The Henryk Niewodniczański
INSTITUTE OF NUCLEAR PHYSICS
Polish Academy of Sciences
ul. Radzikowskiego 152, 31-342 Kraków, Poland.

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Influence of the water content in rock on the thermal neutron diffusion and diffusion cooling coefficients (by Monte Carlo simulations). II: – Quartz

K. Drozdowicz, E. Krynicka, and J. Dąbrowska

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Abstract

The dependence of the thermal neutron diffusion parameters on the water content w in quartz, SiO_2, has been studied by means of Monte Carlo simulations of the pulsed neutron experiments for a number of series of samples. The density-removed diffusion cooling coefficient C^M varies hyperbolically between 39 400 000 and 4940 $cm^4s^{-1}(g/cm^3)^3$ at the water content in the full range $0 \leq w \leq .1$. The obtained function $C^M(w)$ is compared with the analogous dependence for moisturized dolomite.

1. Introduction

Macroscopic parameters of the thermal neutron diffusion in a material depend on the scattering properties of the contributing substances. The diffusion coefficient, D, or the diffusion constant, D_0, is roughly inversely proportional to the macroscopic total scattering cross-section, Σ_s. The diffusion cooling coefficient, C (with the correction, F), depends on Σ_s as well as on the scattering kernel (*i.e.* the differential scattering cross-section, $\Sigma_s(E' \rightarrow E)$, where E' and E are the thermal neutron energies before and after the collision). The relevant definitions, in which also the influence of the thermal neutron energy distribution is taken into account, can be found *e.g.* in [1] and [2]. A calculation of the diffusion cooling coefficient is always difficult (cf. [3], [4], [5]) and results for a wet rock material become uncertain. In this case, not only the values of the scattering cross-section, Σ_s, of the rock and of water are very different but also the character of the energy dependences, $\Sigma_s(E')$ and $\Sigma_s(E' \rightarrow E)$, in the two media is entirely dissimilar. Therefore, even a small change of the water content in a rock material results in a very significant change of the value of the diffusion cooling coefficient of the composed material.

An experimental procedure to determine the thermal neutron diffusion parameters for such complex media is usually most adequate. A pulsed neutron experiment (the so-called variable geometric buckling experiment) is then used. It is based on measurements of the time decay of the thermal neutron flux (after irradiation with the neutron burst) in a series of samples of the same material of varying size. The method is known in the experimental neutron physics, *e.g.* [6]. In the case of a rock material, some problem is created to keep a constant bulk density and homogeneity of samples. An additional serious technical problem appears when the experimental rock material has to have the water content precisely defined and repeatable in consecutive samples. The present-day computer techniques offer a possibility to simulate such experiments using Monte Carlo simulations of the neutron transport in the matter.

An influence of the water content on the thermal neutron diffusion parameters for one of the basic rock constituents, dolomite – $CaMg(CO_3)_2$, was investigated [7] with the Monte Carlo simulations of the variable buckling experiment. As said there, the dependences, which were found, cannot be treated as universal because the scattering properties of different elements are individual and usually very different. Here, we perform a study for another basic rock mineral, quartz – SiO_2. The idea of the simulated series of the experiments was presented in detail in [7], [8], [9]. We remind here only the basic relationship necessary for interpretation of the experiments:

$$\lambda = \langle v\Sigma_a\rangle + D_0 B^2 - C B^4 + F B^6 - \dots \ , \qquad (1)$$

where λ is the decay constant of the fundamental mode of the time distribution of the thermal neutron pulsed flux, v is the thermal neutron speed, Σ_a is the macroscopic absorption cross-section, D_0 is the diffusion constant, C is the diffusion cooling coefficient, F is a correction term, and B^2 is the geometric buckling. It is defined [6] by the shape and size of the sample (including the extrapolation length) and for basic geometries is expressed by simple formulae [10]. Here, the spherical geometry of the experiment is kept and the buckling B^2 is defined as in [9] with a comment on the extrapolation length given in [7].

A fit of the function $\lambda(B^2)$ to the 'experimental' data λ_i obtained for different samples (different B_i^2) at the given water content, w, determines the values of the thermal neutron diffusion parameters, D_0, C, F. The absorption rate, $\langle v\Sigma_a\rangle$, can be calculated with a high precision (cf. [1], [6]) and set into Eq.(1) as the known constant. A repetition of the simulations at the varying water content allows us to find the respective functions, $D_0 = D_0(w)$, $C = C(w)$, and $F = F(w)$.

