

**H. Niewodniczański**  
**INSTITUTE OF NUCLEAR PHYSICS**  
**Kraków, Poland.**

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THERMAL NEUTRON DIFFUSION PARAMETERS  
IN HOMOGENEOUS MIXTURES

Krzysztof Drozdowicz and Ewa Krynicka

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INSTYTUTU FIZYKI JĄDROWEJ  
IM. HENRYKA NIEWODNICZAŃSKIEGO  
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## THERMAL NEUTRON DIFFUSION PARAMETERS IN HOMOGENEOUS MIXTURES

Krzysztof Drozdowicz and Ewa Krynicka

*Henryk Niewodniczański Institute of Nuclear Physics  
ul. Radzikowskiego 152, 31-342 Kraków, Poland*

### **Abstract**

A physical background is presented for a computer program which calculates the thermal neutron diffusion parameters for homogeneous mixtures of any compounds. The macroscopic absorption, scattering, and transport cross sections of the mixture are defined which are generally functions of the incident neutron energy. The energy-averaged neutron parameters are available when these energy dependences and the thermal neutron energy distribution are assumed. Then the averaged diffusion coefficient and the pulsed thermal neutron parameters (the absorption rate and the diffusion constant) are also defined. The absorption cross section is described by the  $1/v$  law and deviations from this behaviour are considered. The scattering cross section can be assumed as being almost constant in the thermal neutron region (which results from the free gas model). Serious deviations are observed for hydrogen atoms bound in molecules and a special study in the paper is devoted to this problem. A certain effective scattering cross section is found in this case on a base of individual exact data for a few hydrogenous media. Approximations assumed for the average cosine of the scattering angle are also discussed. The macroscopic parameters calculated are averaged over the Maxwellian energy distribution for the thermal neutron flux. An information on the input data for the computer program is included.

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## 1. Introduction.

The macroscopic parameters of thermal neutrons have to be known to describe their diffusion in composed media. The macroscopic cross sections are usually easy available basing on the elemental composition of the medium and on nuclear data tables which contain the microscopic cross sections for thermal neutrons. The absorption cross sections are given at the standard thermal neutron velocity, 2200 m/s. For the scattering the so-called free atom scattering cross section is reported. These data are sufficient for a rough approximation of the thermal neutron parameters for a medium. When the thermal neutron group is treated more accurately the energy (or velocity) spectrum of thermal neutrons has to be taken into account and the energy-averaged parameters have to be defined. Additionally, for mixtures of compounds it is easy to do a mistake in the simple arithmetical calculation when the contributions of each element have to be included and the individual microscopic cross sections have to be taken from data tables. In the present report we offer a user a computer program which performs the calculation automatically using a cross section data file and a chemical-like notation for stoichiometric formulae of compounds. The following thermal neutron parameters, averaged over the energy spectrum, are obtained for a homogeneous mixture of compounds: the macroscopic absorption, scattering and transport cross sections, the diffusion coefficient, and the pulsed parameters: the absorption rate and the diffusion constant. The basic definitions of these parameters and their averaging over the thermal neutron energy are presented in the report.

A special study is devoted to the scattering of thermal neutrons by hydrogen nuclei which are bound in molecules. In such a case the table free atom cross section is irrelevant for calculation of the macroscopic parameters. The hydrogen scattering cross section is strongly dependent on the incident neutron energy and, moreover, this dependence is different for different compounds. Therefore, it is impossible to give a single exact formula to calculate the macroscopic scattering and transport cross sections and the diffusion coefficient for materials which contain the hydrogenous compounds. An idea to use certain effective values is presented in the report to get some general expressions which give a reasonable accuracy (on the order of a few per cent).

Some peculiarities of the thermal neutron absorption cross section for certain elements are also discussed in the paper.

The aim of the approach used is to get a general procedure which allows to obtain the energy-averaged thermal neutron macroscopic parameters for any material of a known composition. In most cases the results are exact. For hydrogenous media they must be approximate (the computer code produces a warning message) but are on an acceptable level of accuracy which is much better than while using the free atom cross section. A better

result in this case can be obtained only if each hydrogenous compound is treated individually. However, the necessary data exist only for a few materials.

Another approach has been presented by CZUBEK (1988a). His method is oriented to geological media which can contain water and the approximation given has been elaborated including only that hydrogenous medium. Therefore, Czubek's formalism can give better results for materials containing water but does not distinguish other hydrogenous media.

## 2. Basic definitions and relations.

### 2.1. Maxwellian distribution.

The thermal neutron energy flux distribution  $\Phi(E)$  in a thermal equilibrium with the medium is well described by the Maxwellian distribution:

$$M_{\Phi}(E)dE = M_{\Phi}(W)dW = We^{-W}dW \quad , \quad (1)$$

where:

$$W = \frac{E}{E_0} \quad , \quad (2)$$

$$E_0 = \frac{1}{2}k_B T = \frac{1}{2}m_n v_0^2 \quad (3)$$

with:

$k_B$  - Boltzmann constant,

$T$  - absolute temperature,

$m_n$  - neutron mass,

$v_0$  - the most probable velocity of the Maxwellian density distribution:

$$M_n(v)dv = \frac{4}{\sqrt{\pi}} \frac{v^2}{v_0^3} \exp\left(-\frac{v^2}{v_0^2}\right)dv \quad . \quad (4)$$

The distributions in Eqs (1) and (4) are normalized to unity.

Any magnitudes  $x(E)$  averaged over the Maxwellian flux distribution are defined as:

$$\langle x \rangle \equiv \langle x(E) \rangle = \int_0^{\infty} x(E)M_{\Phi}(E)dE \quad . \quad (5)$$

## 2.2. Thermal neutron cross sections.

The linear macroscopic cross sections  $\Sigma(E)$  are connected to the microscopic ones by the simple dependence

$$\Sigma(E) = N\sigma(E) , \quad (6)$$

where  $N$  is the volume concentration of nuclei of the microscopic cross section  $\sigma(E)$ . For a single chemical compound (or for a mixture of elements) the relation is:

$$\Sigma(E) = N_s \sum_i n_i \sigma_i(E) , \quad (7)$$

where:

$\sigma_i(E)$  – energy-dependent microscopic cross section of the  $i$ -th element,

$n_i$  – number of atoms of the  $i$ -th element in the stoichiometric formula of the compound,

$$N_s = \rho(T) \frac{N_A}{M} , \quad (8)$$

where:

$\rho(T)$  – bulk density of the material at temperature  $T$ ,

$N_A$  – Avogadro's number,

$M$  – gram-molecule of the compound.

For a mixture of  $J$  chemical compounds Eq.(6) leads (cf. CZUBEK *et al.* 1991) to:

$$\Sigma(E) = \rho(T) N_A \sum_{j=1}^J \left[ \sum_{i=1}^I \frac{\sigma_i(E)}{M_j} n_{ij} \right] q_j , \quad (9)$$

where:

$M_j = \sum_{i=1}^I n_{ij} A_{ij}$ , and  $A_{ij}$  is a gram-atom of the  $i$ -th element in the  $j$ -th compound,

$q_j$  – weight content of the  $j$ -th compound in the mixture, and  $\sum_{j=1}^J q_j = 1$ .

The mass macroscopic cross section is defined as

$$\Sigma^M(E) = \frac{\Sigma(E)}{\rho(T)} , \quad (10)$$

and can be found without knowledge of the material density:

$$\Sigma^M(E) = N_A \sum_{j=1}^J \left[ \sum_{i=1}^I \frac{\sigma_i(E)}{M_j} n_{ij} \right] q_j . \quad (11)$$

The relations given in Eqs (6) to (11) are valid for the absorption and scattering cross sections. Similar relations are sometimes quoted in literature, *e.g.* Bussian *et al.* (1991), but they do not take into account the energy dependence of the cross sections within the thermal neutron energy group. Eqs (6) to (11) define the macroscopic cross sections for neutrons of energy  $E$  and have to be used in a more careful description of the thermal neutron diffusion in materials when the neutron energy spectrum is included into the consideration. On this basis the energy-averaged neutron parameters will be defined in further parts of the paper.

