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PROGRAM FOR CALCULATION OF
THERMAL AGE OF NEUTRONS

by

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PROGRAM FOR CALCULATION OF
THERMAL AGE OF NEUTRONS

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PROGRAM FOR CALCULATION OF THERMAL AGE OF NEUTRONS

A. General Description of the Calculation

The calculation is based on equation (108) in the article "Theory of the Slowing Down of Neutrons by Elastic Collision with Atomic Nuclei," by Robert E. Marshak, Reviews of Modern Physics 19, 185 (1947). This equation, which applies to a mixture of hydrogen and one other heavy component, is given below.

$$\begin{aligned}
 L_s^2 = & \frac{1}{3} \left\{ \frac{\lambda^2(a)}{c(a)} + \frac{\lambda^2(\tau)}{c(\tau)} + \lambda(a) \lambda(\tau) e^{-\int_a^\tau \left[\frac{3}{2} - c(u') \right] du'} \right. \\
 & + \int_a^\tau \frac{\lambda^2(u')}{c(u')} du' + \lambda(\tau) \int_a^\tau \lambda(u') du' e^{-\int_{u'}^\tau \left[\frac{3}{2} - c(u'') \right] du''} \\
 & + \lambda(a) \int_a^\tau \lambda(u') du' e^{-\int_a^{u'} \left[\frac{3}{2} - c(u'') \right] du''} \\
 & \left. + \int_a^\tau \lambda(u') du' \int_a^{u'} \lambda(u'') du'' e^{-\int_{u''}^{u'} \left[\frac{3}{2} - c(u''') \right] du'''} \right\}
 \end{aligned}
 \tag{1}$$

τ = lethargy of neutrons from some arbitrary initial point

a = lethargy of neutrons at initial energy

L_s^2 = age of neutrons slowing down from lethargy a to lethargy τ

$$\lambda(u) = \frac{1}{\sum_T^{(H)}(u) + \sum_{Tr}^{(O)}(u)} = \text{total mean free path}$$

$\sum_T^{(H)}(u)$ = total macroscopic cross section for hydrogen, not the transport cross section

$\sum_{Tr}^{(0)} (u)$ = macroscopic transport cross section for the heavy component

$$c(u) = \frac{\sum_T^{(H)} (u)}{\sum_T^{(H)} (u) + \sum_{Tr}^{(0)} (u)} = \frac{\text{total mean free path}}{\text{mean free path for hydrogen}}$$

The assumptions made in the derivation of the formula are the following:

- (1) The scattering of neutrons by the hydrogen is symmetric in the center of mass frame of reference. No absorption of neutrons by the hydrogen is included. Furthermore, the cross section appearing in the formula for the age is the total cross section and not the transport cross section.
- (2) The heavy component scatters neutrons but does not moderate them. The energy of a neutron after a collision with a heavy atom is considered to be the same as before the collision. Marshak also assumed that the scattering of neutrons by the heavy component was spherically symmetric and that there was no neutron absorption by the heavy component. These two restrictions can be relaxed by replacing the total cross section for this element by the transport cross section.
- (3) There are only two components present in the mixture, the heavy element and the hydrogen. The calculation can easily be extended to include several heavy components although feeding the data into the program as it is written at present is somewhat more cumbersome in this case. The changes necessary to include several heavy elements will be given below.
- (4) There is no energy loss by inelastic scattering.

In order to improve the speed of the computation the original expression for L_s^2 was rewritten

$$(2) \quad L_s^2 = \frac{1}{3} \left\{ \frac{\ell^2(a)}{c(a)} + \frac{\ell^2(\tau)}{c(\tau)} + \int_a^\tau \frac{\ell^2(u)}{c(u)} du + \ell(\tau) F_-(a) + F_+(a) f_-(a) \right. \\ \left. + \ell(\tau) f_-(a) + F_+(a) F_-(a) - \int_a^\tau f_+(u') F_-(u') du' \right\}$$

$$\text{where } f_-(u) = \ell(u) e^{-\int_u^{\tau} \left[\frac{3}{2} - c(u') \right] du'}$$

