EFFECT OF TEMPERATURE GRADIENTS ON THE DIFFUSION OF THERMAL NEUTRONS

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SUMMARY

The efect of thermal gradients on the diffusion of thermal neutrons in solid media has been obtained, assuming i) classical scattering of neutrons by nuclei ii) particular distribution function for the velocity of nuclei. A correction, linear in grad T, is obtained. Quantum effects have not been taken into account. Thus the better the agreement of the used scattering law with the actual one, the better the obtained results will hold.

1. INTRODUCTION

The aim of this paper is the theoretical derivation of the offects of temperature gradients on the diffusion of thermal neutrons in non-absorbing scattering media.

As a first approximation the Lorentz theory of electrons in metals can be used (1). In order to solve the problem, it is necessary to assume zero electric charge, and resort to maxwellian statistics instead of Fermi's, due to the usually low density of neutrons. Under these conditions one obtains:

$$J = -(v_l/3)\,[\mathrm{grad}\, n_2 + \frac{1}{2}\,(n_2/T)\;\mathrm{grad}\, T]$$

where

$v = \sqrt{8\,k\,T/\pi\, m_2}$ is the maxwellian average for the absolute value of neutrons velocity, and

$l = 1/n_1\,\pi\, s^2$ the mean free path of neutrons in the scattering media.

In the following we shall use subscripts 1 and 2 for nuclei and neutrons respectively, m_1 and m_2 being their masses, n_1 and n_2 their number densities, and s the diameter of the nuclei.

By introducing the scalar flux of neutrons:

$$\phi = n_2 \bar{v}$$

the vector flux

$$J = -(l/3)\ \text{grad}\,\phi$$

is obtaiend.

This equation is identical with the common diffusion law, usually derived from the elementary diffusion theory (2).

However, the fundamental formulae that have been used in this application imply assumptions that do not hold in the case of neutrons in solids, namely: there is no energy exchange between nuclei and neutrons, and the nuclei are at rest.

From a classical point of view, these assumptions are not valid in the case of neutrons since the mass cannot be neglected when compared with those of nuclei.

In order to introduce the velocity of nuclei it should be necessary to resort to the velocity distribution function f_1. The difficulty arises from the fact that f_1 cannot be determined from a transport equation, as would be the case in a gaseous binary mixture. This difficulty can be obviated by assuming a convenient model for the solid in the absence of neutrons; such a distribution function f_1 is assumed not to be appreciably influenced by neutrons, as long as their number density is sufficiently low, this requirement —$n_2 \ll n_1$— being fulfilled n the usual cases.

One may then obtain an integro-differential equation involving the corresponding function f_2 for neutrons, which is equivalent to the Boltzmann transport equation for one component of a gaseous binary mixture. It should be noted that collisions between neutrons are negligible, because $n_2 \ll n_1$.

If f_2 expanded as a series of functions, and the fore-mentioned integro-differential equation is adequately separated in a sequence of integral equations, the solutions of these equations are the functions of the series in which f_2 was expanded.

Just as in the case of Enskog method, a special solution of the transport equation, valid only for nearly thermal neutrons, is obtained in this way. The only necesary values for the determination of f_2 are: n_2 and the temperature distribution throughout the scattering medium.

On the basis of the first two functions of the f_2 series, the diffusion law corrected for the temperature effect has been obtained.

J_+ and J_- have been defined in the usual neutrons diffusion theory way (2), their expressions having been calculated on the basis of the said approximation. With them, boundary conditions for two cases, namely: the interface between two scattering media and between a scattering medium and a vacuum, have been established.

A few examples with and without absorption have also been calculated.

2. DISTRIBUTION FUNCTION FOR NUCLEI

It has already been seen that, on the basis of a conveniently modified Lorentz theory of electrons in metals, the usual law of diffusion is obtained. This is mainly due to the type of f_2 expansion used for solving the problem of electrons in metals.

This treatment fits well in the latter case since the ion-electron energy exchange in negligible, the electron mass being small wiht respect to the ionic one. This assumption, however, does not hold for neutrons and light nuclei; thus it is necessary to take into account the velocities of nuclei.

It should now be necessary to introduce f_1, but it has already been pointed in § 1 that there is no transport equation for nuclei. Consequently it is necessary to obtain it previously to the resolution of the transport equation; in order to that it shall be assumed the following model for nuclei in a solid: they behave like classical harmonic and isotropic oscillators, with a unique frequency, that can be obtained, e.g. from Einstein theory of specific heats. In so far as this frequency does not appear in f_1, its actual value does not affect the obtained distribution function, but, the ratio of frequency to temperature determines the validity of this classical derivation, when the diffaction effect of the lattice is disregarded.

A macroscopically small volume dr is considered. The number of oscillators within this volume is: $n_1\, dr$. If maxwellian statistics is used, the number of oscillators in dr which have their phase space representative points in a cell of energy E, are given by: $(n_1\, dr) \exp(-\beta E)/Z$ where Z is the partition function for an oscillator of frequency ν:

$$Z = (kT/h\nu)^3 \text{ and } \beta = 1/kT.$$

The classical expression for E is $E = (p_1^2/2m_1) + \frac{1}{2}K^2 q_1^2$ where

$p_1 = (p_{1x}, p_{1y}, p_{1z})$ is the momentum,

$q_1 = (q_{1x}, q_{1y}, q_{1z})$ is the coordinate, and

$K^2 = 4\pi^2 m_l \nu^2$ the oscillator force constant.