2. Thermal neutron diffusion parameters of the contributing pure media

In the thermal neutron energy region (about 10^{-3} to 1 eV) the microscopic scattering cross-sections σ_s of quartz and of water differ not only in their values but also in the type of the energy dependence:

$$\text{quartz, } SiO_2 \qquad \sigma_s(E) \approx const. = \sigma_{sf}, \qquad \mu(E) = const, \qquad (2a)$$

$$\text{water, } H_2O \qquad \sigma_s(E) = f_s(E), \qquad \mu(E) = f_\mu(E), \qquad (2b)$$

where μ is the average cosine of the scattering angle, and σ_{sf} is the microscopic scattering cross-section of the molecule built of atoms treated as free. The relevant macroscopic cross--sections are then defined by

$$\left.\begin{array}{l}\Sigma_{\mathrm{s\,f}} = \Sigma_{\mathrm{s}}(v_0) = 0.2541\,\mathrm{cm}^{-1}, \\ \mu = 0.038\end{array}\right\} \qquad \text{for quartz } (\rho = 2.65 \text{ g/cm}^3) \tag{3a}$$

and

$$\left.\begin{array}{l}\Sigma_{\mathrm{s\,f}} = 1.4921 \ \mathrm{cm}^{-1}, \\ \Sigma_{\mathrm{s}}(v_0) \approx 3.98 \ \mathrm{cm}^{-1}, \\ \langle \mu(E) \rangle \approx 0.2\end{array}\right\} \qquad \text{for water } (\rho \approx 1 \text{ g/cm}^3)\,. \tag{3b}$$

The data in Eqs (3) are based on the microscopic cross-sections from [11], and v_0 = 2200 m/s is the most probable thermal neutron velocity, corresponding to the energy $E \approx 0.0253$ eV.

Due to the characteristics summarized in Eqs (2) and (3), the thermal neutron energy-averaged diffusion parameters, D_0, C, F, of the two media are strongly different. They were determined [7], [9] with the same Monte Carlo simulation method as mentioned above and are here quoted in Tables 1a and 2a. Cases marked as (i) contain results of a more accurate (on the order of B^6) fit of Eq.(1). Results given in Cases (ii) correspond to a fit of Eq.(1) with the accuracy of $O(B^4)$. An influence of the neglected correction F is then visible as a change of values of the parameters D_0 and C. They are sometimes helpful in such theoretical consideration of the neutron transport in which the correction F is not present explicitly.

Tables 1b and 2b contain the so-called density-removed equivalents of the thermal neutron pulsed parameters:

$$\langle v\Sigma_a \rangle^{\mathrm{M}} = \langle v\Sigma_a \rangle\, \rho^{-1}\,, \qquad D_0{}^{\mathrm{M}} = \rho\, D_0, \qquad C^{\mathrm{M}} = \rho^3\, C, \qquad F^{\mathrm{M}} = \rho^5\, F\,. \tag{4}$$

Formulae (4) were obtained on the basis of theoretical definitions of the thermal neutron absorption-diffusion macroscopic parameters [1], [2], [6], [12]. More information on a reason for determination the density-removed parameters can be found in [7], [9], [12], [13].

SiO_2

Table 1a. Thermal neutron diffusion parameters of quartz (ρ = 2.65 g/cm^3).

Case	$\langle v\Sigma_a \rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	1001 ± 18	308 500 ± 2 400	2 117 000 ± 73 000	7 060 000 ± 530 000
(ii)		271 000 ± 3 700	1 094 000 ± 44 000	——

Table 1b. Density-removed thermal neutron parameters of quartz.

Case	$\langle v\Sigma_a\rangle^M$ [$s^{-1}/(g/cm^3)$]	D_0^M [$cm^2s^{-1}\,(g/cm^3)$]	C^M [$cm^4s^{-1}\,(g/cm^3)^3$]	F^M [$cm^6s^{-1}\,(g/cm^3)^5$]
(i)	378 ± 7	817 500 ± 6 400	39 400 000 ± 1 360 000	922 000 000 ± 68 000 000
(ii)		718 100 ± 9 800	20 350 000 ± 830 000	——

H_2O

Table 2a. Thermal neutron diffusion parameters of water at 20 °C ($\rho = 0.99762$ g/cm^3).