$$f_+(u) = \ell(u) e^{\int_u^{\tau} \left[\frac{3}{2} - c(u') \right] du'}$$

$$F_-(u) = \int_u^{\tau} f_-(u') du'$$

$$F_+(u) = \int_u^{\tau} f_+(u') du'$$

This latter expression for the age has the disadvantage that the seventh and eighth terms are large with a small difference, and it would be well when calculating a new situation to check the number of significant figures in this difference. In the particular case of the thermal age in Zr H1.2 the answer should be good to better than one per cent as far as this difference is concerned. An earlier code which was based on equation (1) rather than (2) and hence which did not suffer this drawback was discarded because of the long running time (approximately 8 hours compared to 4 minutes for the revised code) involved.

The code is written using the Wolontis Interpretive System, see IBM Technical Newsletter No. 11. The overall procedure is simply to calculate tables

of the quantities $\ell(u)$, $c(u)$, $\frac{3}{2} - c(u)$, $e^{-\int_u^{\tau} \left[\frac{3}{2} - c(u') \right] du'}$, $f_-(u)$, $f_+(u)$, $F_-(u)$, $F_+(u)$ and then to use these tables in evaluating L_s^2 . All integrals are computed numerically as follows. The integrand is given at a series of points u_1 . The quantity $f(u_1) \frac{\Delta u}{2} + f(u_2) \Delta u + f(u_3) \Delta u + \dots + f(u_{n-1}) \Delta u + f(u_n) \frac{\Delta u}{2}$ is

then used as $\int_{u_1}^{u_n} f(u) du$. Pictorially the approximation made appears in the figure below. The crosshatched area is used to approximate the area under the

curve. The value of Δu is in all cases $\frac{\ln 10}{4}$.

The total lethargy interval of interest extends from 10 Mev down to .056 ev, and the total number of lethargy points is 34. Of course not every integral calculated extends over this entire range.

During the course of the calculation, the age L_s^2 is calculated for ten different values of the initial lethargy a . The

smallest value of a is $a = 0$ which is made to correspond to an energy of 10 Mev. The other nine values of a chosen correspond to lower initial energies and are spaced at lethargy intervals of $\frac{\ln 10}{4}$. The a values used are therefore 0, $\frac{\ln 10}{4}$, $2 \frac{\ln 10}{4}$, $3 \frac{\ln 10}{4}$ ..., $9 \frac{\ln 10}{4}$.

After these computations are finished an averaging process is carried out to obtain an average age for the fission spectrum. The fission spectrum used is the well-known Watt spectrum, see The Reactor Handbook, volume 1, p. 69.

$$(3) \quad n(E) = \sqrt{\frac{2}{\pi E}} \sinh \sqrt{2E} e^{-E}$$

where E is in Mev, and $\int_0^\infty n(E) dE = 1$.

This spectrum is used in the form

$$n(E) dE = n(E) Edu = \eta(u) du$$

and the average age is found from

$$\bar{L}_s^2 = \int L_s^2(u) \eta(u) du.$$

B. Using the Code

In order to use the code one should have, in addition to the Wolontis system deck and the memory reset card (which must be used), the set of twenty five instruction cards, the two cards containing the Watt spectrum factors, the transfer card, the set of 18 data cards and the two cards containing the constants used in the calculation.

Nineteen of these cards change from one calculation to another. They are the eighteen data cards and the first constant card. On the first six data cards one should store the 34 values of $\sigma_T^{(o)}(u)$, the total microscopic cross sections in barns for the heavy element. The values of energy for which these cross sections should be tabulated start at 10 Mev and go down through .056 ev in equal lethargy intervals. The cards should be set up according to the Wolontis prescription to feed the 34 values into storage locations 350-383 inclusive. The value corresponding to 10 Mev should be in location 350 and the .056 ev value in location 383.

Into the next six data cards one should place 34 values of the total hydrogen cross section. The energy values should be chosen just as for the heavy element case. The storage locations are 400-433 inclusive.

Into the next six data cards one should store 34 values of $1 - \frac{\sigma_s^o}{\sigma_T^o} \langle \cos \theta \rangle_{av}$ where σ_s^o = the total microscopic scattering cross section for the heavy element in barns and $\langle \cos \theta \rangle_{av}$ is the average value of $\cos \theta$ for scattering by the heavy element. It will in general be a function of energy. The storage locations are 450-483 inclusive.

