Monte Carlo calculations of neutron thermalization in a heterogeneous system

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Summary:

The slowing down of neutrons in a heterogeneous system (a slab geometry) of uranium and heavy water has been investigated by Monte Carlo methods. Effects on the neutron spectrum due to the thermal motions of the scattering and absorbing atoms are taken into account. It has been assumed that the speed distribution of the moderator atoms are Maxwell-Boltzmann in character.

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1. Introduction.

An analytic solution of the space-energy dependent transport equation in the thermal region for a heterogeneous system with an arbitrary moderator is not known. For a heavy monoatomic gas the problem has been treated by M. V. Kazarnovsky et al. (1958).

The neutron spectrum in a homogeneous medium has been studied by employing various methods. Wigner and Wilkins (1944) derived a differential equation for the case of a monoatomic hydrogen gas and they also used this equation for numerical solutions. Coveyou (1955) has used the Monte Carlo method to calculate the neutron spectrum in a monoatomic gas with " $\frac{1}{v}$ " absorption. Brown (1956) and Brown and St. John (1954) have solved the space independent transport equation numerically when one has absorption and a gaseous D_2O or H_2O moderator. Hurwitz et al. (1956) have solved the energy dependent transport equation for a heavy gaseous moderator with " $\frac{1}{v}$ " absorption. Cohen (1957) has studied the same problem.

In this report a Monte Carlo code, which calculates the neutron spectrum in a slab geometry, is described. Calculations have been made for a system of " $\frac{1}{v}$ " absorbing "uranium" plates in gaseous heavy water. The heavy water has been considered as an ideal gas.

2. Brief outline of the Monte Carlo programme.

See flow diagram in fig. 1. The neutron is started with isotropic angular distribution with a velocity which is well above thermal. The starting point may be chosen arbitrarily or the start may occur where a fission has taken place. In the whole energy range the free paths (d_i) are chosen from the distribution $\int_0^{d_i} \Sigma_T e^{-\Sigma_T x}\, dx = \xi$, where ξ is a random number in the interval (0, 1) and Σ_T is the total macroscopic cross section (speed dependent). When the distance, which a neutron may travel, is chosen, the new coordinate for the neutron is calculated.

The events (fission, capture, collision) are chosen proportional to the velocity dependent macroscopic cross sections (capture is noted by the method of weighting).

The scattering angle is chosen isotropically in the center of mass system. In the thermal region one has to choose the velocity vector of the moderator atom. It is now possible to calculate the velocity vector of the neutron. When this is done the data are stored. Subsequently, it is then possible to calculate the space, velocity and angular distributions of the neutrons from the stored data.

3. Reaction probability, reaction rate and cross-section in the thermal region.

In calculating reaction rates, reaction probabilities and cross-sections in the thermal region one must take into account the thermal motion of the moderating atoms. Through employment of the fact that the total cross-section is the same in all Galilei systems one gets for the reaction rate (R) in a neutron beam against a reacting material

$$R = n \cdot v_{rel} \cdot \sigma \cdot N \tag{1}$$

where n is the density of the neutron beam, $\vec{v}_{rel}$ the velocity of the neutrons relative to the scatterer (absorber), σ the total microscopic cross-section calculated in the relative system and N the number of nuclei per cm^3.

Usually, the velocity of the scatterer (absorber) is not constant but distributed according to a certain probability law. If one assumes that the probability density function is $f(\vec{v}_2)$ ($\vec{v}_2$ is the velocity of the scatterer (absorber)), then the probability of finding the scatterer with a velocity between $\vec{v}_2$ and $\vec{v}_2 + d\vec{v}_2$ is $f(\vec{v}_2)d\vec{v}_2$. One gets for the reaction rate

$$R\, f(\vec{v}_2)\, d\vec{v}_2 = n \cdot v_{rel} \cdot \sigma \cdot N \cdot f(\vec{v}_2)\, d\vec{v}_2 \tag{2}$$

On the average we find the reaction rate ($\bar{R}$)

$$\bar{R} = \frac{\int R\, f(\vec{v}_2)\, d\vec{v}_2}{\int f(\vec{v}_2)\, d\vec{v}_2} \tag{3}$$

Now, in an experiment one cannot measure the velocity relative to the scatterer (absorber). Therefore, we must define an experimental cross-section. This is defined by the equation

$$R = n v_1 \sigma_{exp} \cdot N \tag{4}$$

where $\vec{v}_1$ is the neutron velocity. From (1) and (4) one gets

$$\sigma_{exp} = \frac{v_{rel}}{v_1} \sigma \tag{5}$$

The average experimental cross-section ($\bar{\sigma}_{exp}$) will be given by

$$N \bar{\sigma}_{exp} = \frac{\bar{R}}{n \cdot v_1} = \frac{N \int \frac{v_{rel}}{v_1} \sigma f(\vec{v}_2) \, d\vec{v}_2}{\int f(\vec{v}_2) \, d\vec{v}_2} \tag{6}$$

If σ depends on v_{rel} as $\frac{1}{v_{rel}}$ $\bar{\sigma}_{exp}$ will be independent of the velocity distribution of the scatterer (absorber).

$$\bar{\sigma}_{exp} = \frac{\sigma_o v_o}{v_1} \tag{7}$$

where $\vec{v}_o$ is a reference velocity and σ_o the cross section at this velocity.

It is assumed in this report that the microscopic scattering cross sections are constant. Assuming that the scattering particles are in a Maxwell-Boltzmann distribution one gets

$$N \bar{\sigma}_{exp,s} = N \sigma_s \left[\frac{e^{-\frac{m_2}{2kT} v_1^2}}{v_1 \sqrt{\pi \frac{m_2}{2kT}}} + \left(1 + \frac{1}{\frac{m_2}{kT} v_1^2} \right) \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\frac{m_2}{2kT}} v_1} e^{-y^2} dy \right] \tag{8}$$

(See f. ex. Kennard: Kinetic Theory of Gases).

k is the Boltzmann constant, m_2 the mass of the scattering nucleus and T the moderator temperature on the Kelvin scale. In fig. 2 the cross-section for heavy water calculated in this way is compared with the

experimental cross-section. As constant microscopic cross-sections for deuterium and oxygen the cross-sections for the free nuclei are used.

In the Monte Carlo calculations the velocity of the i:th scatterer as seen by the neutron must be chosen from the reaction probability (P_i) defined in analogy with the reaction rate.

$$P_i = \frac{N_i \sigma_i v_{rel,i} f_i(\vec{v_i})\, d\vec{v_i}}{\sum_i \int N_i \sigma_i v_{rel\,i} f(\vec{v_i})\, d\vec{v_i}} =$$

$$= \frac{N_i \sigma_i v_{rel,i} f_i(\vec{v_i})\, d\vec{v_i}}{\sum_i N_i \bar{\sigma}_{exp,i} v_1} \qquad (9)$$

4. Choice of reaction, angle of approach neutron-scatterer and speed of the scattering nucleus.

The choice of event for a neutron with the speed v_1 is made from the probability $p_i = \frac{\Sigma_i}{\Sigma_T}$ ($\sum_i p_i = 1$), where Σ_i is the macroscopic cross-section and Σ_T the total macroscopic cross-section. Capture has been recorded by weighting. Thus the neutron is given a weight w_i which before every event is multiplied by $1 - \frac{\Sigma_c}{\Sigma_T}$.

$$w_{i+1} = w_i \left(1 - \frac{\Sigma_c}{\Sigma_T} \right) \qquad (10)$$

(It is assumed that there is no absorption in the heavy water).