The distribution function $f_1(r, c_1, t)$ is then obtained by adding up $(n_1\,dr)$ exp—$(\beta E)/Z$ over all the phase space cells for an oscillator whose velocities lie between $c_1 = p_1/m_1$ and $c_1 + dc_1 = (p_1 + dp_1)/m_1$.

A good approach to the summation is obtained by integrating

$$\int_v (n_1\,dr)\,[\exp(-\beta E)/Zh^3]\,dp_1\,dq_1 =$$

$$= \int_v [(n_1\,dr)/(kT/h\nu)^3]\,h^3 \exp\left[-\beta\left(\frac{1}{2}\,p_1^2/m_1 + \frac{1}{2}\,k^2 q_1^2\right)\right] dp_1\,dq_1$$

over the volume $v = dr$. The result is then:

$$f_1(r, c_1, t) = \tag{2.2}$$

$$= (n_1 m_1^3/h^3)\,(h\nu/kT)^3 \exp(-m_1 c_1^2/2kT) \int_v \exp(-K^2 q_1^2/2kT)\,dq_1$$

It should be noted that the integration must be extended over a volume, although macroscopically small, sufficiently great as to assure the condition $K^2q_1^2/2kT \gg$ *all* over the volume surface. This condition is obviously satisfied if the volume contains a sufficiently high number of nuclei, and in this case the integration can be extended to infinity without introducing any appreciable error. The expression for f_1 comes to be

$$f_1(r, c_1, t) = n_1\,(m_1/2\pi kT)^{3/2} \exp(-m_1 c_1^2/2kT) \tag{2.3}$$

It is easily seen that it appears to be the same as that for a perfect monoatomic gas.

Had we considered quantum oscillators, the distribution function would be the same as 2.3 if the medium temperature were high enough so that the oscillators stayed in high quantum number states. The fulfillment of the last condition would justify the classical treatment of the neutrons-nuclei collisions if the difraction with the lattice were not taken into account.

The scattering law obtained from the assumption done, that neutrons make independent collisions with each one of nuclei, must then be replaced by the sum of the Bragg scattering plus the incoherent scattering.

Bragg scattering is higly anisotropic, but for a nearly isotropic distribution of neutron velocities, the number of neutrons scattered from a given volume of a polycristalline medium is independent of the direction in a first approximation and proportional to the scalar neutrons flux. This follows from the fact that the number of neutrons of a given speed scattered by each of the Bragg reflections in a given direction is proportional to the number of incoming neutrons with velocities making the corresponding Bragg angle with the outgoing velocity. This number being in a first approsach independent of the direction of the scattered neutrons, due to the assumed isotropy of the neutron velocity distribution, the integration over all the speeds and Bragg angles is again direction-independent. The isotropic scattering proportional to the neutrons scalar flux leads to the usual diffusion law.

The corrections due to thermal gradients must be obtained from the temperature dependence of the scattering law, arising from the neutrons-phonon scattering, included in the incoherent scattering. Therefore, the classical model assumed for the scattering of neutrons must be taken only as a particular scattering law.

The results obtained will hold if the assumed scattering law is a good approximation to the actual one.

3. THE EQUATION

The neutrons transport equation is formally the same as that for one component of a binary mixture of gases, the nuclei playing the role of the other component (3).

In the following the notation of Chapman and Cowling shall be used.

The fact that $n_2 \ll n$, makes it possible to 1) neglect neutron-

neutron collisions, and 2) assume that f_1 will not be modified by the presence of neutrons. In such a case:

$$\frac{\partial f_2}{\partial t} + c_2 . \frac{\partial f_2}{\partial r} + F . \frac{\partial f_2}{\partial c_2} = \iint [f_1' f_2' - f_1 f_2] g_{21} \, b \, db \, d\epsilon \, dc_1 \qquad 3.1$$

It is sometimes advisable to make the following variable transformation (see (3) 3.45 and 3.5).

$$g_{21} \, b \, db \, d\epsilon = k_{21} \, dk$$

It is necessary to introduce the integral operators $L(f_2)$ and $I_{21}(\phi_2)$ defined by

$$L(f_2) = \iint (f_1' f_2' - f_1 f_2) \, g_{21} \, b \, db \, d\epsilon \, dc_1 = \iint (f_1' f_2' - f_1 f_2) \, k_{21} \, dk \, dc_1 \qquad 3.3$$

$$I_{21}(\phi_2) = - L(f_2{}^0 \phi_2)/n_1 n_2 \qquad 3.4$$

where

$$f_2{}^0 = n_2 (m_2/2\pi kT) \exp(- m_2 c_2{}^2/2kT) \qquad 3.5$$

4. STUDY OF THE HOMOGENEOUS INTEGRAL EQUATION AND ITS KERNEL

The solution of the integral equation:

$$I_{21}(\phi_2) = 0 \qquad 4.1$$

is $\Phi_2 =$ constant, It is obtained by methods only slightly different from those used in (3) Chapter IV (4).

