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SLOWING-DOWN SPECTRA OF NEUTRONS IN HEAVY WATER AND LIGHT WATER MIXTURES

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ABSTRACT

The slowing down spectra of neutrons are obtained for heavy water, light water, and mixtures of heavy water and light water. It is assumed that fission neutrons are produced uniformly throughout an infinite moderator and the only process considered is elastic scattering, spherically symmetric in the centre of mass system. The (n, 2n) reaction with the deuterium nucleus and absorption are assumed negligible.

The average transfer cross section, fast diffusion coefficient, the slowing down area, and average velocity ratio are obtained for two-group calculations using the epi-thermal spectra.

CONTENTS

1. INTRODUCTION

The collision density of neutrons slowing down in an infinite homogeneous moderator consisting of n different nuclides is investigated in this report. It is assumed that fission neutrons are produced uniformly throughout an infinite moderator and the only reaction considered is elastic scattering, spherically symmetric in the centre of mass system. The general equation is solved for D_2O, H_2O, and mixtures of D_2O and H_2O using a direct numerical solution of the equation on a digital computer. Two-group quantities are obtained from the spectra so obtained.

2. THEORY

2.1 Slowing Down Spectra

The number of neutrons lost by scattering in the energy region dE around E per cm^3 per sec is

$$\phi(E)\Sigma_s(E)\,dE \quad .$$

The number of neutrons arising from fission in the region per cm^3 per sec is

$$Ss(E)dE \quad .$$

The number of neutrons per cm^3 per sec which enter the region as a result of scattering from higher energies is

$$dE\sum_{i=1}^{n}\frac{1}{1-\alpha_i}\int_{E}^{E/\alpha_i}\phi(E')\,\Sigma_{si}(E')\,\frac{dE'}{E'} \quad .$$

The appropriate neutron balance equation is therefore

$$\phi(E)\Sigma_s(E) = Ss(E) + \sum_{i=1}^{n}\frac{1}{1-\alpha_i}\int_{E}^{E/\alpha_i}\phi(E')\Sigma_{si}(E')\,\frac{dE'}{E'} \qquad (1)$$

which on introducing the collision density and scattering probability simplifies to

$$F(E) = s(E) + \sum_{i=1}^{n}\frac{1}{1-\alpha_i}\int_{E}^{E/\alpha_i}F(E')\,H_i(E')\,\frac{dE'}{E'} \quad . \qquad (2)$$

Changing the variable of integration from energy to lethargy in equation 2 we get

$$F(E) = s(E) + \sum_{i=1}^{n}\frac{1}{1-\alpha_i}\int_{u-u_i}^{u}F(E')H_i(E')\,du' \quad , \qquad (3)$$

which has been found to be the most convenient form of the slowing down equation for solution on a digital computer when a particular moderator is being investigated.

The scattering probabilities $H_i(E')$ may be calculated for a particular moderator from the compilation of Hughes and Schwartz (1958), and the fission spectrum $s(E)$ may be calculated from the expression given by Cranberg et al. (1956). It is therefore possible to solve equation 3 for the collision density $F(E)$, subject to the restriction placed on the fission spectrum,

$$s(E) = 0 \text{ for } E > E_m \quad ,$$

$$\therefore\ F(E) = 0 \text{ for } E > E_m \quad . \tag{4}$$

Equation 4 may be combined with equation 3 by replacing negative lethargies by zero when they occur for the lower integral limit.

2.2 Two-group Epithermal Quantities

The two-group epithermal quantities are obtained using the following equations whose derivation is given in the Appendix. The spectra are obtained by solving equation 3:

$$\Sigma_{se} = \left\{ E_o^{1/2} \int_o^{ou} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}}\, du \right\}^{-1} \quad ,$$

$$D_e = \int_o^{ou} \frac{F(u)}{3\,\Sigma_{tr}(E)\,\Sigma_s(E)}\, du \Big/ \left\{ E_o^{1/2} \int_o^{ou} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}}\, du \right\} \quad ,$$

$$\frac{\tilde{v}_e}{v_o} = \int_o^{ou} \frac{F(u)}{\Sigma_s(E)}\, du \Big/ \left\{ E_o^{1/2} \int_o^{ou} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}}\, du \right\} \quad ,$$

$$L_s^2 = De/\Sigma_{se}^* \quad .$$

2.3 Asymptotic Solution

The slowing down density and collision density are connected through the following equation derived by Glasstone and Edlund (1952),

$$q(E) = \sum_{i=1}^{n} \frac{1}{1-\alpha_i} \int_E^{E/\alpha_i} (E-\alpha_i E')\, F(E')\, H_i(E')\, \frac{dE'}{E'} \quad . \tag{5}$$