The angle of approach (α) (see fig. 4) is chosen at random by $\mu = \cos \alpha = 1 - 2\,\xi$, where ξ is a random number in the interval (0, 1). Since any azimuthal angle is equally likely the angle δ in fig. 4 is chosen at random by $\delta = 2\,\pi\,\xi$.

The speed of the scatterer has been chosen by a method due to H. Kahn (1954) (see p. 10-15, "The Rejection Technique"). Coveyou et al. (1955) have employed the same method in calculating the energy spectrum of the neutrons in a homogeneous medium. The reaction rate for neutrons of speed v_1 is written in the form

$$R = \left[4 \pi N_2 \left(\frac{\alpha_2}{\pi}\right)^{3/2} \sigma_2 \cdot v_1 v_2^2 e^{-\alpha_2 v_2^2} dv_2 \frac{d\mu}{2} + \right.$$

$$\left. + 4 \pi N_2 \left(\frac{\alpha_2}{\pi}\right)^{3/2} \sigma_2 v_2^3 e^{-\alpha_2 v_2^2} dv_2 \frac{d\mu}{2} \right] \frac{\left|\vec{v}_1 - \vec{v}_2\right|}{v_1 + v_2} \qquad (11)$$

where $\alpha_2 = \frac{m_2}{2kT}$. It is assumed that the thermal speed distributions are Maxwell-Boltzmann in character. One of the distributions in brackets is chosen by the following test

$$\xi \lessgtr \frac{N_2 \sigma_2 v_1}{N_2 \sigma_2 v_1 + \frac{2 N_2 \sigma_2}{\sqrt{\frac{\pi m_2}{kT}}}} = p_1 \qquad (12)$$

where ξ is a random number in the interval (0, 1). If $p_1 > \xi$ the first distribution is chosen and if $p_1 < \xi$ the second. Finally, one chooses a random number ξ (0, 1) and checks whether

$$\xi \gtrless \frac{\left|\vec{v}_1 - \vec{v}_2\right|}{v_1 + v_2} \; ; \quad \text{if} \quad \frac{\left|\vec{v}_1 - \vec{v}_2\right|}{v_1 + v_2} < \xi$$

the scattering parameters are to be rejected, if not, they are accepted. If one has an absorption as in the uranium one can in principle use the same method.

Calculation of the neutron velocity after collision.

See fig. 3. Suppose that the neutron has the velocity $\vec{v}_1$ before collision and that it collides with a moderator atom with velocity $\vec{v}_2$. With data from the last section it is now possible to calculate the velocity of the center-of-mass:

$$(m_2 + 1)\,\vec{v}_c = m_2\,\vec{v}_2 + \vec{v}_1 = m_2\,\vec{v}_2' + \vec{v}_1' \tag{13}$$

where the masses are expressed in atomic mass units and primed quantities represent post-collisions variables. The velocities of the neutron and the scatterer in the center-of-mass system ($\vec{v}_{1c}$ and $\vec{v}_{2c}$ respectively) are given by:

$$\vec{v}_{1c} = -\frac{m_2}{1 + m_2}\,\vec{v}_r \tag{14}$$

$$\vec{v}_{2c} = \frac{1}{1 + m_2}\,\vec{v}_r \tag{15}$$

where

$$\vec{v}_r = \vec{v}_2 - \vec{v}_1$$

In order to determine the velocity of the neutron after the collision one must know the scattering law. It is supposed that the scattering is isotropic in the center of mass system. As the scattering is elastic, one gets $v_{1c} = v_{1c}'$. $\vec{v}_{1c}'$ is then determined if one chooses $\cos\beta$ and φ (see fig. 4) uniformly in the intervals $(-1, 1)$ and $(0, 2\pi)$ respectively. From equation (13) one gets

$$v_c = \frac{1}{1+m_2}\,(v_1^2 + m_2^2\,v_2^2 + 2m_2\,v_1\,v_2\cos\alpha)^{1/2} \tag{16}$$

With $v_{1c} = \frac{m_2}{1+m_2}\,v_r$ from (14) and

$$v_r^2 = v_1^2 + v_2^2 - 2\,v_1\,v_2\cos\alpha \tag{17}$$

one gets

$$v_1' = (v_c^2 + v_{1c}^2 + 2v_{1c}\,v_c\cos\beta)^{1/2} \tag{18}$$

6. Calculation of the direction of the neutron in the reference frame.

See fig. 3 and 4. If one knows the direction of the neutron before the collision (ϑ_i) the direction after the collision can be calculated from the formula

$$\cos \vartheta_{i+1} = \cos \vartheta_i \cos \theta + \sin \vartheta_i \sin \theta \cos (\psi + \delta) \quad (19)$$

One gets θ from

$$\cos \theta = \cos \alpha_1 \cos \alpha_2 + \sin \alpha_1 \sin \alpha_2 \cos \varphi \quad (20)$$

where

$$\cos \alpha_1 = \frac{(v_1')^2 + v_c^2 - v_{1c}^2}{2 v_1' v_c} \quad (21)$$

$$\cos \alpha_2 = \frac{v_1^2 + v_c^2 - v_{1c}^2}{2 v_1 v_c} \quad (22)$$

and ψ from

$$\cos \alpha_1 = \cos \alpha_2 \cos \theta + \sin \alpha_2 \sin \theta \cos \psi \quad (23)$$

δ and φ are chosen at random at the interval $(0, 2\pi)$.

7. Calculation of coordinates in the laboratory system. Sampling of distance travelled by the neutron.

The slab geometry in which the calculations have been worked out is given in fig. 5. As the geometry is symmetric all the lattice cells are equivalent. Therefore, it is convenient to work out the calculations in one lattice cell only.

Suppose that the coordinate of the neutron is z_i in range (1) or (2) in fig. 5. If $\cos \vartheta_i$ is negative one has

$$z_i^{(1)} = a_1 - z_i \qquad \text{(Range 1)} \quad (24)$$

$$z_i^{(2)} = a_1 + a_2 - z_i \qquad \text{(Range 2)} \quad (25)$$

Now one can use $|\cos \vartheta_i|$ in the calculations. The random distance (d_i) which a neutron may travel is chosen from the distribution

$$\xi = \int_0^{d_i} \Sigma_T \, e^{-\Sigma_T x} \, dx \tag{26}$$

where Σ_T is the total cross-section, or

$$e^{-\Sigma_T d_i} = 1 - \xi = \xi_1 \tag{27}$$

where ξ_1 is a random number (0. 1). As Σ_T is different for different ranges a technique suggested by A. J. Mayne (1955) is employed. According to this one tests if a new material is reached, and if so the sampling is repeated.