### *Absorption cross section.*

The energy dependence of the absorption cross section  $\sigma_a(E)$  for almost all nuclei is described for thermal neutrons by the  $\frac{1}{v}$  law. Therefore, it is sufficient to know the microscopic absorption cross sections at only one energy. The values of the  $\sigma_a$  listed in the nuclear data tables are given for the most probable neutron velocity  $v_0 = 2200$  m/sec (the corresponding thermal neutron energy  $E_0 = 0.0253$  eV, the temperature  $T = 293.6$  K). Let introduce here the following notation:

$$\begin{aligned} v_{00} &= 2200 \text{ m/sec} , \\ E_{00} &= 0.0253 \text{ eV} , \\ T_{00} &= 293.6 \text{ K} , \\ \sigma_a^{00} &= \sigma_a(v_{00}) , \\ \sigma_a^0 &= \sigma_a(v_0) , \end{aligned} \quad (12)$$

and then

$$\sigma_a(E) = \frac{v_0}{v} \sigma_a^0 = \frac{v_{00}}{v} \sigma_a^{00} = \sigma_a^{00} \sqrt{\frac{E_{00}}{E}} . \quad (13)$$

The energy-dependent macroscopic absorption cross section  $\Sigma_a(E)$  for a mixture is defined by Eq.(9) where the individual microscopic cross sections  $\sigma_{a,i}(E)$  are given by the above Eq.(13).

The problem of some particular elements, for which the function  $\sigma_a(E)$  deviates from the  $\frac{1}{v}$  dependence, is discussed in paragraph 4.2.

### *Scattering cross section.*

For most elements the energy-dependent scattering cross section  $\sigma_s(E)$  is very well approximated by the formula of the free gas model. In practice this is reduced to a value of the constant scattering cross section  $\sigma_{sf}$  for the free atom:

$$\sigma_s(E) = \sigma_{sf} . \quad (14)$$

The macroscopic cross section  $\Sigma_s(E)$  for a mixture is then given by Eq.(9).

However, for light nuclei, especially for hydrogen, the energy-dependent cross section  $\sigma_s^H(E)$  cannot be approximated in this way. In the thermal neutron energy region it is not constant and differs even strongly from the behaviour described by the free gas model when the hydrogen atoms are bound in molecules. The problem is discussed in paragraph 4.3.

### **2.3. Thermal neutron diffusion coefficient.**

In the case of the anisotropic scattering (cf. BECKURTS and WIRTZ 1964) the transport cross section  $\Sigma_{tr}(E)$  is defined:

$$\Sigma_{tr}(E) = [1 - \mu(E)] \Sigma_s(E) , \quad (15)$$

where  $\mu(E)$  is the average cosine of the scattering angle, given by

$$\mu(E') = \frac{\int_0^{\infty} \Sigma_1(E' \rightarrow E) dE}{\int_0^{\infty} \Sigma_0(E' \rightarrow E) dE} , \quad (16)$$

where  $\Sigma_l(E' \rightarrow E)$  for  $l = 0, 1$  are the zero and first Legendre components of the scattering kernel and

$$\int_0^{\infty} \Sigma_0(E' \rightarrow E) dE = \Sigma_s(E') . \quad (17)$$

Then the thermal neutron diffusion coefficient is defined as:

$$D(E) = \frac{1}{3[\Sigma_a(E) + \Sigma_{tr}(E)]} , \quad (18)$$

which means that knowledge of the energy-dependent cross sections,  $\Sigma_a(E)$  and  $\Sigma_s(E)$ , and of the average cosine of the scattering angle  $\mu(E)$  is required to determine the exact energy dependence of the diffusion coefficient  $D(E)$ . Some approximations are considered in paragraph 3.1.

**Note:** Sometimes another definition of the transport cross section is used, namely:

$$\Sigma_{tr} = \Sigma_a + (1 - \mu)\Sigma_s , \quad (19)$$

(cf. *e.g.* CZUBEK 1988b) and then

$$D = \frac{1}{3\Sigma_{tr}} , \quad (20)$$

which is only formally different from relation (18) but leads to the same value:

$$D = \frac{1}{3[\Sigma_a + (1 - \mu)\Sigma_s]} . \quad (21)$$

## 2.4. Energy-averaged thermal neutron parameters.

The thermal neutron parameters averaged over the energy spectrum,

$$\langle \Sigma_a \rangle, \langle \Sigma_s \rangle, \langle \Sigma_{tr} \rangle, \langle D \rangle,$$

are given by the general definition (5). For the neutrons in a thermal equilibrium with the medium the Maxwellian distribution (1) is then given at the medium temperature. This is a case of the source-free infinite medium, *i.e.* the case of the flux decaying after the neutron pulse. When a steady state neutron source is present a heating (or hardening) of the neutron spectrum is observed and the Maxwellian has to be defined for a higher temperature, cf. AMALDI (1959), CZUBEK (1988b). In a source-free finite medium the diffusion cooling occurs and then the neutron energy spectrum can be approximated by the Maxwellian of the temperature lower than of the medium. Only the averages corresponding to the thermal equilibrium are calculated in the presented computer program because the mentioned problems are individual in each particular application (the material, the geometry, the steady state or pulsed source, etc.).

## 2.5. Pulsed thermal neutron parameters.

### *Absorption rate.*

The absorption rate  $\langle \nu \Sigma_a \rangle$  is equal to the decay constant of thermal neutrons in an infinite medium and defines their lifetime:

$$\tau = \frac{1}{\langle \nu \Sigma_a \rangle} . \quad (22)$$

The value of the absorption rate, according to the general definition (5), is given as:

$$\langle \nu \Sigma_a \rangle \equiv \int_0^{\infty} \nu \Sigma_a(E) M_{\Phi}(E) dE . \quad (23)$$

For the cross section of the  $\frac{1}{v}$  type the macroscopic absorption cross section follows Eqs (13) and (9):

$$\Sigma_a(E) = \frac{\rho(T)}{\rho(T_{00})} \frac{v_{00}}{v} \Sigma_a^{00} \quad (24)$$

and the absorption rate is

$$\langle v \Sigma_a \rangle = \frac{\rho(T)}{\rho(T_{00})} v_{00} \Sigma_a^{00} \quad (25)$$

### *Diffusion constant.*

The relation between the thermal neutron diffusion constant  $D_0$  and the diffusion coefficient  $D(E)$  was defined by NELKIN (1960) as

$$D_0 = \frac{\langle D(E) \rangle}{\langle \frac{1}{v} \rangle} = \frac{\int_0^{\infty} D(E) M_{\Phi}(E) dE}{\int_0^{\infty} \left( \frac{1}{v} \right) M_{\Phi}(E) dE} \quad (26)$$

Note: The relation defined in Eq.(26) is sometimes given in the form:

$$D_0 = \bar{v} \langle D(E) \rangle, \quad (27)$$

where the average  $\bar{v}$  is referred to the Maxwellian density distribution:

$$\bar{v} = \int_0^{\infty} v M_n(E) dE \quad (28)$$

[cf. Eq.(4)]. The using of this confusing relation (27) is justified only by the fact that for the pure Maxwellian flux and density distributions the following relations are observed:

$$\left\langle \frac{1}{v} \right\rangle = \frac{\sqrt{\pi}}{2v_0}, \quad (29)$$

$$\bar{v} = \frac{2}{\sqrt{\pi}} v_0, \quad (30)$$

which makes it possible to substitute

$$\frac{1}{\left\langle \frac{1}{v} \right\rangle} = \bar{v} , \quad (31)$$

but it is necessary to remember that

$$\bar{v} \neq \langle v \rangle . \quad (32)$$

## 2.6. Density-removed parameters.

For a calculation of the thermal neutron macroscopic or pulsed parameters the density of the material has to be known. Sometimes this value is unknown during some test calculations for a mixture of materials. Then the so-called "density-removed parameters" can be calculated and when the density is known later it is easy to obtain from them the usual neutron parameters.