Case	$\langle v\Sigma_a\rangle$ [s^{-1}]	D_0 [cm^2s^{-1}]	C [cm^4s^{-1}]	F [cm^6s^{-1}]
(i)	4882 ± 10	35 450 ± 150	4970 ± 580	1530 ± 520
(ii)		35 064 ± 89	3340 ± 130	——

Table 2b. Density-removed thermal neutron parameters of water.

Case	$\langle v\Sigma_a\rangle^M$ [$s^{-1}/(g/cm^3)$]	D_0^M [$cm^2s^{-1}\,(g/cm^3)$]	C^M [$cm^4s^{-1}\,(g/cm^3)^3$]	F^M [$cm^6s^{-1}\,(g/cm^3)^5$]
(i)	4894 ± 10	35 360 ± 150	4940 ± 570	1510 ± 510
(ii)		34 981 ± 89	3320 ± 130	——

3. Determination of the thermal neutron diffusion parameters for quartz containing water

The variable buckling experiment has been simulated at various water contents in quartz samples, in the same way as described in [7]. The thermal neutron transport parameters, D_0, C, F, have been determined in each case. The thermal neutron absorption rate, $\langle v\Sigma_a\rangle$, can be calculated exactly from the elemental composition and the microscopic absorption cross--sections of the contributing elements, and has been always used in the fitting procedure as the known constant. The results of the individual simulated series of experiments (*i.e.* the decay constants λ_i and the neutron parameters obtained finally) are collected below. The same nomenclature as in [7] is kept here:

Moisturized quartz – material which contains quartz, SiO_2, and an amount of water,

Water content – mass contribution of water in the moisturized material, *i.e.* the ratio of the mass of water to the mass of quartz+water, given as
w – weight fraction, or as
p – weight per cent.

The experiments have been simulated for the water contents equal to 1, 2, 4, 6, 8, 10, and 20 per cent.

3.1. Moisturized quartz, $p = 1$ %

The material density is $\rho = 2.633$ g/cm^3. The thermal neutron decay constants λ_i obtained from the simulations for individual spheres are listed in Table 3 (where R_g is the geometric radius of the sphere, and $\sigma(\lambda)$ is the standard deviation of the λ value determined). The resulting plot $\lambda = \lambda(B^2)$ is shown in Fig. 1. The corresponding thermal neutron diffusion parameters from the fits (i) and (ii), defined in paragraph 2, are collected in Table 4a. The related density-removed parameters are given in Table 4b.

The same scheme of presentation of the results is used for all following simulations of the pulsed thermal neutron flux at the varying water content in quartz.

Table 3. Decay constants λ obtained from the simulated experiment for quartz with the 1 % water content.

R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]	R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]	R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]
5.2	27 267 150	6.5	22 633 88	10.0	14 336 52
5.5	26 153 123	7.0	21 195 199	13.0	10 406 45
6.0	24 134 104	8.0	18 388 31	20.0	5 865 18