In the asymptotic energy region ($E < 0.01$ MeV), where a negligible number of fission neutrons are entering the region and the scattering cross sections are constant $[H_i(E') = H_i]$, the solution of equation 3 is given by

$$F(E) = k/E, \text{ where } k \text{ is a constant}$$

$$\text{or}\quad F(u) = EF(E) = k \quad .$$

Substituting this equation in equation 5 and remembering that all fission neutrons will eventually slow down into the asymptotic region (i.e. $q(E) = 1$),

$$k = \left\{ \sum_{i=1}^{n} H_i \xi_i \right\}^{-1} = 1/\bar{\xi} \quad ,$$

and therefore

$$F(u) = 1/\bar{\xi} \tag{6}$$

in the asymptotic region.

2.4 Numerical Technique

The technique adopted for a particular moderator was to expand the epithermal range into sub-collision ranges of lethargy width Δu starting at $u = 0$ ($E = Em$). Δu was chosen so that the 1^{th} nuclide collision range was divided into exactly n_1 equal lethargy steps ($\Delta u = u_1/n_1$). The collision range for the i^{th} nuclide then consisted of n_i equal lethargy steps of width Δu and one remaining step which was only a fraction of Δu in width (n_i = truncated part of $\frac{u_i}{\Delta u}$. Numbering the sub-collision boundaries from the boundary at $u=0$ starting with $j = 1$, and introducing ,

E_j = the energy corresponding to the j^{th} sub-collision boundary

$= E_m e^{-(j-1)\Delta u}$,

and

$F_j = F(E_j)$

$s_j = s(E_j)$

$H_{ij} = H_i(E_j)$

allows equation 3 to be written

$$F_j = s_j + \sum_{i=1}^{n} \frac{\Delta u}{1-\alpha_i} \sum_{k=j-(n_i+1)}^{j} A_{ik} F_k H_{ik} \quad , \tag{7}$$

where A_{ik} are constants which express the integral rule used in evaluating the integral in equation 3 and allow for both the sharp cut off expressed in equation 4 and linear interpolation required at the low lethargy end of the collision ranges.

For example:

$A_{1,\, j-(n_1+1)} = 0$, as no interpolation is required for the 1^{th} nuclide at the end of the collision range, and when the trapezoidal rule is used

$A_{ij} = 1/2$

$A_{i,j-1} = 1$, provided $j>2$, etc.

Equation 7 may be rewritten as a recurrence relation for F_j, as follows:

$$F_j = \frac{s_j + \sum_{i=1}^{n} \frac{\Delta u}{1-\alpha_i} \sum_{k=j-(n_i+1)}^{j-1} A_{ik} F_k H_{ik}}{1 - \sum_{i=1}^{n} \frac{\Delta u}{1-\alpha_i} A_{ij} H_{ij}} , \tag{8}$$

which relates F_j to previously evaluated collision densities.

The sharp cut-off assumed for the fission spectrum allows the calculation to start at $j = 1$ with

$$F_1 = s_1 = s(E_m) \tag{9}$$

and $$F_j = 0 \text{ for } j < 1 . \tag{10}$$

The two-group quantities are given in terms of integrals with the form

$$G_m(E) = \int_0^u Y_m(E')F(u')\,du' , \tag{11}$$

Where $Y_m(E')$ depends on the moderator and the neutron energy. The numerical evaluation of this type of integral is quite straightforward and may be carried out as the collision density becomes available from the relation 8.

3. DATA USED

The epithermal range was divided up so that 50 lethargy steps comprised one collision range for deuterium. The collision range for oxygen then consisted of slightly less than 6 sub-collision steps, and the collision range for hydrogen covered all the sub-collision steps from $u = 0$, as a neutron may lose all of its energy on collision with a proton.

The scattering cross sections for hydrogen, deuterium, and oxygen were obtained from the compilation of Hughes and Schwartz (1958) at energies corresponding to the sub-collision boundaries. To allow for chemical binding, the low energy cross sections for hydrogen and deuterium were obtained from the H_2O and D_2O curves.