The non-homogeneous integral equation, associated with 4.1 can be written

$$I_{21}(\phi_2) = f(c_2) \qquad 4.2$$

In order to resort to well-known theorems dealing with integral equation, it is advisable to write 4.2 as a Fredholm equation. Following Chapman and Cowling (3) the equivalence

$$I_{21}(\phi_2) = K_0(c_2) \, \phi_2(c_2) - \int K(c_2, c) \, \phi_2(c) \, dc \qquad 4.3$$

can be shown, where

$$K_0(c) = \exp(-m_2 c^2/2kT) . (-4\pi s^2 A/b^2) .$$
$$. \{(1 + bc^2) [\tfrac{1}{2}\sqrt{\pi}\, Erf(\sqrt{b/2}\, c)/\sqrt{b/2\, c}] - \exp(-m_1 c^2/2kT)\} \qquad 4.4$$

being $A = -(m_1 m_2)^{3/2}/(2kT)^3$; $b = m_1/kT$ and $K(c_2, c)$ a symetrical kermel.

Equation 4.2 has a solution if, and only if

$$\int f(c_2)\, \psi_i(c_2)\, dc_2 = 0 \qquad 4.5$$

where the $\Psi_i(c_2)$ are the linearly independent solutions of 4.1. Since the unique solution of 4.1 is $\Phi_2 = \alpha(r, t)$, the condition for 4.2 to be solved is

$$\int f(c_2)\, dc_2 = 0 \qquad 4.6$$

It should be remarked that the only solution of 4.1 is $\phi_2 = \alpha$. This is a consequence of two related facts; i) f_1 was obtained independently of the transport equation, and ii) f_2 was the only unknown in the equation. This imposes at the same time, that the only conservation equation that can be directly derived from the transport equation is that for the number of neutrons.

5. METHOD FOR THE SOLUTION OF THE TRANSPORT EQUATION

It is advisable to define D as in

$$D f_2 = \frac{\partial f_2}{\partial t} + \frac{\partial f_2}{\partial r} . c_2 + F . \frac{\partial f_2}{\partial c_2} \qquad 5.1$$

Resorting to 3.3, equation 3.1 can be rewritten as follows:

$$\mathrm{D} f_2 = L(f_2) \qquad 5.2$$

On setting

$$f_2 = \sum_{r=0}^{\infty} f_2^{(r)} \qquad 5.3$$

and introducing 5.3 in 5.2

$$D f_2 = L\left(\sum_{r=0}^{\infty} f_2^{(r)}\right) = \sum_{r=0}^{\infty} L\left(f_2^{(r)}\right) \qquad 5.4$$

is obtained.

The first member of 5.2 can be expanded according to

$$D f_2 = -n_1 n_2 \sum_{r=0}^{\infty} D^{(r)} \qquad 5.5$$

where $D^{(r)}$ are functions obtained operating on f_2 with some differential operators that will be defined in §7. From 5.4, 5.5 and 3.4 it follows:

$$\sum_{r=0}^{\infty} \{I_{21}(\Phi_2^{(r)}) - D^{(r)}\} = 0 \qquad 5.6$$

The new unknowns $\Phi_2^{(r)}$ are defined according to $f_2^{(r)} = f^0_2 \Phi_2^{(r)}$ where f^0_2 has been defined in 3.5. It should be emphasised that f^0_2 can be made identical with $f_2^{(o)}$, provided $D^{(o)}$ is conveniently chosen, as will be shown in §6.

Equation 5.3 is a solution of 5.2 if the equations

$$I_{21}(\Phi_2^{(r)}) = D^{(r)} \qquad 5.7$$

are satisfied for all values of r.

If $D^{(s)}$ is defined in such a way that the only $f_2^{(r)}$ appearing are those for $r = 0, 1, \ldots s-1$, the second member of 5.7 will be known after having solved all equations for $r < s$.

The general solution for 5.7 is

$$\Phi_2^{(r)} = X_2^{(r)} + \Psi_2^{(r)} \qquad 5.8$$

where $X_2^{(r)}$ is a particular solution for 5.7 and $\Psi_2^{(r)}$ is the general solution for 4.1.

The only solution for 4.1, as it has already been seen in §4, is $\alpha\ (r,t)$. The condition 4.6 for solving 5.7 then reads:

$$\int D^{(r)} dc_2 = 0 \qquad 5.9$$

One should demostrate that $D^{(r)}/\sqrt{K_0(c_2)}$ is integrable and of integrable square for each r.

Two problems arise: i) to separate 5.5 conveniently and ii) to determine $\Phi_2^{(r)} = \alpha^{(r)}(r,t)$ for each value of r.

6. FIRST ORDER APROXIMATION

In order to obtain the first approximation, $D^{(o)}$ will be defined by:

$$D^{(0)} = 0 \qquad 6.1$$

or according to 5.7

$$I_{21}(\Phi_2^{(0)}) = 0 \qquad 6.2$$

for which the only solution is $\Phi_2^{(o)} = \alpha$. Consequently the first approximation will be

$$f_2^{(0)} = \alpha^{(0)} f_2^{(0)} \qquad 6.3$$

Setting $\alpha^{(o)} = 1$, the so—obtained first approximation is that of the maxwellian distribution for the each—point temperature of the scattering media, and for a number density of particles equal to the number density of neutrons at each point.

The setting of $\alpha^{(0)}$ makes it posible to obtain the remaining $\alpha^{(r)}$. Then

$$\int f_2 \, dc_2 = \sum_{r=0}^{\infty} \int f_2^{(r)} \, dc_2 = n_2$$

and consequently

$$\sum_{r=1}^{\infty} \int f_2^{(r)} \, dc_2 = 0$$

This equation is satisfied when

$$\int f_2^{(r)} \, dc_2 = \int f_2^{0} X_2^{(r)} \, dc_2 + \alpha^{(r)} n_2 = 0 \qquad 6.4$$

Equation 6.4 will be taken as the condition determining the values of $\alpha^{(r)}$.