The macroscopic mass cross sections  $\Sigma^M$  (of the absorption, scattering, and transport) do not contain the material density from the definition itself (cf. Eq.(11)). For other parameters a relation between them and the density removed parameters is available from the relevant definitions given in paragraphs 2.2 to 2.5. The following relationships exist where the density-removed parameters are marked with the asterisk:

$$\Sigma^*(T) = \Sigma(T) / \rho(T) , \quad (33a)$$

where  $\Sigma$  means  $\Sigma(E)$  or  $\langle \Sigma \rangle$  for the neutron absorption, scattering, and transport, and  $\rho(T)$  is the material density at the temperature  $T$ . The same type of the relation holds for the neutron absorption rate:

$$\langle v \Sigma_a \rangle^* = \langle v \Sigma_a \rangle(T) / \rho(T) . \quad (33b)$$

For the diffusion coefficient:

$$D^*(T) = \rho(T) D(T) , \quad (33c)$$

where  $D$  means  $D(E)$  or  $\langle D \rangle$ , and for the diffusion constant:

$$D_0^*(T) = \rho(T) D_0(T) . \quad (33d)$$

The expressions which are obtained from Eqs (33) and from relevant definitions for particular parameters do not contain the material density  $\rho$ .

### 3. Calculation of the neutron parameters.

#### 3.1. Average cosine of the scattering angle $\mu(E)$ .

The energy-dependent average cosine of the scattering angle,  $\mu(E)$ , is given by Eq.(16). That means that one has to know the kernels  $\Sigma_0(E' \rightarrow E)$  and  $\Sigma_1(E' \rightarrow E)$  to determine accurately the dependence  $\mu(E)$ . This is usually a difficult task. A certain simple approximation can be used instead. Basing on the general relationship (7) we calculate directly the macroscopic transport cross section:

$$\Sigma_{tr}(E) = N_s \sum_i n_i \sigma_{tr_i}(E) = N_s \sum_i n_i [1 - \mu_i(E)] \sigma_{st_i}(E) . \quad (34)$$

Then the individual scattering cosines  $\mu_i(E)$  are substituted as usually (cf. BECKURTS and WIRTZ 1964) by the approximate relation:

$$\mu_i = 2 / (3A_i) . \quad (35)$$

However, this is not the case for thermal neutrons scattered in hydrogenous media where the dependence on the energy is very strong and each material should be treated individually. The problem becomes more complicated when a mixture of  $J$  compounds is considered, where some compounds are the hydrogenous media. We have then to do further approximations. For each  $j$ -th hydrogenous material we assume

$$\langle \mu_j(E) \rangle = \mu_j = 0.2 \quad (36)$$

and the transport cross section is

$$\Sigma_{tr_j}(E) = (1 - \mu_j) \Sigma_{st_j}(E) . \quad (37)$$

Finally, the cross section of the mixture is

$$\Sigma_{tr}(E) = \sum_j \Sigma_{tr_j}(E) , \quad (38)$$

where for the hydrogenous components the cross section  $\Sigma_{tr_j}$  is given by Eq.(37) and for the others is defined by Eq.(34) with (35).

If necessary one can determine then the average scattering cosine  $\mu$  for the mixture from the obvious relation:

$$(1 - \mu) = \frac{\Sigma_{tr}(E)}{\Sigma_s(E)} , \quad (39)$$

where  $\Sigma_{tr}(E)$  is given by Eq.(38) and  $\Sigma_s$  is obtained from Eq.(9).

### 3.2. Averaged parameters.

The cross sections averaged over the thermal neutron energy spectrum,  $\langle \Sigma_a \rangle$ ,  $\langle \Sigma_s \rangle$ ,  $\langle \Sigma_{tr} \rangle$ , and the pulsed parameters,  $\langle \nu \Sigma_a \rangle$  and  $D_0$ , are easy to calculate according to the definitions given in paragraph 2. In particular, from Eq.(5) the following useful general relation can be obtained for the absorption cross section:

$$\langle \Sigma_a \rangle = \left\langle \frac{1}{\nu} \right\rangle \langle \nu \Sigma_a \rangle . \quad (40)$$

For a calculation of the averaged diffusion coefficient  $\langle D \rangle$  we assume the constant scattering cross section

$$\Sigma_s(E) \approx \Sigma_{sf} \quad (41)$$

(the assumption (41) does not hold for the hydrogen cross section which will be considered in paragraph 4.3). We use here the notation

$$\Sigma_s(E) = \Sigma_s^{00} , \quad (42)$$

which results from Eq.(41). Making use of Eqs (13) and (2) we obtain

$$\Sigma_a(E) = \frac{\Sigma_a^{00}}{\sqrt{W}} , \quad (43)$$

and

$$D(E) = \left[ 3 \left( \frac{\Sigma_a^{00}}{\sqrt{W}} + \Sigma_{tr}^{00} \right) \right]^{-1} . \quad (44)$$

For a calculation of the averaged diffusion coefficient the limits  $[0, \infty)$  of the integral in Eq.(5) are substituted for numerical purposes by  $[0, E_\infty]$ . For the thermal neutrons the  $E_\infty$  value can be assumed as  $E_\infty \approx 1$  eV and then for  $E_0 = E_{00}$  the limit  $W_\infty = 40$ . Using the independent variable  $W$  [as in Eq.(44)] we obtain

$$W_\infty = \frac{E_\infty}{E_0} \quad (45)$$

and for  $E_0 = E_{00}$  the limit  $W_\infty = 40$ . Then the averaged diffusion coefficient is calculated as

$$\langle D \rangle = \frac{1}{3} \int_0^{40} \frac{W e^{-W}}{\frac{\Sigma_a^{00}}{\sqrt{W}} + \Sigma_{tr}^{00}} dW, \quad (46)$$

where the constant transport cross section  $\Sigma_{tr}^{00}$  used is obtained from Eqs (34), (37), (38), following the constant  $\Sigma_s^{00}$  introduced in Eq.(42).

### 3.3 Standard deviations of the calculated parameters.

The standard deviations of the calculated parameters are found with the variance method using the obtained relationships. The standard deviation  $\sigma(X)$  of the parameter  $X$  which is a function of  $I$  independent random variables  $x_i$  is given by

$$\sigma^2(X) = \sum_{i=1}^I \left( \frac{\partial X}{\partial x_i} \right)^2 \sigma^2(x_i), \quad (47)$$

where the relevant formulae for  $\langle \Sigma_a \rangle$ ,  $\langle \Sigma_s \rangle$ ,  $\langle \Sigma_{tr} \rangle$ ,  $\langle \nu \Sigma_a \rangle$ ,  $D_0$  are used as  $X$ . A simplified formula has been used only to obtain the standard deviation of the diffusion coefficient  $\sigma(\langle D \rangle)$ . Certain simplifying approximations have been assumed to obtain this parameter and the next assumption, to make the estimation of the error easier, is here possible. Namely, the following formula:

$$\langle D \rangle \approx \frac{1}{3[\Sigma_a^{00} + \Sigma_{tr}^{00}]} \quad (48)$$

can be used in Eq.(47) when  $X = \langle D \rangle$ .

The standard deviations of the microscopic cross sections,  $\sigma_a^{00}$ ,  $\sigma_{sf}$ , and of the weight contributions  $q_j$  of compounds in the mixture (see Eq.(9)) have been taken into account during the estimation of the accuracy. The standard deviations of the mass density  $\rho$  of the material and of the average cosine  $\mu$  of the scattering angle have been neglected.