Six values were chosen for the ratio of the number of molecules of H_2O to the number of molecules of the D_2O–H_2O mixture, $R = 0$ (D_2O), 0.01, 0.05, 0.2, 0.5 and $R = 1$ (H_2O). The density of each mixture was calculated from the two extremes of pure D_2O and pure H_2O given by Condon and Odishaw (1958).

4. RESULTS

A programme was written in FORTRANSIT for an IBM 650 electronic computer. This programme used the trapezoidal rule, both for integration involved in equation 8 to give the collision density starting at $E = E_m = 12$ MeV, and for integration involved in calculating integrals of the form given by equation 11, which were required for calculating the two-group quantities.

The spectra obtained as output from the programme are shown in Figures 1 and 2. For comparison, Figure 1 also shows the spectra for hydrogen and deuterium obtained from the Greuling-Goertzel approximation below, which is exact for hydrogen:

$$F(u) = \frac{1}{\xi_i}\left\{\int_o^u s(u')\,du' + \gamma_i\, s(u)\right\} , \qquad (12)$$

where $\gamma_i = \left\{1-\alpha_i(1+u_i+1/2\ u_i^2)\right\} / \left\{(1-\alpha_i)\ \xi_i\right\}$.

This comparison shows the bumps in the spectra obtained from the computer output to be due to the presence of the oxygen, which has many wild fluctuations present in the scattering cross section at high energies. The storage limitation of the computer did not enable these fluctuations to be followed in great detail.

The asymptotic values of the collision density F(u) obtained from the computer output agree with the values given in Table 2, which were obtained from equation 6.

The epithermal constants Σ^*_{se}, $\tilde{v}_e/v_o$, De, and L_s^2 calculated down to the epithermal cut-off energy, 0.0711 eV, for various D_2O - H_2O mixtures are given in Table 1. The corresponding graphs are given in Figures 3 and 4.

Also the calculated L_s^2 to indium resonance, 1.44 eV, is given as a function of H_2O content of the mixture in Figure 4. This is compared with the experimental results of Wade (1956) though it should be noted that Wade's experimental points are determined from the slowing down density of neutrons derived from a point fission source measured by point indium detectors.

5. SUMMARY

The method described in this report was used to obtain the collision density F(u) for D_2O, H_2O, and four mixtures of D_2O and H_2O and gave the results shown in Figures 1 and 2. Two-group epithermal quantities were obtained from these spectra and gave the results shown in Figures 3 and 4 as well as Table 1. The spectra obtained are exact for the conditions assumed, but are inaccurate due to neglect of the anisotropy of elastic scattering, the (n,2n) reaction in deuterium and 1/v - absorption in hydrogen.

6. NOTATION

A_i = mass ratio of i^{th} nuclide to neutron

α_i = $\left(\frac{A_i - 1}{A_i + 1}\right)^2$. Minimum energy of a neutron, initial energy E, after a single collision with an i^{th} nuclide is $\alpha_i E$.

E = neutron energy

E_M = maximum energy of neutrons considered in the calculation

= 12 MeV; it is assumed that s (E) = 0 for $E > E_M$

E_o = energy of neutrons having a velocity v_o = 2200m/sec

= 0.0253 eV

${}_oE$	=	assumed cut off energy of epithermal spectrum
	=	0.0711 eV; i.e. 2.81 E_o
u	=	neutron lethargy
	=	$\ln (E_M/E)$
${}_ou$	=	$\ln (E_M/{}_oE)$
u_i	=	lethargy of neutrons having an energy of $\alpha_i E_M$
	=	$\ln(1/\alpha_i)$
S	=	total number of neutrons (of all energy)
		produced in the moderator by fission per cm^3 per sec
$\Sigma_{si}(E)$	=	macroscopic scattering cross section for i^{th} nuclide at energy E
$\Sigma_s(E)$	=	total macroscopic scattering cross section at energy E
$\Sigma_{tr}(E)$	=	total macroscopic transport cross section at energy E
$s(E)$	=	normalized fission spectrum at energy E suggested by Cranberg et al. (1956)
	=	$0.45270 \exp(-E/0.965) \sinh (2.29E)^{1/2}$;
		$\int_o^\infty s(E)\, dE = 1$
$N(E)$	=	neutron density per unit energy at energy E
$\phi(E)$	=	neutron flux per unit energy at energy E
	=	$vN(E)$
$F(E)$	=	collision density per unit energy at energy E derived from sources emitting 1 neutron per cm^3 per sec
	=	$\phi(E)\, \Sigma_s(E)/S$
$q(E)$	=	slowing down density, the number of neutrons per cm^3 per sec that slow down past a given energy E from sources emitting 1 neutron per cm^3 per sec
ξ_i	=	average gain of lethargy for neutrons colliding with the i^{th} nuclide
	=	$1 - \frac{\alpha_i}{1-\alpha_i} \ln(1/\alpha_i)$
$H_i(E)$	=	probability of scattering by the i^{th} nuclide
	=	$\Sigma_{si}(E)/\Sigma_s(E)$