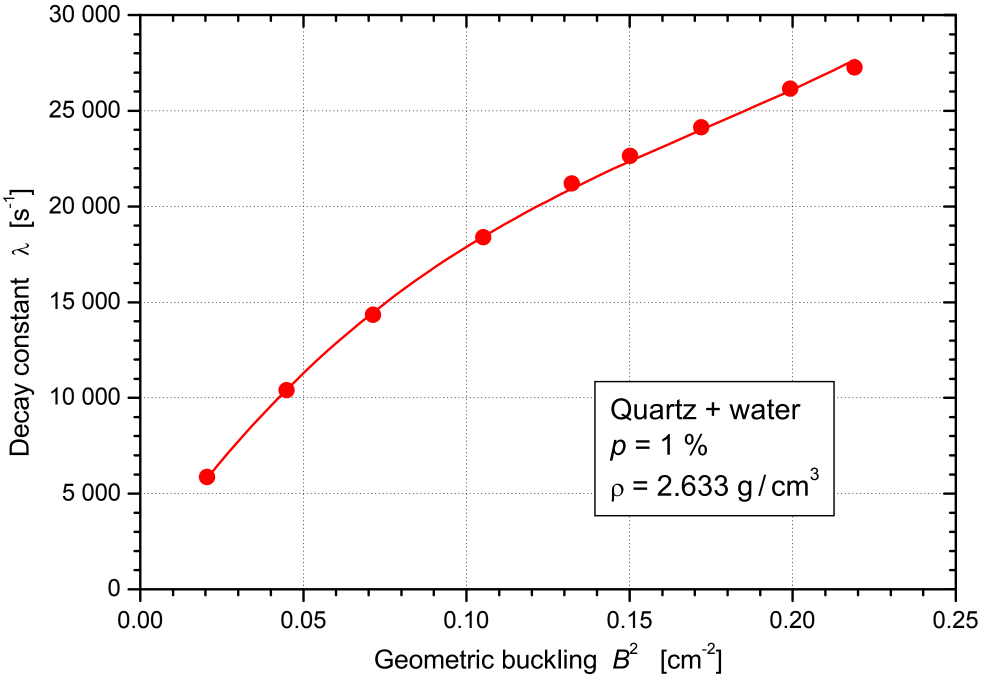

Fig. 1. Results of the simulations of the variable buckling experiment for quartz with the 1 % water content.

Table 4a. Thermal neutron diffusion parameters determined for quartz with the 1 % water content ($\rho = 2.633$ g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a\rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	5.2 ÷ 20	0.021 ÷ 0.219	1114 ± 17	249 000 ± 2 400	1 004 000 ± 39 000	1 920 000 ±150 000
(ii)		0.022 ÷ 0.229		214 700 ± 6 600	477 000 ± 46 000	——

Table 4b. Density-removed thermal neutron parameters of quartz with the 1 % water content.

Case	$\langle v\Sigma_a\rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	423 ± 6	655 500 ± 6 400	18 320 000 ± 720 000	243 000 000 ± 19 000 000
(ii)		565 000 ± 17 000	8 700 000 ± 840 000	——

3.2. Moisturized quartz, *p* = 2 %

The material density is $\rho = 2.617$ g/cm^3.

Table 5. Decay constants λ obtained from the simulated experiment for quatrz with the 2 % water content.

R_g [cm]	λ σ(λ) [s^{-1}]
4.5	32 635 153
4.7	31 454 104
5.0	29 805 122
5.5	27 470 85
6.0	24 990 103
6.5	23 014 86
7.0	21 164 36
8.0	18 183 35
10.0	13 833 21
13.0	9 792 18
20.0	5 436 10