## 4. Particular cases.

### 4.1. Absorption cross section of boron.

The isotopic composition of natural boron fluctuates and, therefore, it is not known exactly in an individual case. The microscopic absorption cross sections of the boron isotopes,  $^{10}\text{B}$  and  $^{11}\text{B}$ , are given in nuclear data tables with a high accuracy but their unknown isotopic abundance in a compound of interest can be a source of an extra error. A certain abundance of the isotopes is assumed in data tables and the corresponding microscopic absorption cross section  $\sigma_a^{\text{B}}$  of natural boron is given. For example, MUGHABGHAB *et al.* (1981) "improved" the value given earlier in MUGHABGHAB and GARBER (1973). For boron in boric acid  $\text{H}_3\text{BO}_3$  which is used in routine experiments in our laboratory we have found experimentally the cross section  $\sigma_a^{\text{B}}$ . We had no data on this acid (produced by the former USSR). We have made comparative measurements (WOŹNICKA 1989) of the absorption by CZUBEK'S (1981) method using this acid and a reference  $\text{H}_3\text{BO}_3$  sample (from the Joint Research Centre, Geel, Belgium) for which the isotopic ratio  $^{10}\text{B}/^{11}\text{B}$  was exactly known. The absorption cross section  $\sigma_a^{\text{B}}$  of our natural boron has been calculated from the result obtained for our boric acid after a subtraction of the well defined absorption cross sections of hydrogen and oxygen. The data for boron are collected in Table 1.

**Table 1.** Variation of the absorption cross section of boron.

	$\sigma_a^{\text{B}}$ [b]
MUGHABGHAB and GARBER (1973)	$759 \pm 2$
MUGHABGHAB <i>et al.</i> (1981)	$767 \pm 8$
Boron in our Lab (1989)	$782 \pm 2$

Our program, which calculates the thermal neutron parameters, performs two runs in the case of a presence of boron in a compound: in one run the  $\sigma_a^B$  value given by MUGHABGHAB *et al.* (1981) is used and in the second run the value is used which has been found for boron in our laboratory. Then two corresponding sets of the calculated parameters,  $\langle \Sigma_a \rangle$ ,  $\langle \Sigma_s \rangle$ ,  $\langle \Sigma_{tr} \rangle$ ,  $\langle D \rangle$ ,  $D_0$ , are given as the result.

#### 4.2. Non- $\frac{1}{v}$ absorption cross section.

Calculation of the macroscopic absorption cross section  $\Sigma_a(E)$  for the material containing elements for which the function  $\sigma_a(E)$  deviates from the  $\frac{1}{v}$  dependence requires introducing a special correction. Let use the following notation:

$$\sigma_v(E) = \sigma_a(E) \sim \frac{1}{v} . \quad (49)$$

Thus, according to Eq.(13):

$$\sigma_v = \frac{v_{00}}{v} \sigma_a^{00} , \quad (50)$$

which averaged over the Maxwellian flux distribution is

$$\langle \sigma_v \rangle = v_{00} \sigma_a^{00} \left\langle \frac{1}{v} \right\rangle = \frac{\sqrt{\pi}}{2} \sigma_a^{00} . \quad (51)$$

The Westcott factor,  $g_w$ , shows how much the function  $\sigma_a(v)$  deviates from the  $\frac{1}{v}$  dependence (*e.g.* due to an existence of positive and/or negative energy resonances in the thermal region). The  $g_w$  factor is defined as:

$$g_w = \frac{\langle \sigma_a(v) \rangle}{\langle \sigma_v \rangle} . \quad (52)$$

Thus:

$$\langle \sigma_a(v) \rangle = g_w \langle \sigma_v \rangle = g_w \frac{\sqrt{\pi}}{2} \sigma_a^{00} . \quad (53)$$

Let assume that during the calculation of the energy averaged neutron parameters the deviation of the  $\sigma_a(v)$  from the  $\frac{1}{v}$  dependence is included in the following way. The  $\frac{1}{v}$  dependence is still used but with a changed value of the  $\sigma_a(v_{00}) \neq \sigma_a^{00}$ , namely:

$$\sigma_a(v_{00}) = g_w \sigma_a^{00} \quad (54)$$

and then

$$\sigma_a(v) = g_w \frac{v_{00}}{v} \sigma_a^{00} . \quad (55)$$

While averaging the cross section  $\sigma_a(v)$  over the Maxwellian distribution one obtains:

$$\langle \sigma_a(v) \rangle = g_w \frac{\sqrt{\pi}}{2} \sigma_a^{00} , \quad (56)$$

which reproduces the averaged  $\langle \sigma_a(v) \rangle$  value given in Eq.(53). In this way, the averaged values of quantities which are proportional to  $\sigma_a(v)$  are always correct. However, one has to remember that the true  $\sigma_a(v)$  function is different from that assumed in Eq.(55) and values of other averaged parameters [which are not proportional to  $\sigma_a(v)$ ] are only approximate.

The Westcott factor ought to be included into the calculation of the thermal neutron parameters such as the absorption rate  $\langle v\Sigma_a \rangle$ , the averaged diffusion coefficient  $\langle D \rangle$ , and the diffusion constant  $D_0$  [cf. Eqs (25), (18) and (26)]. The values of these parameters depend the macroscopic absorption cross section of the investigated mixture [Eq.(9)]. In the computing program, for each  $i$ -th element of the mixture the  $\sigma_{ai}^{00}$  or  $g_{wi} \sigma_{ai}^{00}$  values are chosen automatically, depending the  $\frac{1}{v}$  or non- $\frac{1}{v}$  dependence of the absorption cross section  $\sigma_{ai}(v)$ , respectively. The values of the Westcott factor used in the calculation are taken from MUGHABGHAB *et al.* (1981) and included into the program data array.

### 4.3. Scattering cross section of hydrogen.

The scattering cross section for most elements can be regarded as constant or, better, described by the free gas model. But for light nuclei, especially for hydrogen, the energy dependence for the atom of the same element changes depending on the molecular structure

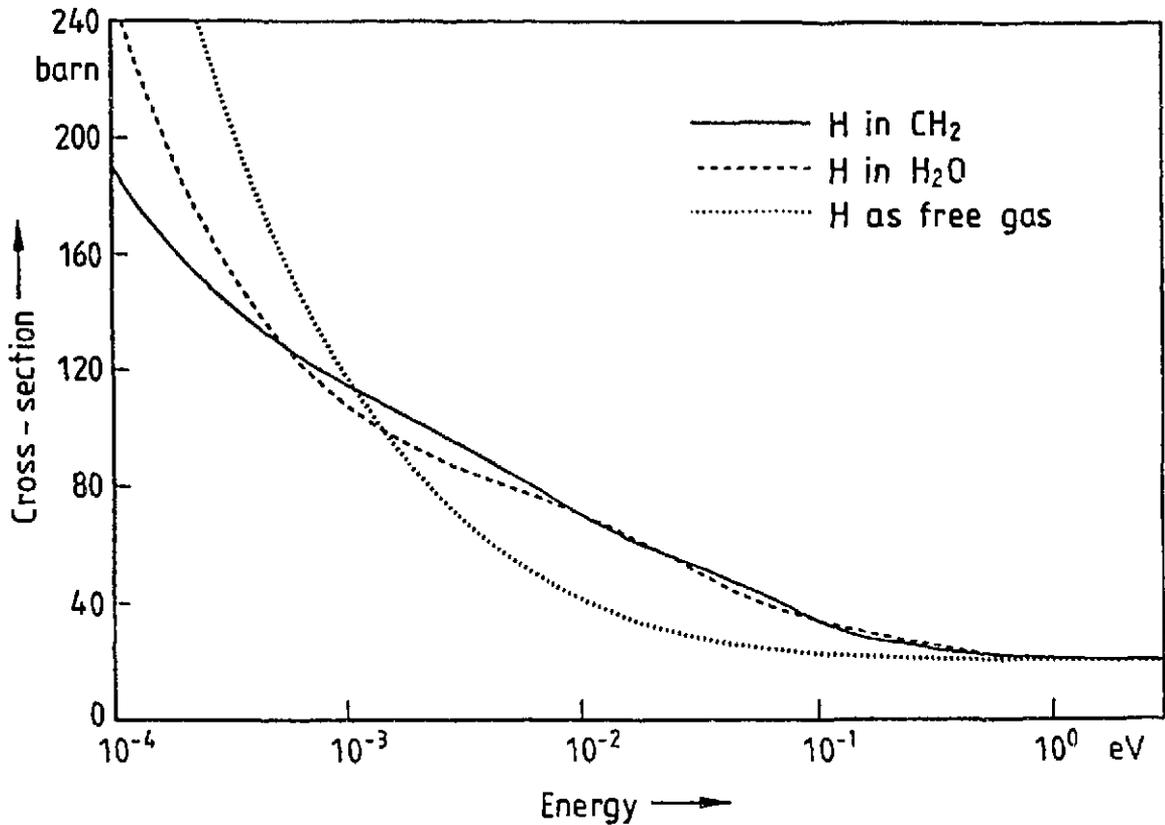


Fig. 1. Energy-dependent scattering cross section  $\sigma_s^H(E)$  of hydrogen gas and of hydrogen bound in water and in polyethylene at 293 K (after HEHN *et al.* 1992).