Σ_{se}^* = macroscopic cross section for transfer of neutrons from the epithermal to the thermal group - see Appendix

De = diffusion coefficient for the epithermal group - see Appendix

L_s^2 = slowing down area defined as D_e/Σ_{se}^*

$\tilde{v}_e$ = epithermal neutron velocity averaged over the neutron density spectrum for the epithermal range - see Appendix

R = ratio of number of molecules of H_2O to the number of molecules of the D_2O - H_2O mixture

7. REFERENCES

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APPENDIX

TWO-GROUP EPITHERMAL QUANTITIES

It is convenient to introduce Ne, ϕe, $\tilde{x}$, and $\bar{x}$ by means of the following definitions

$$Ne = \int_{oE}^{E_m} N(E)dE \quad ,$$

$$\phi_e = \int_{oE}^{E_m} \phi(E)dE = \int_{oE}^{E_m} v(E)N(E)dE \quad ,$$

$$\tilde{x} = \frac{1}{N_e} \int_{oE}^{E_m} x(E)N(E)dE \quad ,$$

$$\bar{x} = \frac{1}{\phi_e} \int_{oE}^{E_m} x(E)\phi(E)dE \quad ,$$

where x(E) is any parameter that depends on the neutron energy and N(E) is the neutron density per unit energy at energy E. When x(E) = v, the neutron velocity,

$$\tilde{v}_e = \frac{1}{N_e} \int_{oE}^{E_m} v\, N(E)dE = \phi_e/N_e \quad .$$

W_e, an effective flux for the epithermal group, may be defined by the relation

$$W_e = v_o N_e \quad .$$

Then $\tilde{v}_e/v_o = \phi_e/W_e$.

An effective cross section for transfer of neutrons from the epithermal to the thermal group, Σ^*_{se}, may also be introduced through the relation

$$W_e \Sigma^*_{se} = S$$

which expresses the fact that all fission neutrons are eventually transferred to the thermal group when absorption and leakage are absent.

$$\therefore \Sigma^*_{se} = S/W_e = S/(v_o N_e) \quad .$$

Introducing F(u) the collision density per unit lethargy, the following series of identities follow from basic definitions

$$-F(u)du = F(E)dE = \frac{\Sigma_s(E)\phi(E)dE}{S} = \frac{\Sigma_s(E)\, v(E)N(E)dE}{S} \quad ,$$

$$\therefore \Sigma^*_{se} = \left\{ E_o^{1/2} \int_o^{o^u} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}} du \right\}^{-1} \quad .$$

It is also possible to introduce a transfer cross section through the relation

$$\phi_e \Sigma_F = S$$

$$\therefore \quad \Sigma_F = \Sigma^*_{se} / (\tilde{v}_e / v_o) \quad .$$

In agreement with this equation the velocity ratio $\tilde{v}_e/v_o$ may also be given in terms of the collision density per unit lethargy as

$$\tilde{v}_e / v_o = \int_o^{ou} \frac{F(u)}{\Sigma_s(E)} \, du \Big/ \left\{ E_o^{1/2} \int_o^{ou} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}} \, du \right\} .$$

The diffusion coefficient for epithermal neutrons may be obtained by applying diffusion theory to 1 cm^3 of the moderator. The leakage rate of epithermal neutrons from the element is then given by

$$L_e = \int_{oE}^{E_m} \nabla \cdot \{ - D(E) \nabla \phi(E) \} \, dE \quad ,$$

$$= \quad - \nabla^2 \int_{oE}^{E_m} D(E) \, \phi(E) dE \quad ,$$

where $D(E) = \{ 3 \, \Sigma_{tr} (E) \}^{-1}$ from the transport theory correction to diffusion theory. For convenience $D_e(E) = v\, D(E)$ is also introduced.