7. SEPARATION OF THE TRANSPORT EQUATION

In the case of gaseous mixtures, five differential equations are obtained from the transport equation without resolving it explicitely, namely, the equations that state the conservation of mass, momentum and kinetic energy (3).

From these equations the time derivatives of the density of particles, mean velocity and temperature, are obtained. These equations must then be introduced in Df_2 in order to perform the separation 5.5 (3).

It has been seen n §4 that, according to this, only one continuity equation can be derived: the one which refers to the number of neutrons:

$$\frac{\partial n_2}{\partial t} + \frac{\partial}{\partial r} \cdot n_2 \overline{c_2} = 0 \qquad 7.1$$

The equation for the mean velocity:

$$n_2 \overline{c_2} = \int f_2 c_2 d c_2 \qquad 7.2$$

is just the required one, as the vectorial flux of neutrons can be expressed:

$$J_2 = n_2 \overline{c_2} \qquad 7.3$$

The mean velocity will be obtained from the second approximation since the first one is maxvellian and, being isotropic, does not contribute to $\overline{c_2}$.

As long as the transport equation only determines the neutrons distribution function, it cannot lead to a differential equation for the conservation of kinetic energy, as the involved integrals do not vanish. It should be noted that this limitation does not lead into troubles since, neutrons being approximately thermal, the temperature that appears in $f_2^{(o)}$ is the one of the scattering medium. Therefore, the time derivative of temperature follows from the medium properties.

It is now posible to write the separation 5.5 explicitly. It is posible to write:

$$-n_1 n_2 D^{(r)} = \frac{\partial_0 f^{(r-1)}}{\partial t} + \dots + \frac{\partial_{r-1} f^{(0)}}{\partial t} + c_2 . \frac{\partial f^{(r-1)}}{\partial r} + F . \frac{\partial f^{(r-1)}}{\partial c_2} \qquad 7.4$$

for $r \neq 0$, where

$$\frac{\partial_s f_2^{(r)}}{\partial t} = \frac{\partial f_2^{(r)}}{\partial n_2} \cdot \frac{\partial_s n_2}{\partial t} + \frac{\partial f_2^{(r)}}{\partial T} \cdot \frac{\partial_s T}{\partial t} \qquad 7.5$$

being

$$\frac{\partial_s n_2}{\partial t} = -\frac{\partial}{\partial r} \cdot [n_2 \overline{c_2^{(s)}}] \qquad 7.6$$

$$n_2 \overline{c_2^{(s)}} = \int f_2^{(s)} c_2 dc_2 \qquad 7.7$$

The symbol $\delta_s T / \delta t$ is an arbitrary function in t and r satisfying

$$\sum_{s=0}^{\infty} \frac{\partial_s T}{\partial t} = \frac{\partial T}{\partial t} \qquad 7.8$$

As it is seen in 7.4 the only $f^{(k)}$ that appear in $D^{(r)}$ are those for k between 0 and r-1. Otherwise, it is not difficult to show (4) that 7.4 satisfies 5.5 and 5.9; consequently, the integral equations 5.7 admit a solution for every r. Each one of them could be solved once the solutions for every foregoing equations where known.

It remains still to be shown for every case that $D^{(r)}/\sqrt{K_0(c_2)}$ is integrable and of integrable square.

8. SECOND ORDER APPROXIMATION

From 5.7 the equation

$$I_{21}(\phi_2^{(1)}) = D^{(1)} \qquad 8.1$$

is obtained for $r = 1$.

The external forces acting upon neutrons are in general negligible, and then $F = O$. Also: $\partial_0 T / \partial t = O$ which is equivalent to considering this effect being of higher order with respect to the second order approximation. With this simplification, it follows

$$-n_1 n_2 D^{(1)} = \left\{ (c_2/n_2) . \frac{\partial n_2}{\partial r} + [(m_2 c_2^2/2kT) - 3/2] (c_2/T) . \frac{\partial T}{\partial r} \right\} f_2^0 \qquad 8.2$$

It is necesary to find a particular solution for 8.1, called $X_2^{(1)}$ in § 5; it has already been seen in § 6 that $\acute{a}(^1)$ is entirely determined by 6.4. The expression:

$$X_2^{(1)} = A . \frac{\partial \ln n_2}{\partial r} + \frac{\partial \ln T}{\partial r} . B \qquad 8.3$$

is tried as a particular solution, in which A and B appear to be the new unknowns. Resorting to 8.1 and 8.2 the following equation is obtained

$$\frac{\partial \ln n_2}{\partial r} . I_{21}(A) + \frac{\partial \ln T}{\partial r} . I_{21}(B) =$$

$$= -(f_2^0/n_1 n_2) \left\{ (c_2/n_2) . \frac{\partial n_2}{\partial r} + [(m_2 c_2^2/2kT) - 3/2] (c_2/T) . \frac{\partial T}{\partial r} \right\}$$

8.4

Equation 8.3 is a solution if A and B are themselves solutions for the following integral equations

$$-n_1 n_2 I_{21}(A) = c_2 f_2^0 \qquad 8.5$$

$$-n_1 n_2 I_{21}(B) = [(m_2 c_2^2/2kT) - 3/2] c_2 f_2^0 \qquad 8.6$$

As it has been shown in § 5 these equations can be solved when

$$\int c_2 f_2^0 \, dc_2 = 0 \qquad 8.7$$

and

$$\int [(m_2 c_2^2/2kT) - 3/2] c_2 f_2^0 \, dc_2 = 0 \qquad 8.8$$

respectively. It can be shown, considering the symetry of the integrands that these conditions are satisfied; therefore, 8.5 and 8.6 admit a solution.