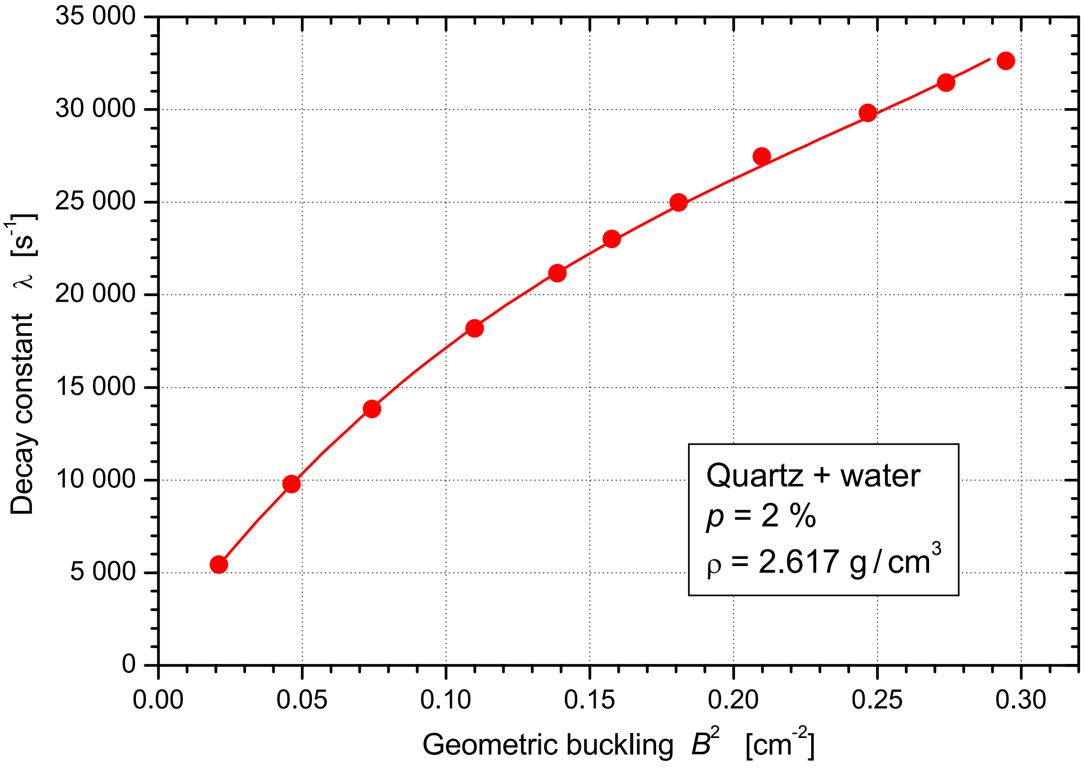

Fig. 2. Results of the simulations of the variable buckling experiment for quartz with the 2 % water content.

Table 6a. Thermal neutron diffusion parameters determined for quartz with the 2 % water content ($\rho = 2.617$ g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a \rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.021 ÷ 0.295	1225 ± 17	210 100 ± 1 500	593 000 ± 21 000	840 000 ± 64 000
(ii)		0.021 ÷ 0.304		190 200 ± 3 800	313 000 ± 23 000	——

Table 6b. Density-removed thermal neutron parameters of quartz with the 2 % water content.

Case	$\langle v\Sigma_a \rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	468 ± 6	549 700 ± 3 900	10 620 000 ± 380 000	103 100 000 ± 7 900 000
(ii)		498 000 ± 10 000	5 600 000 ± 400 000	——

3.3. Moisturized quartz, *p* = 4 %

The material density is $\rho = 2.584$ g/cm^3.

Table 7. Decay constants λ obtained from the simulated experiment for quartz with the 4 % water content.

R_g [cm]	λ σ(λ) [s^{-1}]	R_g [cm]	λ σ(λ) [s^{-1}]	R_g [cm]	λ σ(λ) [s^{-1}]
4.5	33 888 96	6.5	22 231 69	13.0	8 715 17
5.0	30 189 164	7.0	20 206 23	20.0	4 874 13
5.5	27 089 62	8.0	16 996 21		
6.0	24 421 51	10.0	12 570 27		

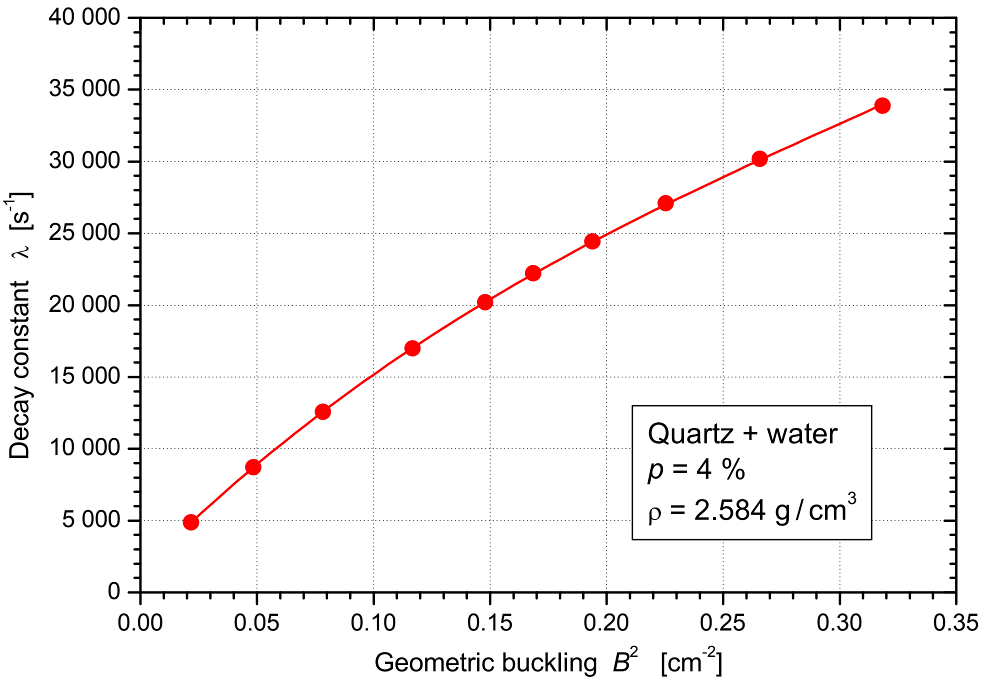

Fig. 3. Results of the simulations of the variable buckling experiment for quartz with the 4 % water content.