The above expression for L_e may then be written in two ways

$$L_e = - \frac{\tilde{D}_e}{v_o} \nabla^2 w_e \quad ,$$

and $$L_e = - \bar{D} \, \nabla^2 \phi_e \quad .$$

The effective diffusion coefficient is therefore given by

$$D_e = \frac{\tilde{D}_e}{v_o}$$

$$= \int_o^{ou} \frac{F(u)}{3 \Sigma_{tr}(E) \Sigma_s(E)} \, du \Big/ \left\{ E_o^{1/2} \int_o^{ou} \frac{F(u)}{\Sigma_s(E)\, E^{1/2}} \, du \right\},$$

which may be derived in the same way as the equation for Σ^*_{se} .

The second expression above for L_e shows that the alternative definition of diffusion coefficient satisfies a relation similar to that for Σ_F , namely

$$D = D_e / (\tilde{v}_e / v_o) \quad .$$

Two–group theory gives the slowing down area as

$$L_s^2 = D_e / \Sigma^*_{se} \quad ,$$

which may also be written

$$L_s^2 = D / \Sigma_F \quad .$$

TABLE 1

Two-group Epithermal Constants at 20.4°C

R	Σ^*_{se} cm^{-1}	D_e cm	L_s^2 cm^2	$\frac{\tilde{v}_e}{v_o}$
0	0.159	20.3	127	15.8
0.01	0.174	20.6	119	16.2
0.05	0.223	21.8	98	17.4
0.20	0.409	25.2	61.5	21.0
0.50	0.785	31.0	39.5	25.5
1.00	1.368	42.5	31.1	29.5