Consequently d_i is chosen according to (26) and one compares

$$d_i \gtrless \frac{a_1 - z_i}{\cos \vartheta_i} \quad \text{and} \quad d_i \gtrless \frac{a_2 - z_i}{\cos \vartheta_i} \tag{28}$$

respectively.

If less (<) the new coordinate is calculated

$$z_{i+1} = z_i + d_i \cos \vartheta_i \tag{29}$$

If greater (>) a new sampling is performed and after which it is tested whether

$$d_i \lessgtr \frac{a_1}{\cos \vartheta_i} \quad ; \qquad d_i \lessgtr \frac{a_2 - a_1}{\cos \vartheta_i} \tag{30}$$

respectively.

If less (<)

$$z_{i+1} = d_i \cos \vartheta_i \quad ; \qquad z_{i+1} = a_1 + d_i \cos \vartheta_i \tag{31}$$

is calculated. If greater (>) the sampling is proceeded with in the next range.

8. An example of the use of the Monte Carlo code.

The Monte Carlo programme has been divided into two parts, one calculating the neutron velocities and coordinates and the other doing statistics on these data. Subsequently, it is possible to vary the statistical part. As a first example of the use of the Monte Carlo code the average neutron spectrum has been calculated in different zones in the slab geometry (see fig. 5).

The neutrons have been started at an energy of 100 eV uniformly over the lattice cell. (A separate investigation into the validity of this method of proceeding is planned). The neutron density (n) and the flux (ϕ) are calculated from the definition of the collision density ρ

$$\rho = \Sigma_T (\vec{r}, v)\ \phi\ (\vec{r}, \vec{v}) \tag{32}$$

with the normalising condition

$$\int \rho\, d\vec{v}\, d\vec{r} = 1$$

The result of the calculations is given in fig. 6-10. The calculated values are marked out with a cross. The curves in fig. 6-9 are least square fits of the following form of the spectrum:

$$n(v) = \frac{4n}{\sqrt{\pi}} \left[(1 - c_1 r) \frac{v^2}{v_T^3} e^{-\left(\frac{v}{v_T}\right)^2} + r \frac{v_T}{v^2} \left\{ 1 + \left(\frac{a v_T^2}{v^2} \right)^m \right\}^{-1} \right] \tag{33}$$

where

$$c_1 = \frac{4}{\sqrt{\pi}} \int_0^\infty \frac{v_T}{v^2} \left\{ 1 + \left(\frac{a v_T^2}{v^2} \right)^m \right\}^{-1} dv$$

and v_T is the modal velocity of the Maxwellian distribution of temperature T^oK. r is defined by Westcott (1958). One cannot expect this form of the energy distribution to fit very well if one has heavy absorption, but as one often uses such a spectrum in calculating

effective cross-sections for reactors it may be interesting to see how well it fits. Westcott (1958) has used the values a = 5. 02 and m = 16. The following values were obtained:

	zone			
	1	2	3	2 + 3
r	0,18	0,14	0,10	0,12
a	5,9	3,7	3,2	3,4
v_T	2610	2270	2230	2250
m	4	4	6	5

The values must be regarded as approximate as the square fits was not very sensitive to the parameters.

In the calculations the temperature of the uranium and the heavy water was assumed to be 293°K.

As can be seen from the diagrams the assumed form of the spectrum fits well in the heavy water. In the "uranium" there is a considerable hardening and it is a question whether one can speak of a "neutron temperature" in the sense in which it is defined above. — The code has been checked by calculating the neutron spectrum in a non-absorbing ideal gas. More detailed calculations with the code are in progress.

The Monte Carlo code has been programmed for BESK (Matematikmaskinnämnden, Stockholm, Sweden) by Mr P. E. Persson. Mr Persson also made a programme for the least square fits.

Acknowledgements.

The author wishes to thank Mr P. E. Persson for the programming and operation of the BESK code. He also wishes to thank Dr. K. Loimaranta, Mr B. Pershagen and Mr P. E. Persson for many stimulating discussions.

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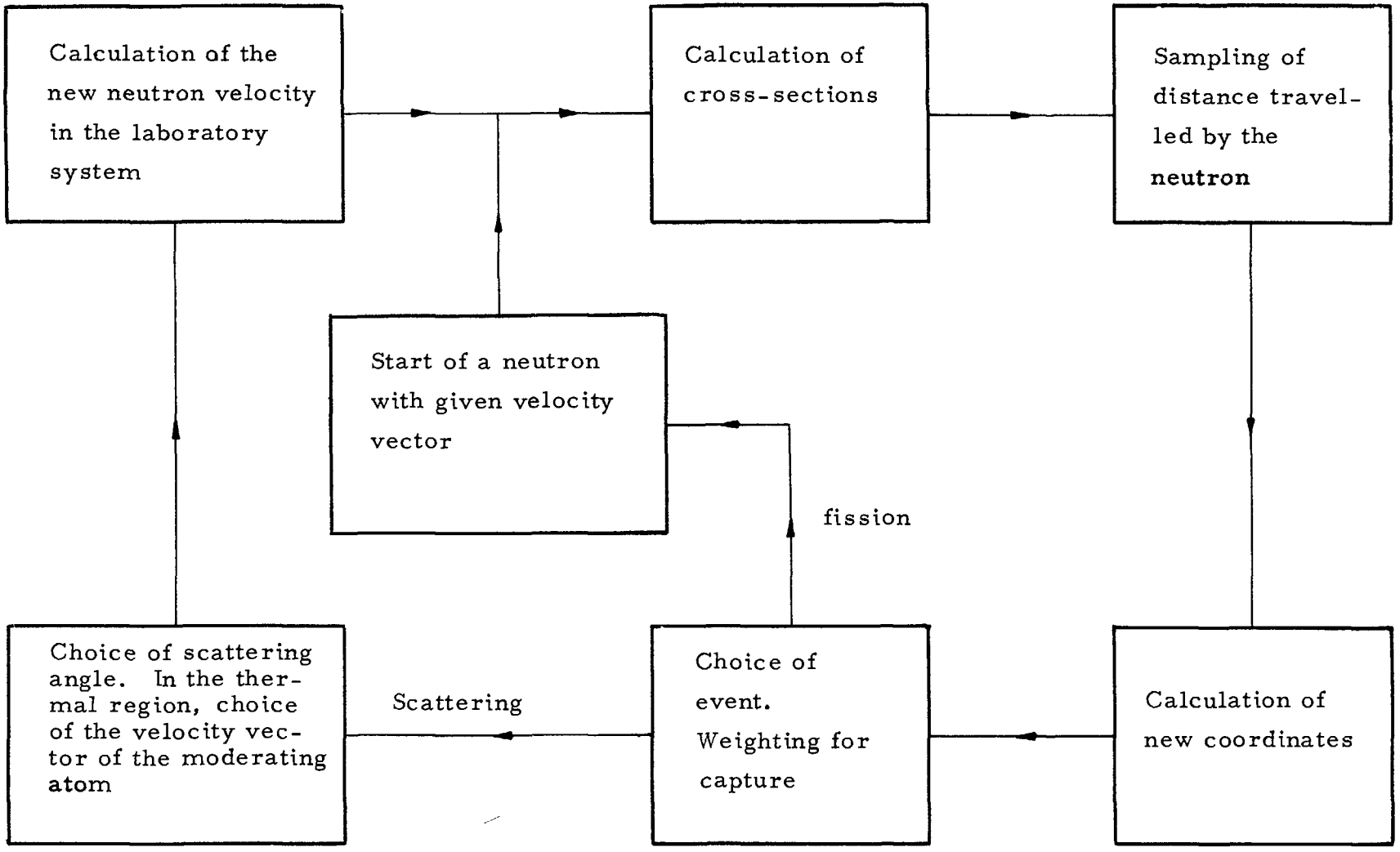