in which the atom is bound and thus changes from one material to another. An example for three hydrogenous materials is shown in Fig. 1. Formula (9) is still valid for a calculation but the individual energy dependence of the microscopic scattering cross section  $\sigma_{s_i}(E)$  of the  $i$ -th atom in a particular molecule has to be known. Therefore, the energy dependence of the  $\sigma_s^H(E)$  for hydrogen cannot be given by a general relationship valid for various chemical bindings. To solve this problem for hydrogen an idea to apply a certain constant effective value  $\sigma_s^{H\text{eff}}$  of the scattering cross section can be used. The calculation of the effective cross section is based on values of the thermal neutron diffusion parameters of some hydrogenous media reported in last few years. The data of benzene and water are taken from GRANADA *et al.* (1987), of Plexiglass from SIBONA *et al.* (1991), of polyethylene from GRANADA *et al.* (1987), and of diphenyl and Dowtherm-A from FLORIDO *et al.* (1991). Details presented by the authors allow us to use the diffusion constants  $D_0$  quoted in the papers as the reference values. They will be called the true parameters.

We have used the following procedure to obtain the effective scattering cross section of hydrogen  $\sigma_s^{H\text{eff}}$ . A constant cross section has been assumed for hydrogen but being individual for each  $k$ -th compound:

$$\sigma_s^H(E) = \sigma_{sk}^H \quad . \quad (57)$$

Then such a value  $\sigma_{sk}^{H\text{fit}}$  was fitted which inserted into the definition of the diffusion constant  $D_0$  [Eqs (26),(46),(34)] reproduces the true parameter  $D_0$  for the compound under consideration. The average scattering cosine used during the calculation was  $\mu = 0.2$  according to the assumption made for the hydrogenous media in paragraph 3.1. As it was expected the effective constant cross section  $\sigma_{sk}^{H\text{fit}}$  is different for each compound because the true energy dependence of the cross section is different in each case. The results are listed in Table 2. In one case (Dowtherm) only the density-removed parameter  $D_0^*$  has been available which is independent of the material density (cf. Eq.(33d)).

**Table 2.** Fitted individual effective cross sections  $\sigma_s^{H\text{fit}}$ .

Compound	Stoichiometric formula	$\rho$ [g/cm <sup>3</sup> ]	True diffusion parameters (from references)		$\sigma_s^{H\text{fit}}$ [b]
			$D_0$ [cm <sup>2</sup> s <sup>-1</sup> ]	$\langle v\Sigma_a \rangle$ [s <sup>-1</sup> ]	
Benzene	C <sub>6</sub> H <sub>6</sub>	0.879	51 488	3 013	44.30
Diphenyl	C <sub>12</sub> H <sub>10</sub>	1.06	48 962	3 038	44.98
Dowtherm-A	73.5 % C <sub>12</sub> H <sub>10</sub> O 26.5 % C <sub>12</sub> H <sub>10</sub>	–	55 300*	2 859	45.12
Plexiglass	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	1.176	37 360	4 167	44.65
Polyethylene	CH <sub>2</sub>	0.92	27 133	5 821	45.52
Water	H <sub>2</sub> O	0.997 62	36 310	4 885	40.45

\*) the density-removed parameter [g cm<sup>-1</sup> s<sup>-1</sup>]

Finally, a single effective value of the hydrogen cross section  $\sigma_s^{H\text{eff}}$  has been determined as the mean of the individual fitted cross sections  $\sigma_{sk}^{H\text{fit}}$  given in Table 2 and the result is:

$$\sigma_s^{H\text{eff}} = 44.17 \pm 1.90 \text{ b} . \quad (58)$$

A scheme of the idea of using the effective values instead of the energy dependent cross section is shown in Fig. 2.

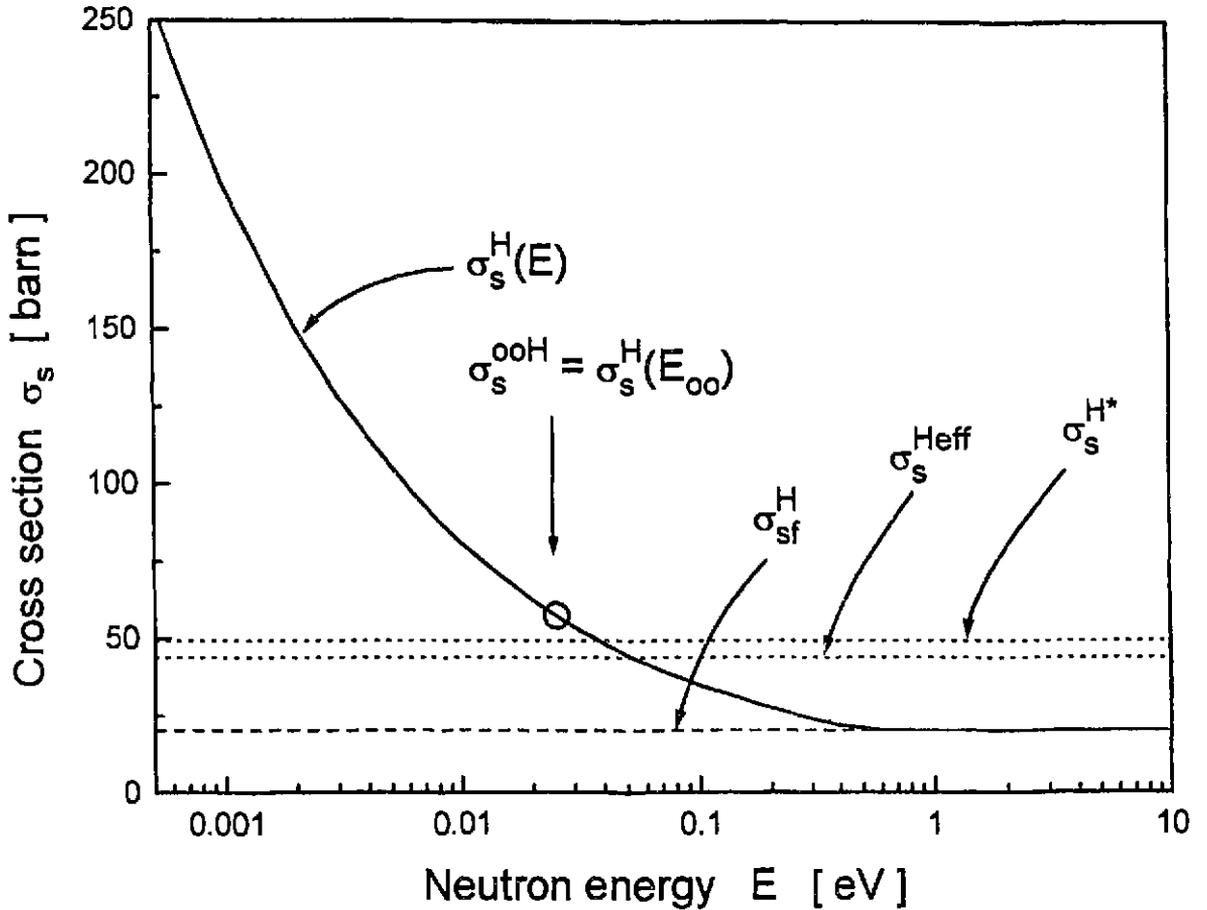


Fig. 2. The energy-dependent  $\sigma_s^H(E)$  and effective ( $\sigma_s^{H\text{eff}}$  and  $\sigma_s^{H*}$ ) and free atom  $\sigma_{sf}^H$  cross sections for hydrogen bound in a molecule.