A and B only depend on c, $n(r,t)$ and $T(r,t)$; as they are the only variables that appear in 8.5 and 8.6, these variables determine vectors according to: $A = A(c_2) . c_2$ and $B = B(c_2) . c_2$, where $A(c_2)$ and $B(c_2)$ are functions of c_2, $n(r,t)$ and $T(r,t)$.

Although it is not necessary to obtain $A(c_2)$ and $B(c_2)$ explicitly, it will be necessary to calculate some coefficients that depend on these functions.

It can be shown that $a^{(1)} = O$, from which

$$f_2^{(1)} = f_2^{(0)} \left[A(c_2) \, c_2 . \frac{\partial \ln n_2}{\partial r} + B(c_2) \, c_2 . \frac{\partial \ln T}{\partial r} \right] \qquad 8.9$$

9. DIFFUSION LAW

The diffusion law can now be derived from the vector flux of neutrons estimated to a second orden approximation, the flux being

$$J = n_2 \overline{c_2^{(1)}} = \int f_2^{(1)} c_2 \, dc_2 \qquad 9.1$$

As the operator $I_{21}(\Phi_2)$ has been defined according to Chapman and Cowling (3), the functional:

$$[G_2; K_2]_{12} = \int G_2(c_2) \, I_{21}[K_2(c_2)] \, dc_2 \qquad 9.2$$

in the same as that of (3) 4.4.9

It follows (4)

$$J = -(1/3 n_1 n_2) \left\{ [A; A]_{12} \cdot \frac{\partial \ln n_2}{\partial r} + [A; B]_{12} \cdot \frac{\partial \ln T}{\partial r} \right\} \qquad 9.3$$

which is the diffusion law. It should be noted that the term on $\partial \ln T / \partial r$ is the one from which the correction to the usual diffusion law if obtained. Coefficients $[A; A]_{12}$ *and* $[A; B]_{12}$ will be computed following Chapman and Cowling.

10. ESTIMATION OF J_+ and J_-

It is useful to introduce magnitudes similar to those used in the theory of neutron diffusion (2).

If dS is a surface element and n its normal unit vector, J_+ is defined in an equivalent manner. It can be shown (4) that

$$J_+ = (1/4) \, n_2 \overline{c_2^{(0)}} + (1/6) \left\{ -(n_1 n_2) \frac{\partial \ln n_2}{\partial r} \cdot [A; A]_{12} + \frac{\partial \ln T_2}{\partial r} \cdot [A; B]_{12} \right\} \cdot n \qquad 10.1$$

$$J_- = (1/4) \, n_2 c_2^{(0)} - (1/6) \left\{ -(n_1 n_2) \frac{\partial \ln n_2}{\partial r} \cdot [A; A]_{12} + \frac{\partial \ln T}{\partial r} \cdot [A; B]_{12} \right\} \cdot n \qquad 10.2$$

On comparing with 9.3 it follows

$$J_+ = (1/4)\, n_2\, \overline{c_2^{(0)}} + \frac{1}{2} J \,.\, n \qquad 10.3$$

$$J_- = (1/4)\, n_2\, \overline{c_2^{(0)}} - \frac{1}{2} J \,.\, n \qquad 10.4$$

These are the formulae 5.17.1 and 5.17.2 from (2), corrected for the influence of temperature gradients.

11. ESTIMATION OF $[A\,;A]_{12}$ AND $[A\,;B]_{12}$

These coefficients are approximately obtained following Chapman and Cowling (3). On defining (5)

$$a^{(r)} = S_{3/2}{}^{(r)}\,(m_2 c_2^2/2\,kT)\, c_2 \qquad 11.1$$

$$a_{rs} = [a^{(r)}\,;\, a^{(s)}]_{12} \qquad 11.2$$

$$\alpha_s = [A\,;\, a^{(s)}]_{12} = -\,(1/n_1 n_2) \int f_2^0\, c_2 .\, a^{(s)}\, dc_2 \qquad 11.4$$

$$\beta_s = [B\,;\, a^{(s)}]_{12} = -\,(1/n_1 n_2) \int f_2^0\, [(m_2 c_2^2/2\,kT) - 3/2]\, c_2 .\, a^{(s)}\, dc_2 \qquad 11.3$$

$$A_r^{(r)} = \begin{vmatrix} a_{0,\,0} & \cdots & a_{r,\,0} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ a_{0,\,r-1} & \cdots & a_{r,\,r-1} \\ 0 & \cdots & r \end{vmatrix} \qquad 11.5$$

$$B_r^{(r)} = \begin{vmatrix} a_{0,\,0} & \cdots & a_{r,\,0} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ a_{0,\,r-1} & \cdots & a_{r,\,r-1} \\ 0 & \cdots & r \end{vmatrix} \qquad 11.6$$

$$A^{(r)} = \begin{vmatrix} a_{0,0} & \cdots & a_{r,0} \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ a_{0,r} & \cdots & a_{r,r} \end{vmatrix} \qquad 11.7$$

It follows (4) according to Chapman and Cowling that

$$[A;A]_{12} = \frac{\alpha_0^2}{a_{0,0}} + \sum_{r=1}^{\infty} \frac{[A_r^{(r)}]^2}{A^{(r)}A^{(r-1)}} \qquad 11.8$$

$$[A;B]_{12} = \frac{\alpha_0\beta_0}{a_{0,0}} + \sum_{r=1}^{\infty} \frac{A_r^{(r)}B_r^{(r)}}{A^{(r)}A^{(r-1)}} \qquad 11.9$$

The values of $[A\,;A]_{12}$ and $[A\,;B]_{12}$ can be obtained with as many terms as wished provided a sufficient number of coefficients α_r, β_r, and a_{rs} are known.