In the first constant card information must be entered which gives the number of hydrogen and heavy element atoms per cm^3 . This information is entered through the first constant card into storage locations 950-952 inclusive. Into storage

location 950 should go the number of atoms of the heavy element per cm^3 measured in units of 10^{24} , that is, if the actual number of atoms is $10^{24} \frac{1}{\text{cm}^3}$, then the number to be entered is 1. Into storage location 951 should go the number of hydrogen atoms per cm^3 measured in the same units and into 952 the ratio of these two numbers, i.e., $\frac{N_H}{N_O}$. It is easy to insert this information into the computer by making an extra constant card which is inserted after the original one and which reloads storage locations 950-952.

During the course of the calculation of the quantity $\overline{L_s^2}$, the average age, the machine will punch 21 cards. These cards will be punched in 11 steps. The first punch order produces two cards on which the terms in equation (2) appear in the order indicated by that equation, and following this in the ninth place appears the age. All of these quantities will be those appropriate for an initial energy of 56 kev (initial lethargy $2.25 \ln 10$) and a final energy of .056 ev. The next punch order produces two more cards containing the same quantities except that they refer to an initial lethargy of $2.00 \ln 10$. Eight more punch orders produce sixteen more cards with a succession of initial lethargies at intervals of $\frac{\ln 10}{4}$. Finally a single card is punched which gives $\overline{L_s^2}$.

The total running time of the program is about four minutes.

C. Changes in the Code for two or more Heavy Elements

If one wants to use the code for the age of neutrons in a mixture of hydrogen and several other heavy materials, the input of data should be modified as follows:

Let the heavy materials be described by numbers 1, 2, ..., i, ..., n. Then into locations 350-383 inclusive should go the quantities

$$\begin{aligned} & \sigma_T^{(0_1)}(u) \left[1 - \frac{\sigma_s^{0_1}}{\sigma_T^{0_1}} \langle \cos \theta \rangle_{av.1} \right] + \frac{M_{02}}{M_{01}} \sigma_T^{(0_2)}(u) \left[1 - \frac{\sigma_s^{0_2}}{\sigma_T^{0_2}} \langle \cos \theta \rangle_{av.2} \right] \\ & + \dots + \frac{M_{0i}}{M_{01}} \sigma_T^{(0_i)}(u) \left[1 - \frac{\sigma_s^{0_i}}{\sigma_T^{0_i}} \langle \cos \theta \rangle_{av.i} \right] + \dots \\ & \dots + \frac{M_{0n}}{M_{01}} \sigma_T^{(0_n)}(u) \left[1 - \frac{\sigma_s^{0_n}}{\sigma_T^{0_n}} \langle \cos \theta \rangle_{av.n} \right] \end{aligned}$$

Into locations 450-483 should go l's.

Into locations 400-433 should go σ_T^H just as before.

Into location 950 should now be fed N_{01} , the number of atoms per cm^3 of element 1.

Into location 951 should go the number of hydrogen atoms and into location 952 should go $\frac{N_H}{N_{01}}$.

Of course the program could easily be revised to make the entry of data simpler in this case. It should be remembered that the same assumptions apply to all heavy elements included, i.e., no moderation of neutrons by them.

A complete list of instructions used in the age program is included below.

