneous lattice in the heavy moderator approximation¹, and then to average specified quantities over that spectrum. Up to 30 elements may be mixed to form the medium which defines the neutron spectrum and up to 230 functions may be averaged over that spectrum. More precise limitations are given later.

1. E. R. Cohen, Nuclear Science and Engineering, 2, 227-245 (1957).

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NAA-SR-MEMO-4220

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Input Data

Reference to the Homad deck arrangement and sample data sheets enclosed will be very useful in understanding the following description.

The input data may conveniently be separated into 6 different sets.

1. Initial Data specifying the total number of energy points, I ; the number of elements mixed to form the medium, N ; the total number of functions to be averaged, M ; a number (0,1) specifying how the input absorption cross sections are specified (σ_a or $\sqrt{E}\sigma_a$); and other related numbers.
2. Energy Points at which all cross sections are specified and at which the neutron flux will be computed.
3. Functions to be Averaged, M in number and specified at the energy values given in 2).
4. Composition of the medium which determines the flux.
5. Cross-Sections of the materials given in 4) specified at the energy points of 2).
6. Temperature of the moderator.

Each of the above sets of input data will now be described in detail.

1. Initial Data. Locations 00000 to 00008 are needed to complete the specification of the initial data. The numbers are entered as floating point numbers at a binary scale of either 35 or 17 as indicated. Location 00000 contains the total number of energy points, I , ($I \leq 200$) at a B.S. of +35. The same number is listed at 00001 except at a B.S. of +17. The code has an option, whereby the absorption cross sections of the materials in the medium may be given either in the form $\sigma_a(E)$ or $\sqrt{E}\sigma_a(E)$. Therefore, the location 00002 must contain a 0, if σ_a is given, or a 1, if $\sqrt{E}\sigma_a$ is given, at a B.S. of +35. 00003 contains N , the number of elements mixed to form the medium, ($N \leq 30$) at a B.S. of 17. 00004 contains M , the number of functions to be averaged, ($M \leq 230$) at a B.S. of +17. 00005 contains 51 at a B.S. of +17 and 00006 contains $2M+6$ also at a B.S. of +17. Location 00007 contains a control number Q which is zero if only one composition is used and is $N(400+I)$ otherwise. The B.S. is +35. The final location 00008 contains $400+I$ at a binary scale of +35.

Summarizing the limitations on the size of various numbers for a 4K core:

$$\begin{aligned} N &\leq 30 \\ I &\leq 200 \\ M &\leq 230 \\ Q+MI &\leq 8192 \end{aligned}$$

2. Energy Points. Locations 00130-00529 are reserved for the energy points at which the various quantities will be specified and computed. These energy points need not be equally spaced but must be in increasing order. The energy values must be in floating point form and in units of ev. The last energy specified determines the maximum energy at which quantities are computed and averages taken. The last card must contain an X-LAST.

3. Functions to be Averaged. The next N blocks of input data contain the values, at each of the energy points, of the functions whose averages are desired. The last card of each function must contain an X-LAST. The data in each block is entered as floating point data in locations 00000-00199. The order of the functions here is the same as the order in which their averages will appear in the output.

4. Composition. The number densities of each constituent of the medium which determines the flux is entered in locations 00001 to 00030. They are floating point numbers in units of 10^{24} atoms/cm³. The last card must contain an X-LAST.

5. Cross-Sections. The cross-section data will consist of N blocks one for each of the constituents of the medium. Their order must coincide with that of the number densities. Each block gives the cross-section data for an individual material. Three quantities are needed for each material: absorption cross section, σ_a , (or $\bar{\sigma}_a$ as previously noted) in locations 00000 to 00199; slowing down power, σ_s , in locations 00200 to 00399, and 3 times the transport cross section; $3\sigma_{tr}$, in locations 00420 to 00599. The numbers are again in floating point and the units are barns. An X-LAST must appear on the last card of each material. Any cross-sections which are zero may be omitted as the locations are cleared to zero before reading in the data. A constant cross section may be read into the appropriate locations by merely putting the number into the first location appropriate to that cross section. (The next number must be blank or zero). Thus only one card is necessary to indicate a constant cross section.

6. Temperature. The temperature of the moderator is specified in two locations by two cards. First in location 00000 T is given in °K in floating point form. Then an alpha-numeric card is used for location 00051.

Again T is in °K. Either an X-LAST or a Y-LAST must appear on the alpha-numeric card. An X-LAST is used if the problem is to be done for several different temperatures with the same composition. The temperature cards then merely follow each other, all the alpha-numeric cards but the last having X-LAST's; the last has a Y-LAST.

It is possible to run several different compositions of the same materials merely by putting the new composition cards and temperatures following the last temperature card of the previous case. A glance at the figure will make this more clear.

The code is simple to run, no tapes or drums being required. The 8KPAT package* must however be placed in front of the deck. A typical running time may be 1½ minutes per case. It should be remarked that the code is still provisional and as such a core dump is taken at the end of each run.