Fig 1. Flow diagram

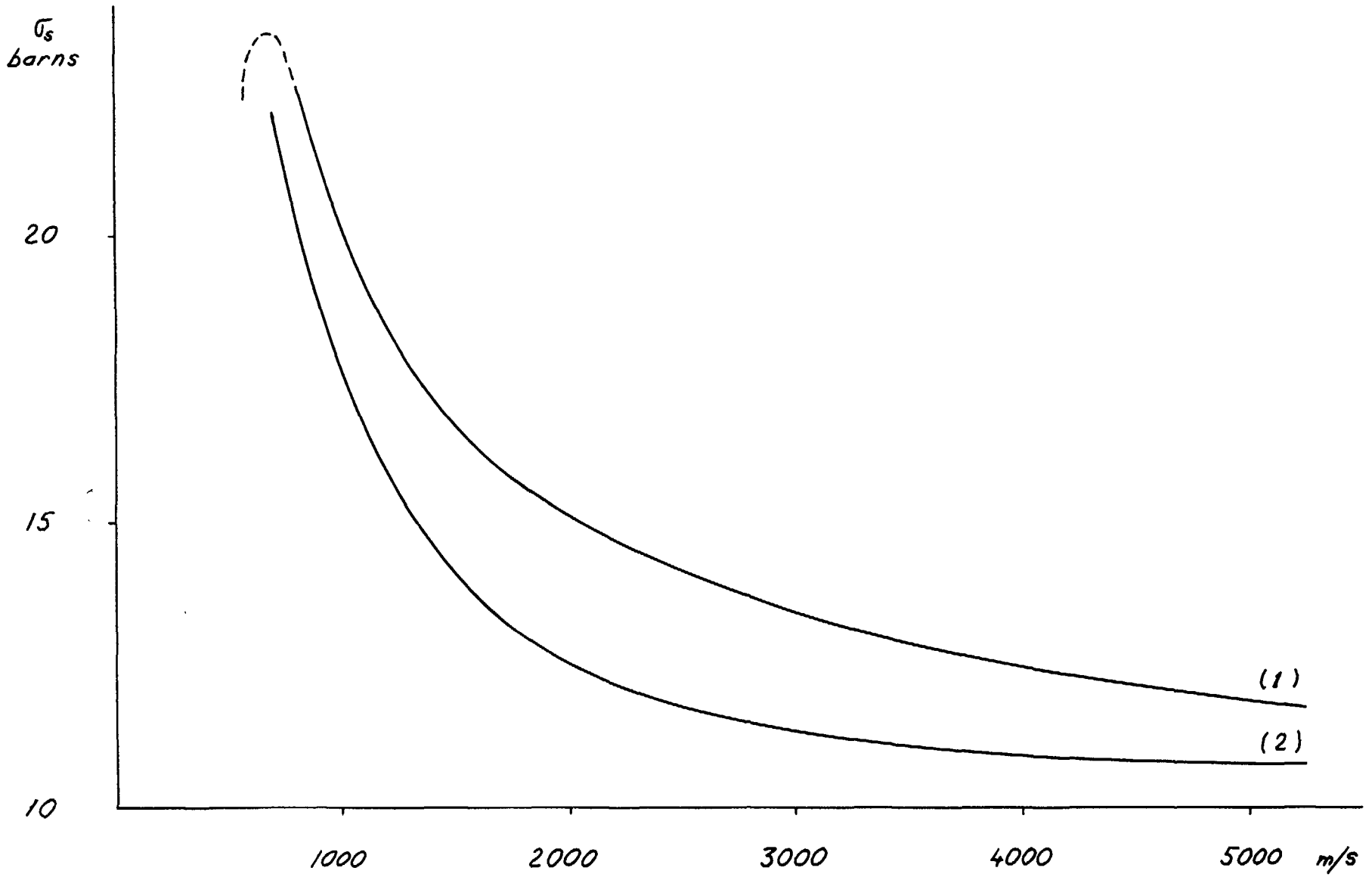