Program for Calculation of Thermal Age of Neutrons

PROBLEM

1-4 5-6 7-9 10 11 76: CARD COLUMNS

CARD No.	DK. No.	LOC. WD.1	N	DRM. LOC.	OP: NO:	+	0	AOR0 ₂	B	C	COMMENTS
						-	X.XXX	X.XX	X	a	
0001	01	90	4								
				90		+	0	500	181	8 59	
				91		+	0	050	181	7 09	
				92		+	0	050	182	7 09	
				93		+	0	500	183	8 09	
0002	01	94	6	94		+	0	050	183	8 59	
				95		+	0	005	191	9 27	
				96		+	0	050	179	3 09	
				97		+	0	050	180	8 09	
				98		+	0	050	192	3 09	
				99		+	0	203	000	2 23	
0003	01	100	6	100		-	3	350	450	3 00	$(\sigma_T)_0 [1 - \langle \cos \theta \rangle_{ave}] \rightarrow 30x$
				101		+	0	111	034	1 00	
				102		-	3	952	400	2 50	$(N_H/N_0)(\sigma_s)_H \rightarrow 25x$
				103		+	0	011	034	1 02	
				104		-	1	300	250	5 00	$(\sigma_s)_0 (1 - \langle \cos \theta \rangle_{ave}) + \frac{N_H}{N_0} \sigma_{SH} \rightarrow 50x$
				105		+	0	111	034	1 04	
0004	01	106	6	106		-	3	950	500	5 00	
				107		+	0	011	034	1 06	
				108		-	4	954	500	5 00	$\ell(u) \rightarrow 50x$
				109		+	0	011	034	1 08	
				110		-	3	951	400	5 50	
				111		+	0	011	034	1 10	
0005	01	112	6	112		-	3	550	500	5 50	$c(u) \rightarrow 55x$
				113		+	0	111	034	1 12	
				114		-	2	955	550	6 00	
				115		+	0	011	034	1 14	$3/2 - c(u) \rightarrow 60x$
				116		-	1	600	601	3 00	
				117		+	0	111	033	1 16	
0006	01	118	6	118		-	5	300	957	6 50	
				119		+	0	101	033	1 18	
				120		-	0	301	650	6 50	$\exp(-\int_u^{u+2u} [3/2 - c(u')] du') - 765x$
				121		+	0	011	033	1 20	
				122		+	9	000	954	6 83	
				123		+	9	000	954	7 33	

I-4 5,6 7-9 10 II 76: CARD COLUMNS

CARD No.	DK. No.	LOC. WD.1	N	DRM. LOC.	OP: NO:	+	O ₁	AORO ₂	B	C	COMMENTS
						-	X.XXX	XXX	X	a	
0007	01	124	6	124		+	9	000	954	7 83	
				125		+	0	500	131	7 83	
				126		+	0	050	131	6 82	
				127		+	0	005	131	7 82	
				128		+	0	500	132	7 83	
				129		+	0	050	132	6 82	
0008	01	130	6	130		+	0	005	132	7 82	
				131		+	3	[000]	[000]	0 00	
				132		+	4	[000]	[000]	0 00	
				133		+	0	700	131	0 01	
				134		+	0	070	131	0 01	
				135		+	0	007	131	0 01	
0009	01	136	6	136		+	0	700	132	0 01	
				137		+	0	070	132	0 01	
				138		+	0	007	132	0 01	
				139		+	8	131	699	1 31	
				140		-	3	700	500	7 00	$f_-(u) \rightarrow 70x$
				141		-	3	750	500	7 50	$f_+(u) \rightarrow 75x$
0010	01	142	6	142		+	0	111	034	1 40	
				143		+	9	000	953	8 33	
				144		+	9	000	953	8 83	
				145		+	0	500	151	8 33	
				146		+	0	050	151	7 33	
				147		+	0	050	152	7 32	
0011	01	148	6	148		+	0	005	152	8 32	
				149		+	0	500	227	8 83	
				150		+	0	203	000	2 33	
				151		+	1	833	733	0 00	
				152		+	1	000	732	8 32	
				153		+	0	203	000	2 27	
0012	01	154	6	154		+	0	070	151	0 01	
				155		+	0	700	151	0 01	
				156		+	0	700	227	0 01	
				157		+	0	070	152	0 01	
				158		+	0	007	152	0 01	
				159		+	7	151	700	1 51	