The energy averaged diffusion coefficient  $\langle D \rangle$  and the diffusion constant  $D_0$  are well approximated while using the effective value  $\sigma_s^{H\text{eff}}$  obtained, Eq.(58). The accuracy of the approximation has been checked and is presented in Table 3. The relative deviations of the estimated  $D_0$  values from the true ones are given:

$$\varepsilon = \frac{D_0(\sigma_s^{H\text{eff}}) - D_0^{\text{true}}}{D_0^{\text{true}}} \quad (59)$$

The deviation  $\varepsilon$  is a measure of a quality of the approximation. The maximum error is observed for water but a special treatment of water is available in CZUBEK'S (1988a) paper which has been prepared especially for geological media with a presence of water. The method presented here is thought to be applied to any hydrogenous material (of an unknown energy dependence of the scattering cross section) and an expected order of errors is visible in Table 3.

**Table 3.** Accuracy of the approximation by using the effective cross section  $\sigma_s^{H\text{eff}}$ .

Compound	$D_0$ [ $\text{cm}^2\text{s}^{-1}$ ]		$\varepsilon$ [%]
	true	using $\sigma_s^{H\text{eff}}$	
Benzene	51 488	51 622	0.26
Diphenyl	48 962	49 748	1.61
Dowtherm-A	55 300*	56 344*	1.89
Plexiglass	37 360	37 732	1.00
Polyethylene	27 133	27 913	2.87
Water	36 310	33 410	-7.99

\*) the density-removed parameter [ $\text{g cm}^{-1} \text{s}^{-1}$ ]

The value  $\sigma_s^{H\text{eff}}$  is accepted as the basic data and is set in our computer program as the 'table' value of the scattering cross section of hydrogen bound in a molecular structure.

However, the effective cross section  $\sigma_s^{H\text{eff}}$  is not fully relevant for an estimation of the averaged cross sections  $\langle \Sigma_s \rangle$  and  $\langle \Sigma_{tr} \rangle$  because they are proportional to the microscopic cross section  $\sigma_s$  while the diffusion constant is inversely proportional. Therefore, the values  $\langle \Sigma_s \rangle$  and  $\langle \Sigma_{tr} \rangle$  would be obtained with a worse accuracy. Unfortunately, these averages were not given in the references and a comparison is not available. The only possibility exists for Plexiglass for which we can calculate the exact averaged macroscopic

scattering cross section  $\langle \Sigma_s^{PLX} \rangle$  using Granada's Synthetic Model (GRANADA 1985, DROZDOWICZ 1995). Then a certain effective cross section of hydrogen  $\sigma_s^{H^*}$  can be fitted (in a similar way as for the diffusion constant) to reproduce the true value  $\langle \Sigma_s^{PLX} \rangle$ . The result is:

$$\sigma_s^{H^*} = 49.13 \text{ b} \quad (60)$$

and a reference to the basic effective value is

$$r^* = \frac{\sigma_s^{H^*}}{\sigma_s^{H \text{ eff}}} = 1.112 \quad (61)$$

One has to remember while using this approximation that the value  $\sigma_s^{H^*}$  is based on the data of only one material.

A relation between the bound hydrogen effective scattering cross sections  $\sigma_s^{H \text{ eff}}$  and  $\sigma_s^{H^*}$  obtained is visible in Fig. 2. The value  $\sigma_s^{H \text{ eff}}$  is used to calculate the energy averaged parameters which are inversely proportional (roughly speaking) to the scattering cross section, *i.e.* the diffusion coefficient and constant,  $\langle D \rangle$  and  $D_0$ , while the value  $\sigma_s^{H^*}$  for the parameters proportional to the scattering cross section, *i.e.* the energy averaged macroscopic scattering and transport cross sections,  $\langle \Sigma_s \rangle$  and  $\langle \Sigma_{tr} \rangle$ .

Another approximation has been made to get an estimate for the value of the hydrogen scattering cross section at the neutron velocity  $v_{00}$ . The method is as follows. For each  $k$ -th compound the value of the cross section of hydrogen  $\sigma_s^{00H}$  has been extracted from the available data. Then the individual ratio:

$$r = \frac{\sigma_s^{00H}}{\sigma_s^{H \text{ fit}}} \quad (62)$$

has been calculated. The results are presented in Table 4. Finally, the cross section at the velocity  $v_{00}$  can be referred to the effective cross section given in Eq.(58) by the relation:

$$\sigma_s^{00H} = \bar{r} \sigma_s^{H \text{ eff}} \quad (63)$$

where  $\bar{r}$  has been found as the mean from the individual ones:

$$\bar{r} = 1.307 \quad (64)$$

**Table 4.** Comparison of the hydrogen cross sections  $\sigma_s^{H \text{ fit}}$  and  $\sigma_s^{00 H}$  in different compounds.

Compound	From references		$\sigma_s^{H \text{ fit}}$	$\frac{\sigma_s^{00 H}}{\sigma_s^{H \text{ fit}}}$
	$\sigma_s^{00}$	$\sigma_s^{00 H}$		
	[b]	[b]		
Benzene	-	61.26#)	44.30	1.38
Diphenyl	-	~62	44.98	1.38
Dowtherm-A	-	56.2	45.12	1.25
Plexiglass	469	54.72	44.65	1.23
Polyethylene	118.4	56.83	45.52	1.25
Water	~113	54.62	40.45	1.35

#) The cross section  $\sigma_s^{00 HC}$  was available from which  $\sigma_s^{00 H} = \sigma_s^{00 HC} - \sigma_s^{00 C}$ .

and the value of this cross section is

$$\sigma_s^{00 H} = 57.73 \text{ b} \quad (65)$$

and can be used during a calculation of the macroscopic cross sections  $\Sigma_s$  and  $\Sigma_{tr}$  at the 'table' neutron velocity  $v_{00}$  for an hydrogenous compound for which an exact energy dependence of the scattering cross section is unknown. An importance to use the effective cross sections and not of the free atom cross section (when the exact energy dependence is unknown) is shown in Table 5 elaborated for Plexiglass. For each neutron parameter  $P$  calculated using a given approximation the relative deviation  $\varepsilon(P)$  from the true value is given:

$$\varepsilon = (P^{Appr} - P^{true}) / P^{true} \quad (66)$$

where the  $P^{true}$  values are calculated using the true energy dependence of the Plexiglass scattering cross section and  $P^{Appr}$  are the values of the parameter obtained within a given approximation. The deviations are of the order of a per cent when the effective hydrogen

**Table 5.** Comparison of the energy-averaged parameters for Plexiglass obtained from different approximations of the hydrogen scattering cross section.