The values of α_r and β_r are (4)

$$\alpha_r = -(3/2n_1)\sqrt{(2kT/m_2)}\,\delta_{r0} \qquad 11.10$$

$$\beta_r = \alpha_0[\delta_{r0} - (5/2)\,\delta_{r1}] \qquad 11.11$$

where $_{kr}$ is the Kronecker's simbol.

Introducing these values into 11.8 and 11.9 the following expressions are obtained

$$[A;A]_{12} = (\alpha_0^2/a_{00})\left\{1 + \frac{[A_{01}^{(1)}]^2}{A^{(1)}A^{(0)}}a_{00} + \dots + \right.$$

$$\left. + \frac{[A_{0m}^{(m)}]^2}{A^{(m)}A^{(m-1)}}a_{00} + \dots + \right\} \qquad 11.12$$

$$[A;B]_{12} - [A;A]_{12} = -(5\,\alpha_0^2/2a_{00})\left\{\frac{A_{01}^{(1)}A_{11}^{(1)}}{A^{(1)}A^{(0)}}a_{00} + \dots + \right.$$

$$\left. + \frac{A_{0m}^{(m)}A_{1m}^{(m)}}{A^{(m)}A^{(m-1)}}a_{00} + \dots + \right\} \qquad 11.13$$

where $A_{rs}^{(m)}$ is a_{rs} cofactor in $A^{(m)}$.

The coeficients a_{00}, a_{01}, a_{11}, a_{02}, a_{12} and a_{22} are known (6).

The first three terms for $[A\,;A]_{12}$ and $[A\,;B]_{12}$ have been calculated on the assumption that both nuclei and neutrons behave like rigid spheres.

Calling

$$P_m\,(M_2)/Q_m\,(M_2) = a_{00}\,[A_{cm}{}^{(m)}]^2/A^{(m)}\,A^{(m-1)} \qquad 11.14$$

$$R_m\,(M_2)/Q_m\,(M_2) = \frac{5}{2}a_{00}\,A_{cm}{}^{(m)}\,A_{1m}{}^{(m)}/A^{(m)}\,A^{(m-1)} \qquad 11.15$$

where $M_2 = m_2/m_2 + m_1$, it follows

$$\alpha_0{}^2/a_{00} = (9\,\pi\,\sqrt{1 - M_2}/32\,n_1)\,\overline{c_2{}^{(0)}}/n_1\,\sigma_{12}{}^2\,\pi \qquad 11.16$$

$$P_1(x) = (1 - x)^2$$

$$P_2(x) = 73728\ \ (1 - x)^4\ \ (18 - 24\,x + 110\mathrm{x}^2 - 68x^3 + 194x^4)$$

$$Q_1(x) = 12 - 8x + 6x^2$$

$$Q_2(x) = 4098\ \ (13824 - 36864x + 84264x^2 - 206104x^3 + \\ + 295662x^4 - 166633x^6 - 61152x^7 + 13482x^8)$$

$$R_1(x) = 5(1 - x)$$

$$R_2(x) = 122880\ \ (1 - x)^3\ \ (36 - 48\mathrm{x} + 232x^2 - 144x^3 + 323\mathrm{x}^{i})$$

By σ_{12} it is meant, as usual, the average diameter of nucleus and neutron; this magnitude having been introduced through coeficients a_{rs}. Quantity $n_1\,\sigma^2{}_{12}\,\pi$ represents the macroscopic geometrical cross section Σ_s . $\overline{c_2{}^{(0)}}$ is the maxwellian mean value for the velocities.

Table I shows several numerical values of

$$\gamma = (n_1\,\Sigma_s/\overline{c_2{}^{(0)}})\,[A;\,A]_{12},\ \ \gamma' = (n_1\,\Sigma_s/\overline{c_2{}^{(0)}})\,[A;\,B]_{12},$$

$a^T = [A\,;B]_{12}\,/\,[A\,;A]_{12}$ and $\beta_T = \alpha_T - ½$ within the M_2 variation range, namely: from 0.0 to 0.5.

TABLE I

M_2	0.0	0.1	0.2	0.3	0.4	0.5
γ	0.97791	0.91379	0.84960	0.78465	0.71823	0.64971
γ'	0.54073	0.52209	0.50285	0.48218	0.45831	0.42579
α_t	0.55294	0.57135	0.59187	0.61451	0.63811	0.65536
β_t	0.05294	0.07136	0.09187	0.11451	0.13811	0.15536

12. BOUNDARY CONDITIONS

It is advisable to express the diffusion law as a function of the scalar flux of neutrons Φ:

$$\phi = n_2 \overline{c_2^{(0)}} \qquad 12.1$$

It is then obtained

$$J = -(\gamma/3\,\Sigma_s)\,[(\partial\,\phi/\partial\,r) + (\beta_T\,\phi/T)\,(\partial\,T/\partial\,r)] \qquad 12.2$$

where γ and β_T have been defined in § 11.