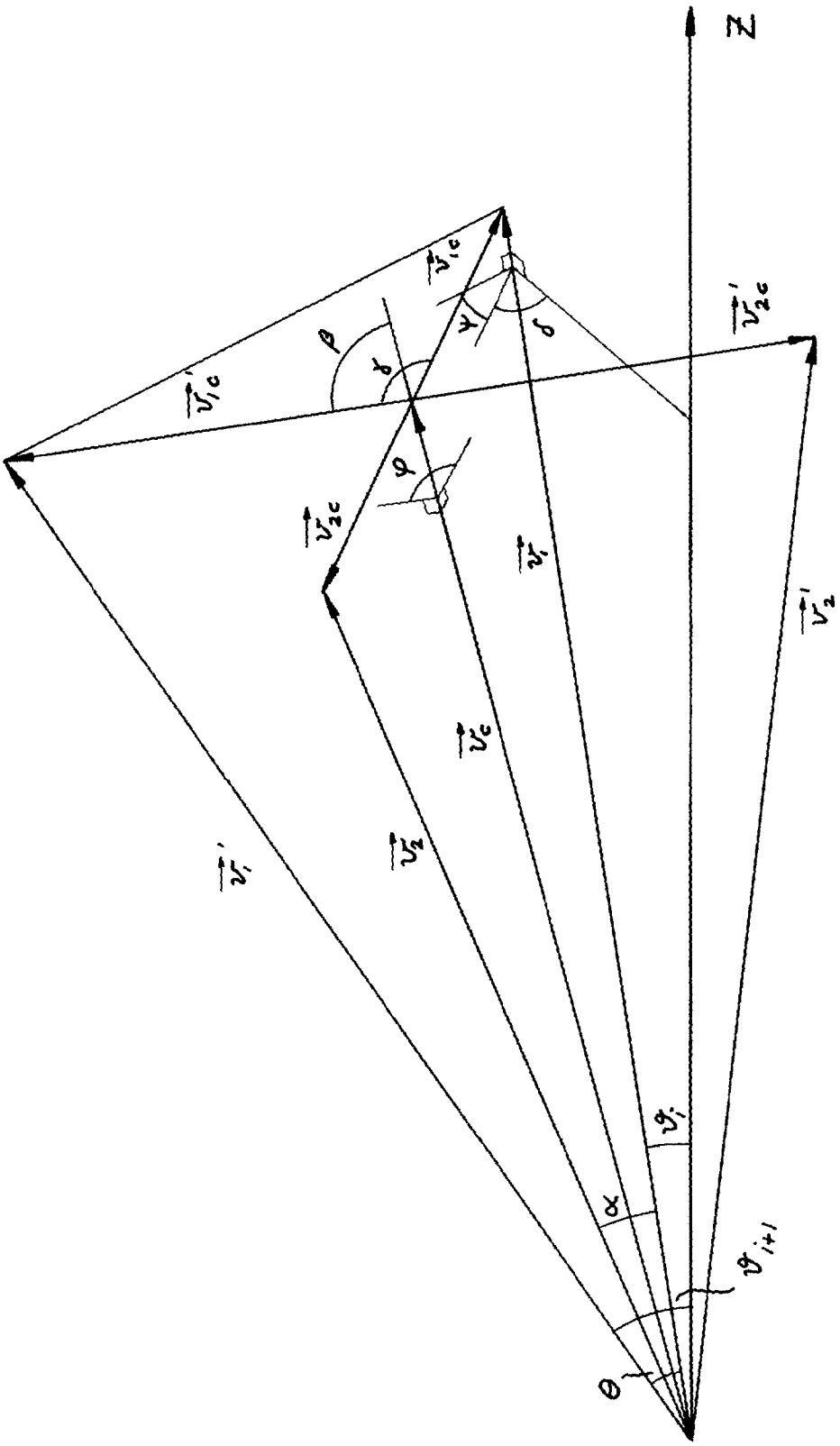
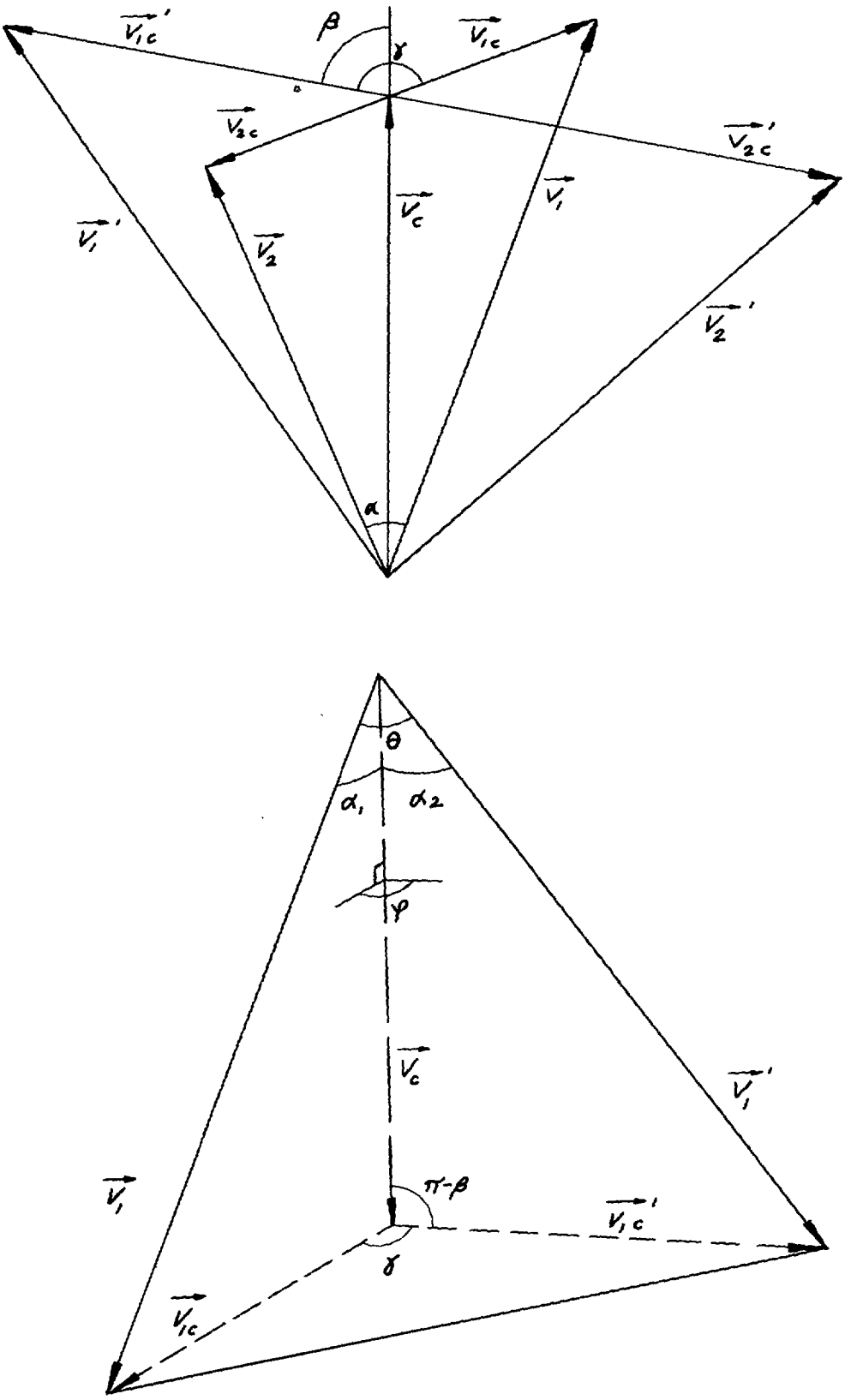