1-4 5-6 7-9 10

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76: CARD COLUMNS

CARD No.	DK No.	LOC. WD.1	N	DRM. LOC.	OP: NO.	+	0	AOR ₀	B	C	COMMENTS
						-		X.XXX,XXX,X		a	
0013	01	160	6	160		-	3	957	800	8:00	$F_-(u) \rightarrow 80x$
				161		-	3	957	850	8:50	$F_+(u) \rightarrow 85x$
				162		+	0	011	033	1:60	
				163		-	3	500	500	3:00	
				164		+	0	111	034	1:63	
				165		-	4	300	550	3:00	$l^2/c \rightarrow 30x$
0014	01	166	6	166		-	3	750	800	2:50	$f_+(u) F_-(u) \rightarrow 25x$
				167		+	0	111	034	1:65	
				168		+	9	000	953	9:62	
				169		-	1	962	309	9:62	
				170		-	1	962	310	9:62	
				171		+	0	010	024	1:69	
0015	01	172	6	172		+	9	000	953	9:67	
				173		-	1	967	259	9:67	
				174		-	1	967	260	9:67	
				175		+	0	010	024	1:73	
				176		+	3	962	957	9:62	$l^2/c \rightarrow 962$
				177		+	5	967	957	9:57	$-\int f_+ F_- \rightarrow 967$
0016	01	178	6	178		+	9	000	333	9:61	$l^2/c(\tau) \rightarrow 961$
				179		+	9	000	{309}	9:60	$l^2/c(a) \rightarrow 960$
				180		+	3	533	{809}	9:63	$l(\tau) F_-(a) \rightarrow 963$
				181		+	3	{859}	{709}	9:64	$F_+ f_- \rightarrow 964$
				182		+	3	533	{709}	9:65	$l(\tau) f_-(a) \rightarrow 965$
				183		+	3	{809}	{859}	9:66	$F_+ f_-$
0017	01	184	6	184		+	9	008	960	9:10	Move to punching loc
				185		-	3	958	910	9:10	1/3 age terms
				186		+	0	011	008	1:85	
				187		+	9	000	953	9:18	
				188		-	1	910	918	9:18	Age sum to 918
				189		+	0	100	008	1:88	
0018	01	190	6	190		+	0	410	910	9:18	Punch
				191		+	9	000	918	{9:27}	Age to 92x
				192		+	1	{309}	{310}	9:90	
				193		+	0	203	000	2:14	
				194		+	0	700	181	0:01	Address 396-
				195		+	0	070	181	0:01	Modification 10

1-4 5-6 7-9 10				11 12 13 14 15 16 17							76: CARD COLUMNS	
CARD No.	DK No.	LOC. WD.1	N	DRM. LOC.	OP: NO:	+	0	AOR ₀	B	C	COMMENTS	
						-	X.XXX	,XXX	X	a		
0019	01	196	6	196		+	0	070	182	0:01	Address Modification	
				197		+	0	700	183	0:01		
				198		+	0	070	183	0:01		
				199		+	0	006	191	0:01		
				200		+	0	070	179	0:01		
				201		+	0	070	180	0:01		
0020	01	202	6	202		+	0	070	192	0:01		
				203		+	0	203	000	2:04		
				204		+	8	191	937	1:79	Test for last "a"	
				205		-	3	927	977	9:27	$L_s^2(u) \eta(u) \rightarrow 92x$	
				206		+	0	111	010	2:05		
				207		+	9	000	953	9:37		
0021	01	208	6	208		-	1	927	937	9:37		
				209		-	1	928	937	9:37		
				210		+	0	100	009	2:08		
				211		+	3	937	957	9:37	$L_s^2 \rightarrow 937$	
				212		+	0	410	937	9:37	Punch	
				213		+	0	000	000	0:00		
0022	01	214	6	214		+	3	990	957	0:00		
				215		+	1	000	962	9:62		
				216		+	1	260	259	0:00		
				217		+	3	000	957	0:00		
				218		+	2	967	000	9:67		
				219		+	0	700	192	0:01		
0023	01	220	6	220		+	0	700	216	0:01		
				221		+	0	070	216	0:01		
				222		+	0	203	000	1:94		
				223		+	0	500	192	3:08		
				224		+	0	500	216	2:59		
				225		+	0	050	216	2:58		
0024	01	226	6	226		+	0	203	000	1:00		
				227		+	1	883	783	0:00		
				228		+	1	000	782	8:82		
				229		+	0	070	227	0:01		
				230		+	0	070	228	0:01		
				231		+	0	007	228	0:01	396 //	

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