The boundary conditions in the separation of two scattering media are taken to be the continuity of J_+ and J_- in the forementioned separation surface, letting n (see § 10) coincide with its normal. It follows from 12.1, 10.3 and 10.4

$$J_+ = (1/4)\,\phi + \frac{1}{2}\,J.\,n \qquad 12.3$$

$$J_- = (1/4)\,\phi - \frac{1}{2}\,J.\,n \qquad 12.4$$

The continuity of Φ and the component of J normal to the separation surface are boundary conditions equivalent to 12.3 and 12.4.

In the separation of a scattering medium and vacuum, the boundary condition is chosen to be

$$J_- = 0 \qquad 12.5$$

taking n directed into vacuum.

APPLICATIONS

13. UNIDIMENSIONAL STEADY-STATE PROBLEM

A planar symetry medium without production or absorption of neutrons is considered. The direction of the maximum variability of medium properties is taked as the x-axis. For the steady state it holds $J_x = J_o =$ constant and $J_y \equiv J_z = O$. Resorting to 12.2 it follows:

$$-(\gamma/3\,\Sigma_s)\left\{\frac{\partial\phi}{\partial x} + \beta_T\,(\phi/T)\,\frac{\partial T}{\partial x}\right\} = J_0 \qquad 13.1$$

for wich the general solution is given by

$$\phi(x) = (3\,\Sigma_s/\gamma)\,J_0\,[T(x)]^{-\beta_T}\int_0^x [T(x)]^{-\beta_T}\,dx + B\,[T\ \ (x)]^{-\beta_T} \qquad 13.2$$

where $T(x)$ is the temperature as a function of x, and B is an integration constant.

An experiment only slightly differing from the conditions assumed above could be performed in the following way: a slab of with $2l$ and equal values for ϕ and T in both sides. Resorting to 12.3 follows:

$$\phi(-l) = (3\,\Sigma_s/\gamma)\,J_0\,[T(-l)]^{-\beta_T}\int_{-l}^{0} [T(x)]^{\beta_T}\,dx + B\,[T(-l)]^{-\beta_T}$$

$$\phi(+l) = (3\,\Sigma_s/\gamma)\,J_0\,[T(+l)]^{-\beta_T}\int_{0}^{+l} [T(x)]^{\beta_T}\,dx + B\,[T(+l)]^{\beta_T}$$

where $x \equiv +l$ and $x = -l$ are the coordinates of both sides of the slab. In order to satisfy the imposed conditions to Φ and T, J_o must vanish, therefore

$$\phi(x)/\phi(l) = [T(x)/T(l)]^{-\beta_T} \qquad 13.3$$

Placing $\beta_T = O$ the ordinary diffusion law is obtained. Then it holds

$$\phi(x)/\phi(l) = 1 \qquad 13.4$$

In order to exemplify the foregoing results, the values $T(O) = 600°K$ and $T(+l) = 300°K$ can be chosen: from 12.2 it follows $0.964 \leq \phi(0)/\phi(l) \leq 0.899$ when β_T varies between 0.05294 and 0.15536, and $\phi(0)/\phi(l) \equiv 1$ when the ordinary law of diffusion is used.

It is seen that the variation recorded for $\Phi(0)/\Phi(e)$ extends from 3.6 % up to 10.1 % as M_2 varies from 0.0 up to 0.5 according to whether the ordinary law of diffusion or the corrected one is used.

14. UNIDIMENSIONAL DIFFUSION EQUATION WITH ABSORPTION

It shall be assumed that the diffusion law 12.2 is still valid even with small absorption of neutrons. Applying the continuity equation for the number of neutrons with absorption, the diffusion equation:

$$\frac{\partial n_2}{\partial t} = -\frac{\partial}{\partial r} . J - \Sigma_a \phi \qquad 14.1$$

is obtained where Σ_a is the macroscopical absorption cross-section. In the unidimensional case, equation 14.1 leads to

$$\frac{\partial n_2}{\partial t} = (\gamma/3\,\Sigma_s)\left[\frac{d^2\phi}{dx^2} + \beta_T \frac{d\phi}{dx}\,\frac{d\,ln\,T}{dx} + \phi\,\beta_T \frac{d^2\,ln\,T}{dx^2}\right] - \Sigma_a \phi \qquad 14.2$$

and for the steady state

$$\frac{d^2\phi}{dx^2} + \beta_T \frac{d\,ln\,T}{dx}\,\frac{d\phi}{dx} + \left[\beta_T \frac{d^2\,ln\,T}{dx^2} - (3\,\Sigma_a\,\Sigma_s/\gamma)\right]\phi = 0 \qquad 14.3$$

A slab of with $2l$ is assumed. One side of the slab limits with vacuum and other side has a fixed neutron flux J_x.

A temperature distribution is given in the slab. Both values of the scalar flux Φ at the side where J_x is fixed shall be calculated, assuming that the ordinary or the corrected diffusion law holds.