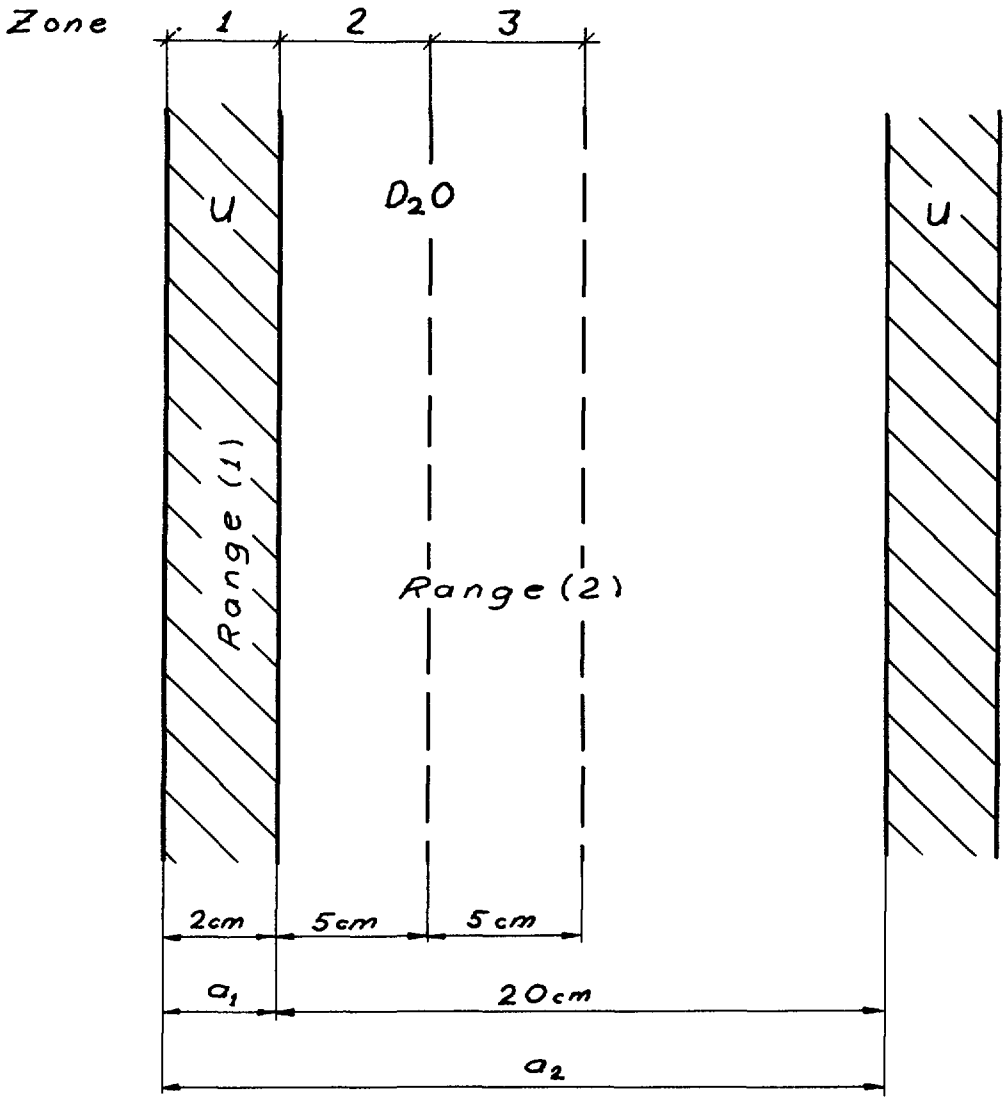
Fig. 2. Comparison between experimental (1) and theoretical (2) scattering cross-sections.