TABLE 2

Asymptotic Values of the Collision Density

R	F(u)
0	1.98
0.01	1.90
0.05	1.70
0.2	1.38
0.5	1.18
1	1.08

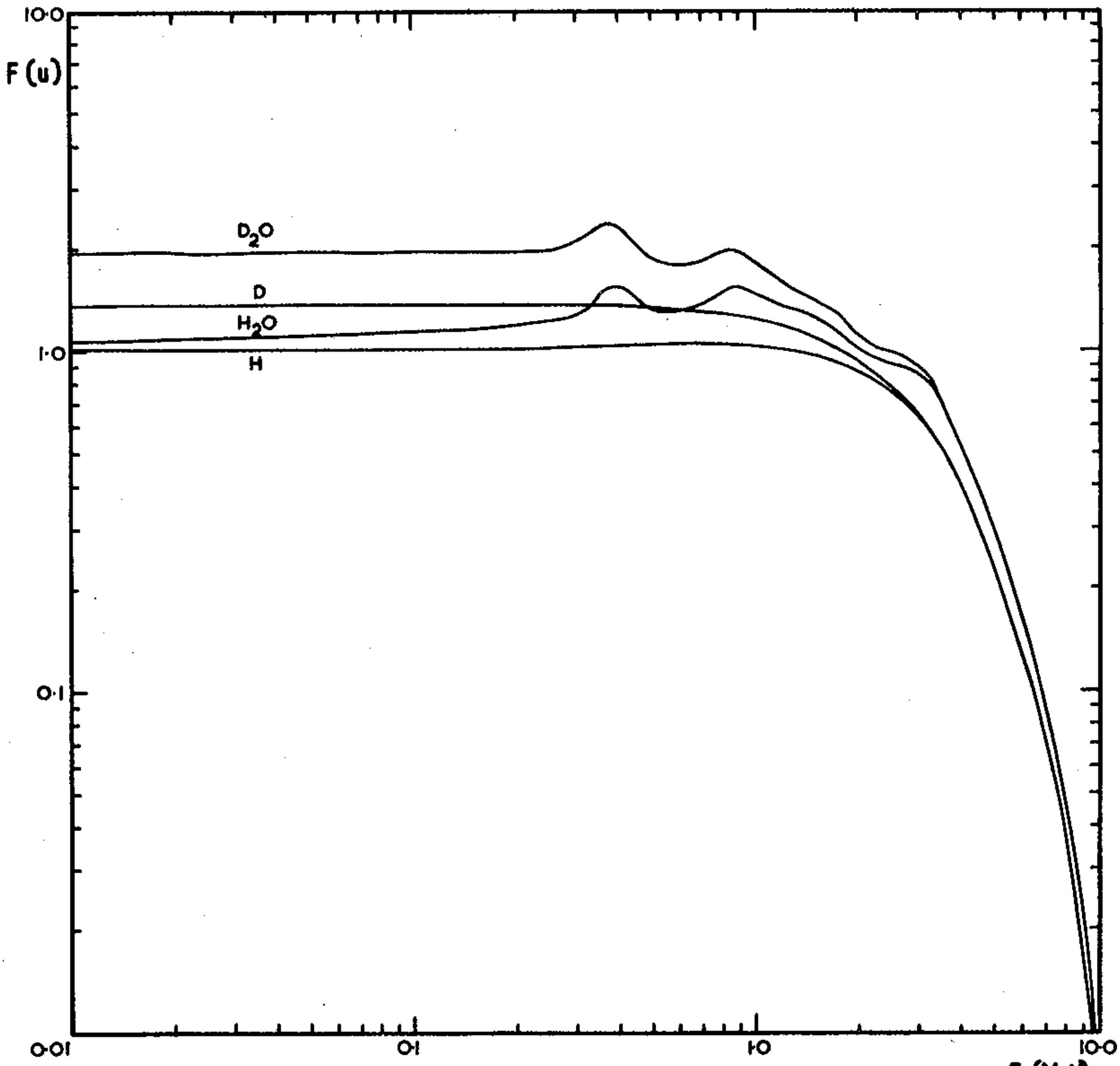

FIG. I COMPARISON OF SLOWING DOWN SPECTRA