Chosing

$$\ln T = -2ax + b \qquad 14.4$$

a simple equation is obtained, since from 14.1 it follows

$$\frac{d^2 \phi}{d x^2} - 2 a \beta_T \frac{d \phi}{d x} - (3\, \Sigma_a \Sigma_s/\gamma)\, \phi = 0$$

the general solution of which is given by

$$\phi = \exp(\alpha x)\,[A \exp(\beta x) + B \exp(-\beta x)] \qquad 14.5$$

$$\text{where } \alpha = a\, \beta_T \text{ and } \beta = \sqrt{a^2 \beta_T{}^2 + (3\, \Sigma_a\, \Sigma_s/\gamma)}$$

Using the ordinary law of diffusion, — or taking $\beta_T = O$, which is equivalent — it follows: $\alpha = \alpha^o \equiv O$ and

$$\beta = \beta_0 = \sqrt{(3\, \Sigma_a\, \Sigma_s/\gamma)}.$$

Calling $x = O$ the coordinate of the first side and $x \equiv l$ the coordinate of the other one the boundary conditions are $J_x\,(O) \equiv = J_o$ and $J_-(l) \equiv O$. Bringing these conditions into 14.5 the following equation holds:

$$\phi(x) = 2 J_0 \exp(\alpha x) \frac{[\alpha - (3\, \Sigma_s/2\gamma)]\, Sh\, \beta\, (l - x) - \beta\, Ch\, \beta\, (l - x)}{[(2\gamma/3\, \Sigma_s)\, (\alpha^2 - \beta^2) - \alpha]\, Sh\, \beta\, l - \beta\, Ch\, \beta\, l}$$

14.6

It is easy to identify the expression $\gamma/3\, \Sigma_s$ appearing in 12.2 with the coefficient D appearing in the common law of diffusion: $J = - D \operatorname{grad} \phi$

If graphite is taken as scattering medium, it holds $D \equiv 0.92$ cm.

Taking $T = 450^o K$ at $x \equiv O$ and $T = 300^o K$ at $x = l$, it follows from 14.4 that

$$l a = 0.20 \qquad 14.7$$

For graphite $\Sigma_a \simeq 3.7\ 10^{-4}\ \mathrm{cm}^{-1}$; hence $\beta_o \equiv 2.01\ 10^{-2}\ \mathrm{cm}^{-1}$.

From Table I and equation 14.7 it follows $a^2 \beta_T{}^2 < 10^{-3}/l$ whence for $l > 10$ cm,

$$\beta = \beta_0 (1 + \delta) \qquad 14.8$$

$$\text{where } \delta = \frac{1}{2} a^2 \beta_T{}^2/\beta_0{}^2 = 0.02\, \beta_T{}^2/\beta_0{}^2\, l^2.$$

Introducing 14.8 into 14.6 and neglecting δ and α with respect to α/β_o, it follows

$$\phi(0) = J_0 \frac{T h \beta_0 l + (2 \gamma \beta_0 / 3 \Sigma_s)}{(\beta_0 \gamma / 3 \Sigma_s)} [1 - (2 \gamma / 3 \Sigma_s) \beta_0 T h \beta_0 l] [1 - (\alpha/\beta_0)]$$

If the value of $\phi(O)$ obtained resorting to the ordinary diffusion law when applied to the same problem, is called $\phi^0(O)$ the relation

$$\phi(0)/\phi^0(0) = 1 - \alpha/\beta_0$$

is obtained.

If $l \equiv 30$ cm, then $\alpha / \beta_o = 0.022$, which is a 2.2 % difference it the values of $\phi(O)$ according to whether the corrected diffusion law ot the ordinary one is used.

15. FINAL REMARKS

It has been shown that the Boltzmann transport equation in the case of a very dilute binary mixture can be solved by a method similar to the one of Enskog, if the velocity distribution function for the more abundant component is previously given as maxwellian and time independent. In such a case there is only one parameter to be given, namely: the number density of the less abundant component at each point at a given time.

These results have been applied to the diffusion of thermal neutrons in a scattering medium. The distribution function for the scattering nuclei has been obtained by assumming that they behave like classical harmonic isotropic oscillators. The frequency of these oscillators does not appear in the so obtained distribution function.

A better model is to assume quantum oscillators instead of the classical ones. For a temperature of the medium such that the oscillators are in high quantum number states, they may be taken as classical, and also the neutrons have enough energy to make the nuclei change their quantum state by collisions. If diffraction effects with the lattice are not considered, the applicability of the model is to be tested by the ratio medium temperature-vs-Deybe temperature, as the latter corresponds to the maximum frequency of the oscillations of the solid.

With the classical oscillators model a diffusion law corrected for the effect of thermal gradients has been obtained. This latter effect appears in the same natural way as thermal diffusion does in gases.

The scattering law assumed for neutron nuclei collisions is that of rigid spheres, which is isotropic in the center of mass system. This law is assumed only for numerical calculation of the diffusion law coeficients and the derivation of some properties of the equations. Other scattering laws could possibly be assumed without changing the analytical form of the obtained diffusion law.

If neutron difraction with the lattice is taken into account, collisions with phonons and Bragg scattering rather than independent collisions with each one of the nuclei must be considered. The transport equation in this case contains the corresponding scattering law and must lead, in a first approximation to the usual diffusion law, if the velocity distribution for neutrons is not far from isotropic (see 2). The temperature corrections to the diffusion law arise from the temperature dependence of the scattering law. The classical model chosen is then equivalent to assume a particular (and easy to menage) scattering law. Therefore, the obtained temperature correction for the diffusion law is valid insofar as the scattering law represents a good approximation.

A few problems representing possible experimental conditions have been calculated, leading to variations of the scalar neutron flux of a few unities per cent, according to whether the ordinary law of diffusion or the corrected one were used.