Velocity diagram 2.
Fig. 3.4

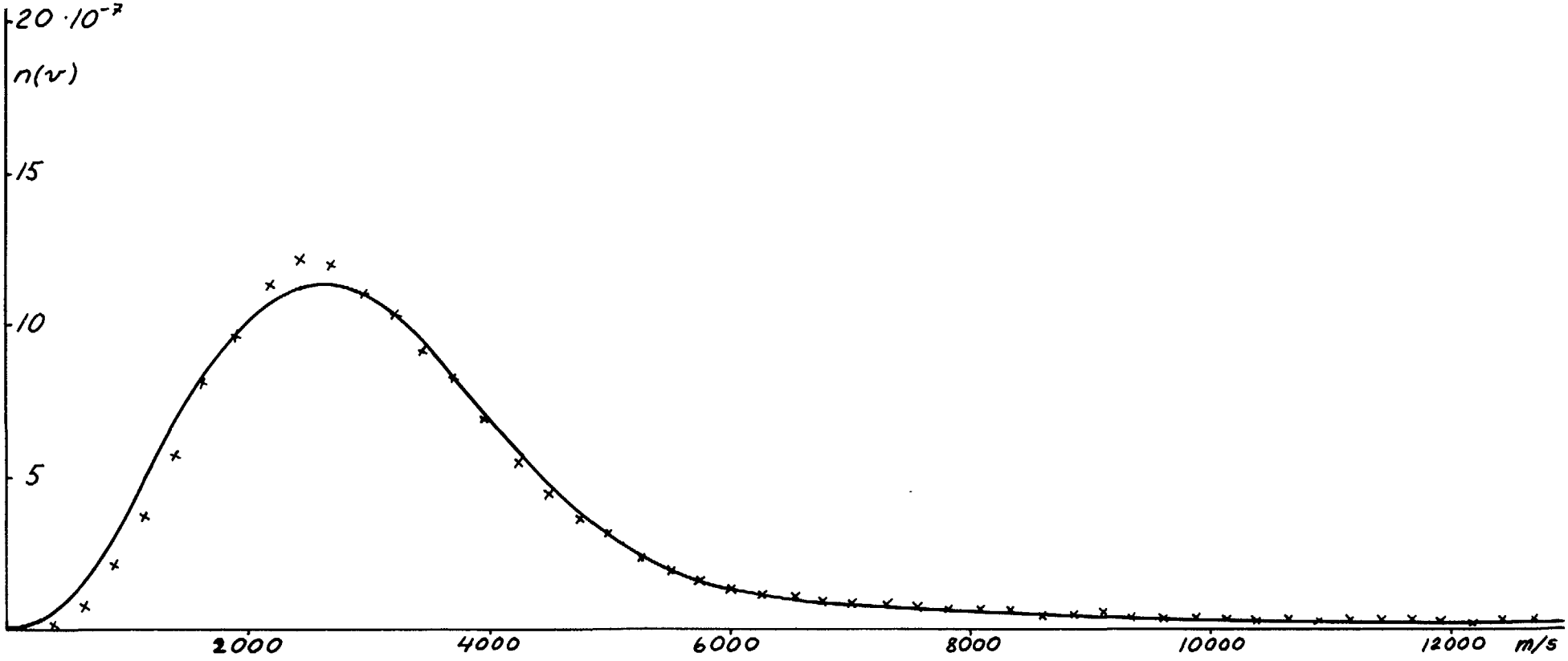


Velocity diagram 1.
Fig. 4.3



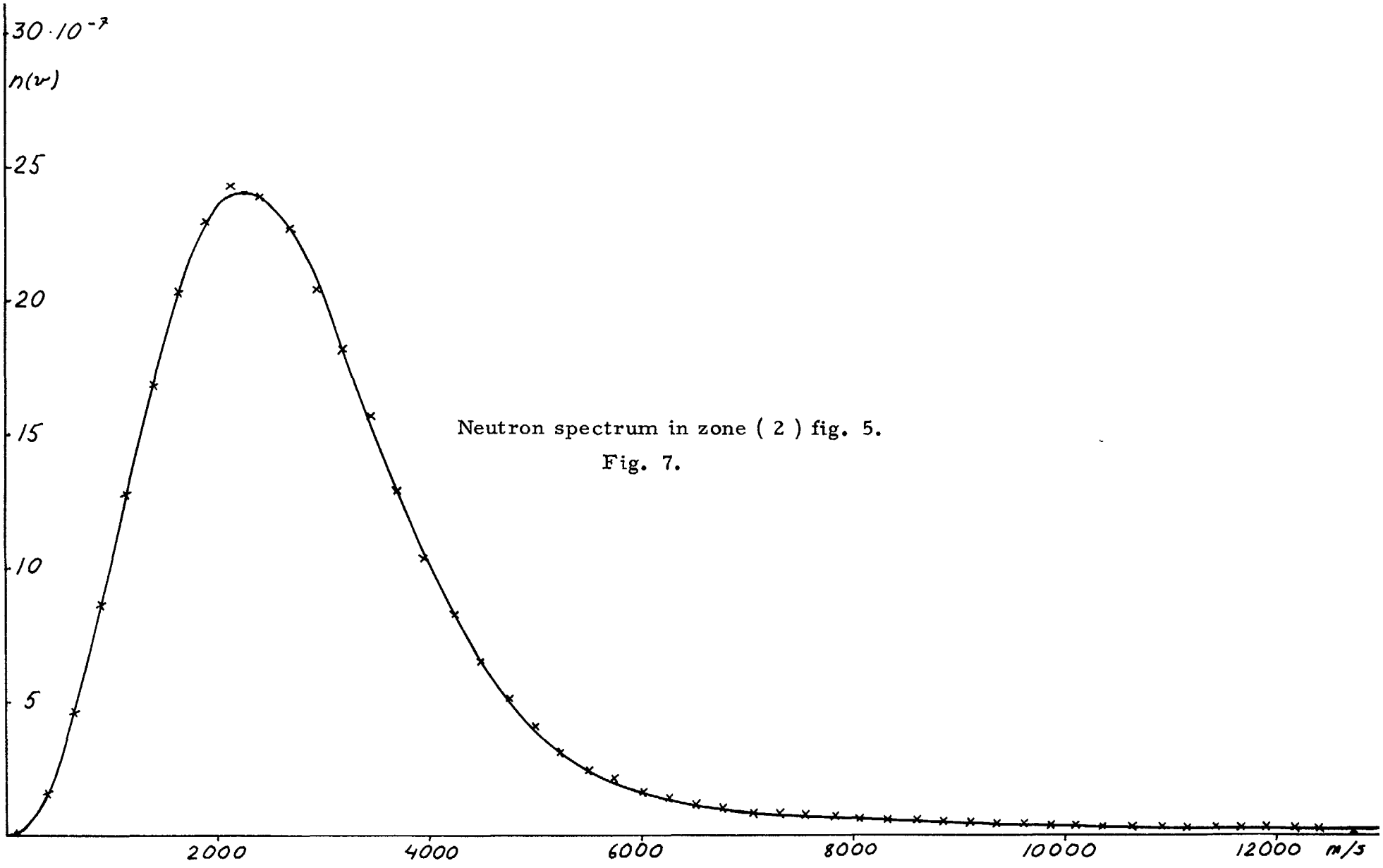
Schematic figure of the slab geometry.

Fig. 5.



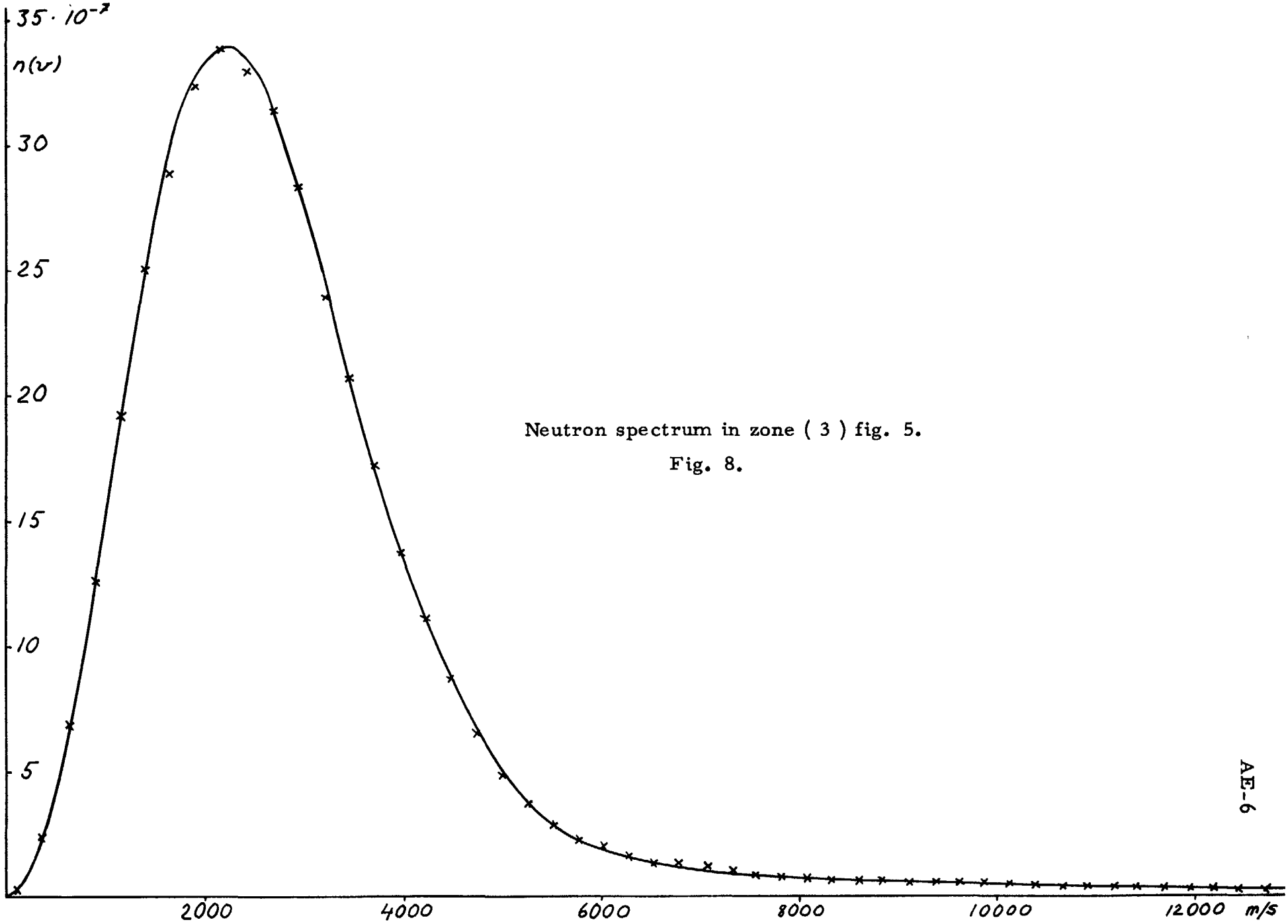
Neutron spectrum in zone (1) fig. 5.

Fig. 6.



Neutron spectrum in zone (2) fig. 5.

Fig. 7.



Neutron spectrum in zone (3) fig. 5.

Fig. 8.