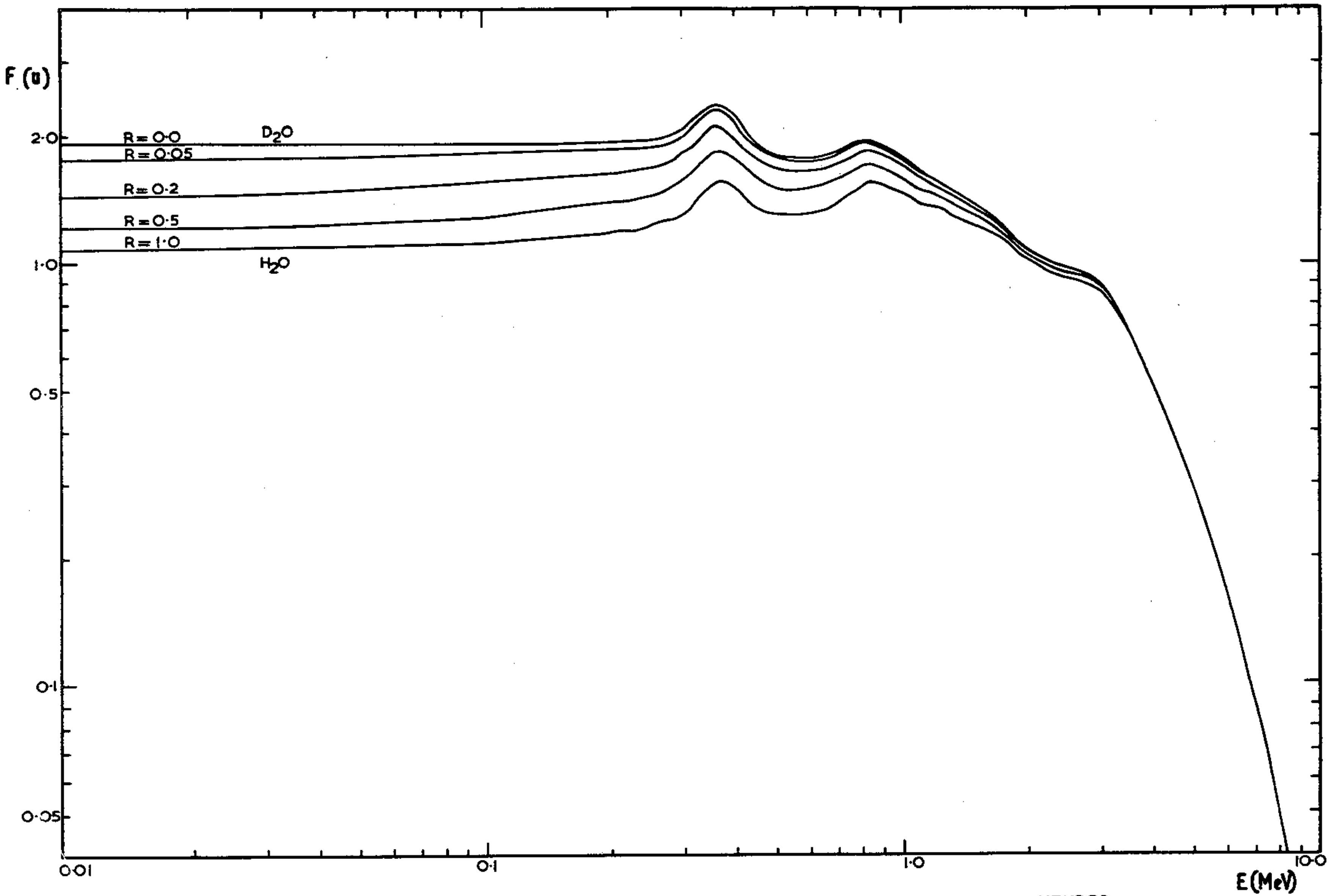

FIG. 2 SLOWING DOWN SPECTRA OF NEUTRONS IN D_2O AND H_2O MIXTURES

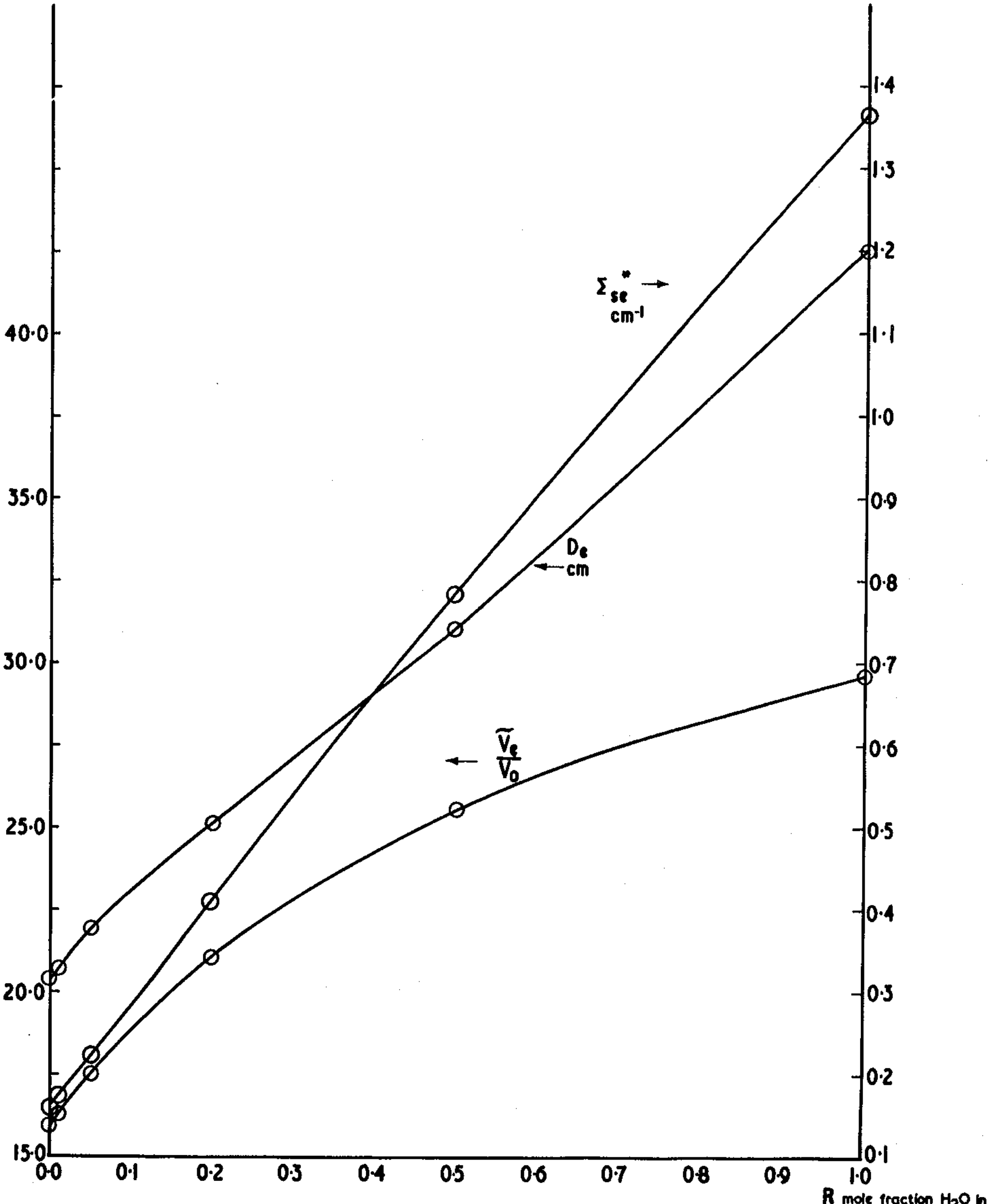