OUTPUT

The Hemad code solves the Wilkins differential equation for the neutron density which can be written in the form:

$$x \frac{d^2 N}{dx^2} + (2x^2 - 1) \frac{dN}{dx} + 4x \sqrt{1 - G(x)} N(x) = 0$$

$$\text{where } G(x) = \frac{\sum_j N_j \sigma_{a_j}(x)}{\sum_j N_j \sum_j \sigma_{s_j}(x)} \quad \text{and} \quad x^2 = \frac{E}{kT}$$

The code will then compute two types of averages; the "flux averaged," and "effective."

$$\bar{g} \text{ (flux averaged)} = \frac{\int_0^{E_{\max}} g(E) \phi(E) dE}{\int_0^{E_{\max}} \phi(E) dE}$$

$$g \text{ (effective)} = \frac{\int_0^{E_{\max}} g(E) \phi(E) dE}{\int_0^{E_{\max}} \sqrt{\frac{kT}{E}} \phi(E) dE}$$

* This package is in the 709 console file and will be placed in position if requested on the job order.

where $KT_0 = .0253$ ev

$\phi(E)$ = the calculated flux

$g(E)$ = the function to be averaged

$E_{\max}$ = the maximum energy specified in the input

In the output under the heading "Average Cross Sections" will appear:

1. $\bar{\Sigma}_a$ for the medium
2. $\bar{\Sigma}_s$ " " "
3. $\bar{D}$ (the diffusion coefficient) for the medium; $D(E) = \frac{1}{3 \Sigma_{tr}(E)}$
However, $D_{(eff)} = \frac{\bar{D}(\text{flux})}{\bar{\Sigma}_a(\text{flux})}$
4. $\left. \begin{array}{l} \text{the functions to be averaged} \\ \text{in the same order as in the} \\ \text{input} \end{array} \right\}$
- 11+3

Final Note: Averages over a Maxwellian spectrum may be obtained by merely setting all absorption cross sections equal to zero.

The following data sheets show a somewhat atypical case. The numbers in parenthesis are the locations available for that quantity. The cards are numbered in the order in which they must follow in the data deck.

HEMAD

Deck Arrangement

TDR No. 4220
Page 6

FIXED OR FLOATING 8 DIGIT DECIMAL DATA

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 1 OF 6 JOB NO. _____

END CLASS	FIRST LOCATION	MAX NO DIGITS	NUMBER	64 52 40 28 16	65 53 41 29 17	67 55 43 31 19	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
2	6	7 8 9			D	B	73	80
1	00000	08	4		+ 01	+ 3.5		I = Number of energy points
			4		+ 01	+ 1.7		" " " " "
			1		+ 01	+ 3.5		Test on input 0 if $\sqrt{a}$ 1 if $\sqrt{b}$
			1		+ 01	+ 1.7		N = Number of elements forming medium
			1		+ 01	+ 1.7	1	M = Number of quantities to be averaged
1	00005	08	2		+ 02	+ 1.7		5I
			8		+ 01	+ 1.7		2M + 6
			0		+ 00	+ 3.5		$Q = \begin{cases} 0 & \text{only one composition used} \\ N(400+I) & \text{otherwise} \end{cases}$
			404		+ 03	+ 3.5		400 + I
							2	
1		08						Limitations:
								$N \leq 30$
								$M \leq 230$
								$I \leq 200$
								$Q + MI \leq 8192$
1		08						

5 DIGIT FLOATING DECIMAL DATA

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 2 OF 6 JOB NO. _____

END CLASS	FIRST LOCATION	MAX. NO. DIGITS	NUMBER	D	IDENTIFICATION	DESCRIPTION DO NOT KEY PUNCH
X2	00130	05	1	-02		Energy Points in ev. (130-329)
			1	-01		
			1	+00		
			1	+01		
X2	00000	05	1	+00		Function to be averaged (0-199)
			2	+00		
			3	+00		
			4	+00		

5 DIGIT FLOATING DECIMAL DATA

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 3 OF 6 JOB NO. _____

[illegible]

5 DIGIT FLOATING DECIMAL DATA

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 4 OF 6 JOB NO. _____

[illegible]

5 DIGIT FLOATING DECIMAL DATA

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 5 OF 6 JOB NO. _____

[illegible]

ALPHANUMERIC DATA, 6 CHARACTERS PER WORD

DECK NO. HEMAD PROGRAMMER Sample Case DATE 7-31-59 PAGE 6 OF 6 JOB NO. _____

END CLASS	FIRST LOCATION	WORDS PER CARD	DATA										IDENTIFICATION	
			43	48	49	54	55	60	61	66	67	72		
2	6	8	13	18	19	24	25	30	31	36	37	42	73	80
X	4	0005101	300.0											
														10
Y	4	0005101	400.0											
														12
4														
4														
4														
4														
4														
4														
4														