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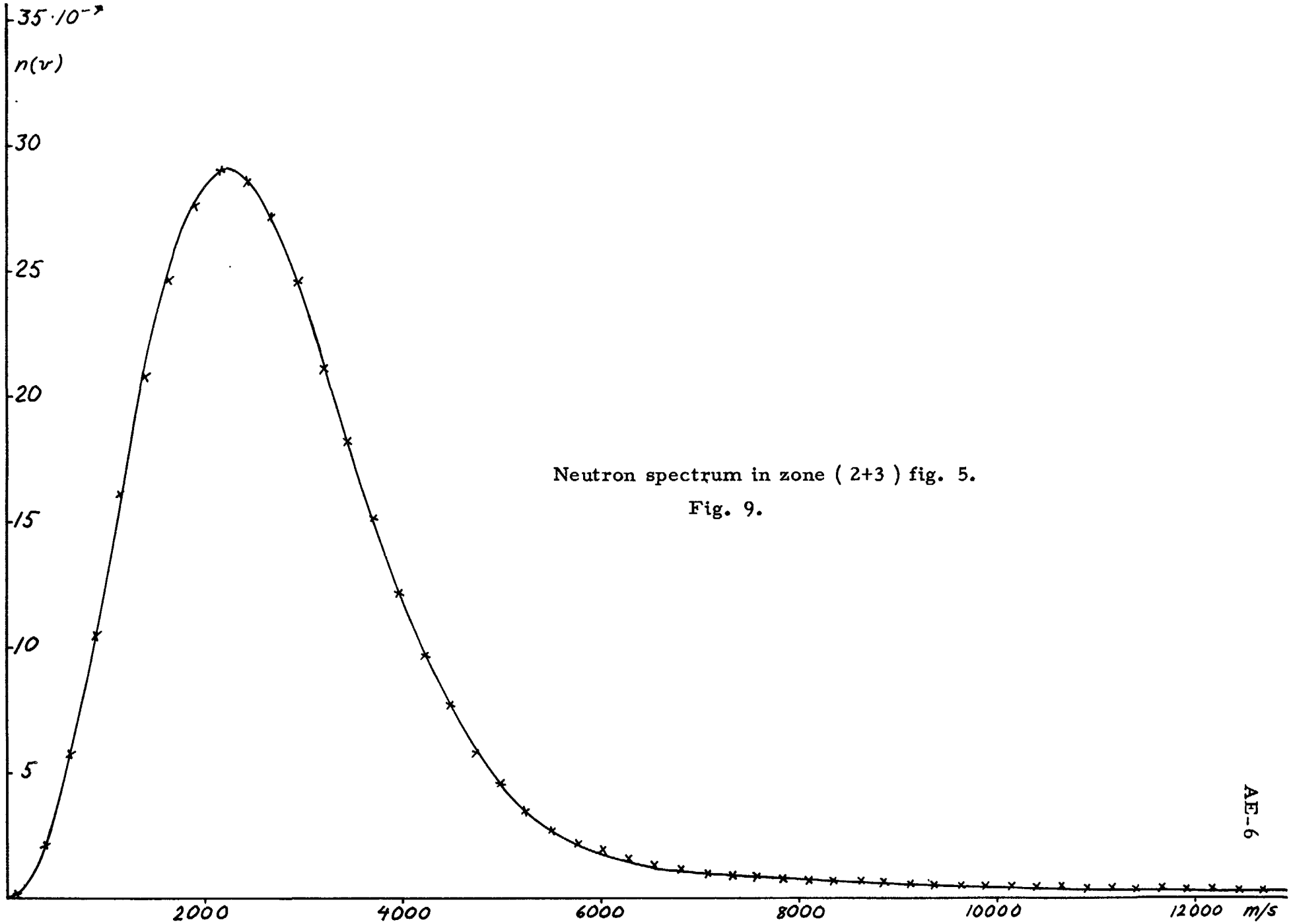
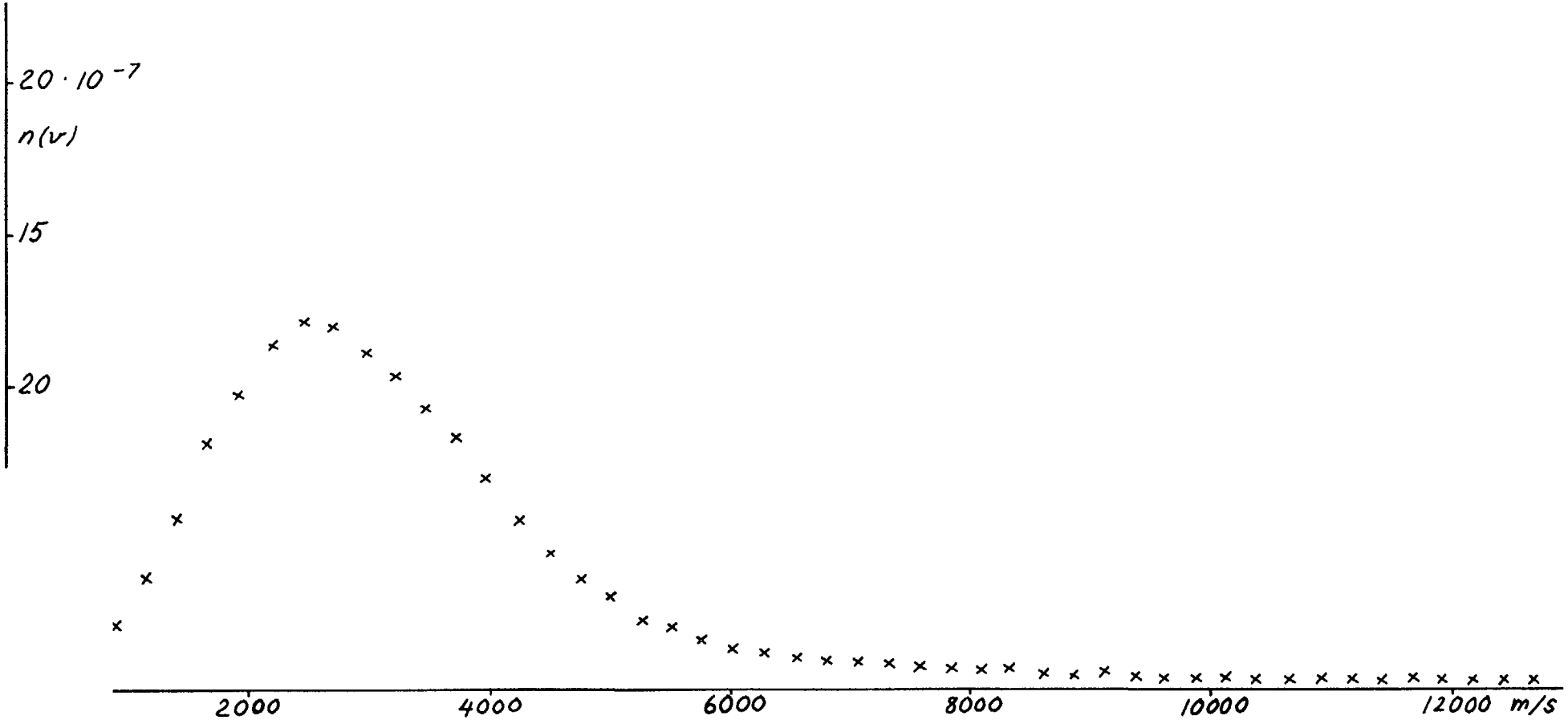


Neutron spectrum in zone (2+3) fig. 5.

Fig. 9.



Neutron spectrum in zone (1) fig. 5 without the fitted curve.

Fig. 10.

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