FIG. 3 TWO-GROUP EPITHERMAL CONSTANTS AT 20·4 °C AS FUNCTIONS OF THE H_2O CONTENT OF THE MIXTURE

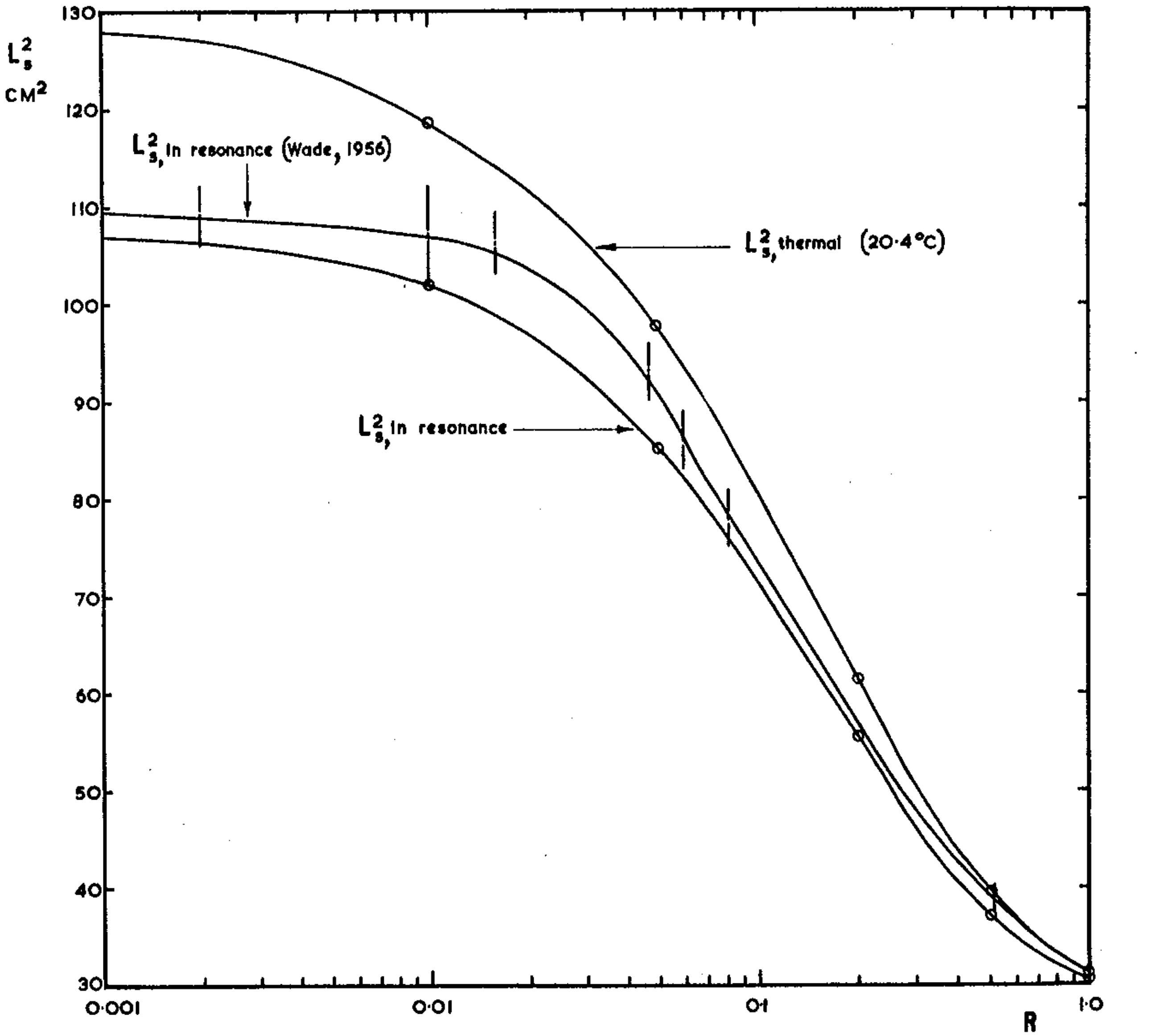

FIG. 4 AGE AS A FUNCTION OF THE H_2O CONTENT OF THE MIXTURE