Parameter	Unit	Approximation			
		True <sup>a)</sup> $\sigma_s^H(E)$	Present work	Free gas model ( $\sigma_{sf}^H = 20.49$ b)	
				energy averaging	constant parameters <sup>b)</sup>
$\Sigma_s^{00}$	cm <sup>-1</sup>	3.3167	3.4877	1.3804	1.3804
$\epsilon(\Sigma_s^{00})$	%		+5.2	-58.4	-58.4
$\langle \Sigma_s \rangle$	cm <sup>-1</sup>	3.0008	3.0003	1.3804	1.3804
$\epsilon(\langle \Sigma_s \rangle)$	%		+0.01	-54.0	-54.0
$\langle \Sigma_{tr} \rangle$	cm <sup>-1</sup>	2.4207 <sup>c)</sup>	2.4003 <sup>d)</sup>	1.1043 <sup>d)</sup>	0.5960
$\epsilon(\langle \Sigma_{tr} \rangle)$	%		-0.8	-54.4	-75.4
$\langle D \rangle$	cm	0.1506	0.1520	0.2974	0.5420
$\epsilon(\langle D \rangle)$	%		+0.9	+97.5	+259.9
$D_0$	cm <sup>2</sup> s <sup>-1</sup>	37 352	37 732	73 816	119 240
$\epsilon(D_0)$	%		+1.0	+97.6	+219.2

a) based on SIBONA *et al.* (1991) and on a calculation after DROZDOWICZ (1992)

b)  $\sigma_{si}^{00} = \sigma_{sfi}$

$$\sigma_{tri} = (1 - \mu_i) \sigma_{sfi}$$

$$\mu_i = 2/(3A_i)$$

$$D = 1 / [3(\Sigma_a^{00} + \Sigma_{sf})]$$

$$D_0 = v_{00} D$$

c)  $\mu^{PLX} = \mu(E)$

d)  $\mu^{PLX} = 0.2$

cross sections are used as proposed in the present work. When the hydrogen scattering is approximated by the free atom scattering cross section the macroscopic cross sections,  $\Sigma_s^{00}$ ,  $\langle \Sigma_s \rangle$  and  $\langle \Sigma_{tr} \rangle$ , are underestimated over 50 per cent and the diffusion coefficients  $\langle D \rangle$  and

$D_0$  are overestimated almost 100 per cent. The worst results are obtained when no energy averaging is used (in the column "constant parameters").

## 5. Computer code.

A computer program (named SIGSA) has been written in FORTRAN77. It calculates for a mixture of  $J$  chemical compounds the thermal neutron parameters averaged over the Maxwellian energy spectrum. The program uses an input data array which for all elements contains the atomic masses and thermal neutron microscopic scattering and absorption cross sections with their standard deviations. The data are generally based on MUGHABGHAB *et al.* (1981). The absorption cross section is taken at the neutron velocity  $v_0 = v_{00} = 2200$  m/s and the Westcott factor is also included. The scattering cross section is used of the free atom for all elements except of hydrogen for which the effective cross section  $\sigma_s^{\text{H eff}}$  is applied as defined in the present work. Basing on these values the averaging over the energy distribution is done as described in the previous paragraphs.

The input data for the program require the formulae of all  $J$  chemical compounds together with the weight contents in the mixture. The formulae should be introduced as stoichiometric-like ones. The lower and upper case letters in the symbols of elements have to be rigorously followed and the subscript numbers are used in the main line. The formulae cannot contain parentheses or dots. For example, the formula  $\text{MgCa}(\text{CO}_3)_2$  can be transformed to  $\text{MgCaCO}_3\text{CO}_3$  or  $\text{MgCaC}_2\text{O}_6$ . A formal check of the syntax is included into the program. The program checks also whether the sum of contributions of components is 100 per cent.

Program SIGSA calculates for the mixture the following thermal neutron parameters with their standard deviations:

1. The mass and linear macroscopic cross sections at the neutron velocity  $v_{00} = 2200$  m/s :
  - $\Sigma_a^{00}$  - absorption,
  - $\Sigma_s^{00}$  - scattering,
  - $\Sigma_{tr}^{00}$  - transport.
2. The energy-averaged mass and linear macroscopic cross sections:
  - $\langle \Sigma_a \rangle$  - absorption [from Eqs (5), (9), and (13) or (55)],
  - $\langle \Sigma_s \rangle$  - scattering [from Eqs (5), (9), and (14) or (60)],
  - $\langle \Sigma_{tr} \rangle$  - transport [from Eqs (5), (34), (9), with (35) or (36), and (14) or (60)].
3. The energy averaged diffusion coefficient  $\langle D \rangle$  (cm)
  - [from Eqs (5), (18) with (14) or (58)].

4. Pulsed neutron parameters:

$\langle v \Sigma_a \rangle$  - absorption rate [from Eqs (23), (9), and (13) or (55)],

$D_0$  - diffusion constant ( $\text{cm}^2 \text{s}^{-1}$ ) [from Eqs (26), (18) with (14) or (58)].

5. Microscopic and mass macroscopic absorption and scattering cross sections of individual compounds of the mixture (available on request) at the neutron velocity  $v_{00} = 2200 \text{ m/s}$  [as results from Eq.(11)].

The density  $\rho$  of the material has to be known to calculate all the macroscopic parameters, except the mass cross sections. When the density is unknown the so-called density-removed parameters are calculated by the program as defined in Eqs (33).

An example of the input data file is given in Fig. 3a and the corresponding results are shown in Fig. 3b. In this example the calculated averaged values of the scattering and

```
-----
Ottawa Sand                                     ! Name, max=char*40
2.633                                           ! Density of mixture - write 0 if unknown
14                                              ! Number of compounds
Na2O                                            ! Stoichiometric formula 1, max=char*20
0.0163 0.                                       ! Contents %, error (real numbers)
MgO                                             ! Stoichiometric formula 2, max=char*20
.270 0.                                         ! Contents %, error (real numbers)
Al2O3                                           ! Stoichiometric formula 3, max=char*20
.0251 0.                                         ! Contents %, error (real numbers)
SiO2                                           ! Stoichiometric formula 4, max=char*20
99.5 0.                                         ! Contents %, error (real numbers)
Cl                                              ! Stoichiometric formula 5, max=char*20
.0002 0.                                        ! Contents %, error (real numbers)
K2O
.0072 0.
CaO
.0494 0.
TiO2
.0089 0.
MnO2
.0165 0.
Fe2O3
.107 0.
SrO
.0007 0.
Cd
0. 0.
Sm2O3
.0029 0.
Gd2O3
0. 0.
```

Fig. 3a. Example of the input data file for program SIGSA.

Mixture: Ottawa Sand

---

Composition [weight %]:				
1	Na2O	.016	+/-	.000
2	MgO	.270	+/-	.000
3	Al2O3	.025	+/-	.000
4	SiO2	99.500	+/-	.000
5	Cl	.000	+/-	.000
6	K2O	.007	+/-	.000
7	CaO	.049	+/-	.000
8	TiO2	.009	+/-	.000
9	MnO2	.017	+/-	.000
10	Fe2O3	.107	+/-	.000
11	SrO	.001	+/-	.000
12	Cd	.000	+/-	.000
13	Sm2O3	.003	+/-	.000
14	Gd2O3	.000	+/-	.000
-----				
100.004 %				

Density = 2.633 [g cm<sup>-3</sup>]

---

-----  
Macroscopic Cross Sections

	Mass [cm <sup>2</sup> /g]		Linear [cm <sup>-1</sup> ]	
	Sigma00	<Sigma>	Sigma00	<Sigma>
Absorption	.00233	.00241	.00613	.00636
	.00003	.00003	.00008	.00008
Scattering	.09592	.09592	.25256	.25256
	.00012	.00012	.00032	.00032
Transport	.09229	.09229	.24301	.24301
	.00012	.00012	.00031	.00031

---

Diffusion Parameters

<D> = 1.33694 [cm]  
.00169

<vSigma\_a> = 1578. [s<sup>-1</sup>]  
20.

D0 = 331887. [cm<sup>2</sup> s<sup>-1</sup>]  
421.

---

Notes: The standard deviations are given under the values  
of the parameters.  
The microscopic cross sections are listed in "SIGSA.MIC".

Fig. 3b. Example of results of program SIGSA.

transport cross sections are the same as at the neutron velocity  $v_{00}$  because the mixture contains only such elements for which the constant scattering cross section is a good approximation. Fig. 3c contains the corresponding listing of the microscopic and mass cross sections of the compounds of the mixture.

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Mixture: Ottawa Sand

---

Individual Microscopic and Mass Macroscopic  
Cross Sections ( $v=2200$  m/s)

---

Compound	Absorption		Scattering	
	Microsc. sigma_j	Mass Macrosc. Kj*sigma_j	Microsc. sigma_j	Mass Macrosc. Kj*sigma_j
#j	[b]	[cm <sup>2</sup> g <sup>-1</sup> ]	[b]	[cm <sup>2</sup> g <sup>-1</sup> ]
1	1.06019	.000002	9.81100	.000016
2	.06319	.000003	7.17500	.000289
3	.46257	.000001	14.10980	.000021
4	.17138	.001709	9.56570	.095394
5	33.50000	.000001	15.80000	.000001
6	4.20019	.000002	7.84100	.000004
7	.43019	.000002	6.69100	.000035
8	6.09038	.000004	11.61200	.000008
9	13.30038	.000015	9.72200	.000011
10	5.12057	.000021	33.98300	.000137
11	1.28019	.000000	13.76100	.000001
12	2520.00000	.000000	5.60000	.000000
13	11340.00057	.000568	87.28300	.000004
14	97780.00057	.000000	355.28300	.000000
Mixture	-	.002327	-	.095920

Kj = number of molecules per gram,  
 $Kj = Nj/\rho$  ( Nj - number of molecules per cm<sup>3</sup>; Nj=NA\*qj/Mj,  
rho - mas density g/cm<sup>3</sup> )

Fig. 3c. Example of the listing of the individual microscopic and mass cross sections of the compounds of the mixture (according to the list in Fig. 3b).

An example for a hydrogenous material (Plexiglass) is shown in Fig. 4. In this case the energy-averaged cross sections are significantly different from the values at  $v_{00}$ .

Mixture: Flexiglass

Warning: the hydrogenous medium - approximate results.

---

Composition [weight %]:

1	C5H8O2	100.000	+/-	.000	
		-----			
		100.000	%		

Density = 1.176 [g cm<sup>-3</sup>]

---

Macroscopic Cross Sections

	Mass [cm <sup>2</sup> /g]		Linear [cm <sup>-1</sup> ]		
	Sigma00	<Sigma>	Sigma00	<Sigma>	
Absorption	.01611	.01428	.01895	.01679	
	.00003	.00003	.00004	.00004	
Scattering	2.96574	2.55128	3.48771	3.00031	approx., effective
	.11950	.10167	.14053	.11956	
Transport	2.37259	2.04103	2.79017	2.40025	approx., effective
	.09560	.08133	.11242	.09565	

---

Diffusion Parameters

<D>	=	.15200	[cm]	approximate
		.00595		
<vSigma_a>	=	4169.	[s <sup>-1</sup> ]	
		9.		
D0	=	37732.	[cm <sup>2</sup> s <sup>-1</sup> ]	approximate
		1477.		

---

Notes: The standard deviations are given under the values of the parameters.  
The microscopic cross sections are listed in "SIGSA.MIC".

Fig.4. Example of the result listing for a hydrogenous medium.

If a compound of the mixture contains boron the calculation is performed twice, for two different values of the microscopic absorption cross section of boron: the one with the value given in MUGHABGHAB *et al.* (1981), and the second with the value obtained experimentally in our Lab.

Executable version of program SIGSA for IBM-compatible PCs is available after a contact with "krynicka@bron.ifj.edu.pl".

## List of symbols.

- $A_i$  – gram-atom of the  $i$ -th element
- $D(E)$  – thermal neutron diffusion coefficient, Eq.(18)
- $D_0$  – thermal neutron diffusion constant, Eq.(26)
- $E$  – neutron energy, Eq.(1)
- $E_{00}$  – thermal neutron energy corresponding to the velocity  $v_{00}$ , Eq.(12)
- $g_w$  – Westcott factor, Eq.(52)
- $k_B$  – Boltzmann constant, Eq.(3)
- $m_n$  – neutron mass, Eq.(3)
- $M$  – gram-molecule of the compound, Eq.(8)
- $M_n(v)$  – Maxwellian distribution of the thermal neutron density, Eq.(4)
- $M_\Phi(E)$  – Maxwellian distribution of the thermal neutron flux, Eq.(1)
- $n_i$  – number of atoms of the  $i$ -th element in the stoichiometric formula of the compound, Eq.(7)
- $N$  – volume concentration of nuclei, Eq.(6)
- $N_A$  – Avogadro's number, Eq.(8)
- $q_j$  – weight content of the  $j$ -th compound in the mixture, Eq.(9)
- $r$  – ratio of the  $\sigma_s^{00H}$  to  $\sigma_s^{Hfit}$  for a given compound, (Table 4)
- $r^*$  – ratio of the  $\sigma_s^{H^*}$  to  $\sigma_s^{Heff}$ , Eq.(61)
- $\bar{r}$  – mean of the ratio  $r$ , Eq.(64)
- $T$  – absolute temperature
- $T_{00}$  – temperature corresponding to the thermal neutron velocity  $v_{00}$
- $v_0$  – the most probable velocity of the Maxwellian density distribution, Eq.(3)
- $v_{00}$  – thermal neutron velocity  $v_0 = 2200$  m/sec, Eq.(12)
- $\bar{v}$  – velocity averaged over the Maxwellian density distribution, Eqs(28), (30)
- $\left\langle \frac{1}{v} \right\rangle$  –  $\frac{1}{v}$  averaged over the Maxwellian flux distribution, Eq.(29)
- $\langle v\Sigma_a \rangle$  – absorption rate, Eq.(23)
- $\langle x \rangle$  – magnitude  $x(E)$  averaged over the Maxwellian flux distribution, *i.e.* over the thermal neutron energy spectrum, Eq.(5)
- $X^*$  – density-removed parameter  $X$ , Eqs(33)

- $X^{00}, X_{00}$  – magnitude  $X$  corresponding to the thermal neutron velocity  $v_{00}$   
 $\mu(E)$  – average cosine of the scattering angle as a function of energy, Eq.(16)  
 $\rho(T)$  – bulk density of the material at temperature  $T$   
 $\sigma(E)$  – energy-dependent microscopic cross section  
 $\sigma(X)$  – standard deviation of the parameter  $X$ , Eq.(47)  
 $\sigma_a^0$  – microscopic absorption cross section at the thermal neutron velocity  $v_0$ , Eq.(12)  
 $\sigma_a^{00}$  – microscopic absorption cross section at the thermal neutron velocity  $v_{00}$ , Eq.(12)  
 $\sigma_a^B$  – microscopic absorption cross section of natural boron  
 $\sigma_a(E)$  – thermal neutron energy-dependent microscopic absorption cross section, Eq.(13)  
 $\sigma_s(E)$  – thermal neutron energy-dependent scattering cross section  
 $\sigma_{sf}$  – thermal neutron scattering cross section for the free atom  
 $\sigma_s^H(E)$  – thermal neutron energy-dependent scattering cross section of hydrogen  
 $\sigma_s^{00H}$  – thermal neutron scattering cross section of hydrogen at the velocity  $v_{00}$   
 $\sigma_s^{H\text{eff}}$  – thermal neutron effective scattering cross section of hydrogen bound in molecules, relevant to  $D_0$  and  $\langle D \rangle$ , Eq.(58)  
 $\sigma_s^{H\text{fit}}$  – individual effective scattering cross section of hydrogen for a given compound (Table 2)  
 $\sigma_s^{H^*}$  – effective scattering cross section of hydrogen, Eq.(60), relevant to  $\langle \Sigma_s \rangle$  and  $\langle \Sigma_{tr} \rangle$   
 $\sigma_{tr}(E)$  – thermal neutron energy-dependent microscopic transport cross section, Eq.(34)  
 $\sigma_v$  – thermal neutron microscopic absorption cross section subject to the  $\frac{1}{v}$  law, Eq.(50)  
 $\Sigma(E)$  – energy-dependent linear macroscopic cross sections, Eq.(6)  
 $\Sigma^M(E)$  – energy-dependent mass macroscopic cross section, Eq.(11)  
 $\Sigma_a(E)$  – energy-dependent macroscopic absorption cross section, Eq.(24)  
 $\Sigma_s(E)$  – energy-dependent macroscopic scattering cross section, Eq.(18)  
 $\Sigma_{tr}(E)$  – energy-dependent macroscopic transport cross section, Eq.(15)  
 $\tau$  – thermal neutron lifetime, Eq.(22)

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