Table 8a. Thermal neutron diffusion parameters determined for quartz with the 4 % water content (ρ = 2.584 g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a \rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.022 ÷ 0.318	1443 ± 16	163 210 ± 450	292 400 ± 5 200	316 000 ± 14 000
(ii)		0.022 ÷ 0.325		152 700 ± 2 000	175 000 ± 11 000	——

Table 8b. Density-removed thermal neutron parameters of quartz with the 4 % water content.

Case	$\langle v\Sigma_a \rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	558 ± 6	421 700 ± 1 200	5 045 000 ± 90 000	36 400 000 ± 1 600 000
(ii)		394 500 ± 5 100	3 030 000 ± 190 000	——

3.4. Moisturized quartz, *p* = 6 %

The material density is $\rho = 2.551$ g/cm^3.

Table 9. Decay constants λ obtained from the simulated experiment for quartz with the 6 % water content.

R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]
4.5	33 269 134
5.0	29 206 71
5.5	25 938 56
6.0	23 211 48
6.5	20 876 45
7.0	18 870 27
8.0	15 691 19
10.0	11 484 16
13.0	7 949 12
20.0	4 544 12

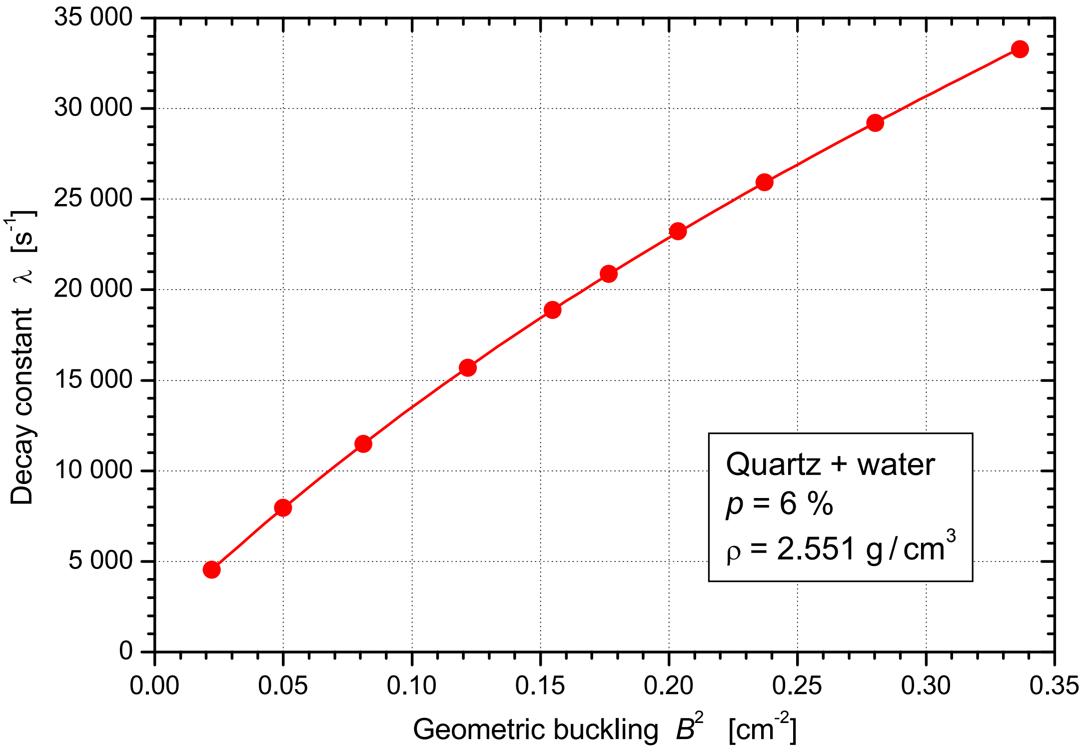

Fig. 4. Results of the simulations of the variable buckling experiment for quartz with the 6 % water content.

Table 10a. Thermal neutron diffusion parameters determined for quartz with the 6 % water content ($\rho = 2.551$ g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a \rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.022 ÷ 0.337	1655 ± 16	133 890 ± 240	169 500 ± 3 000	152 500 ± 8 300
(ii)		0.022 ÷ 0.340		129 550 ± 870	116 400 ± 5 000	——

Table 10b. Density-removed thermal neutron parameters of quartz with the 6 % water content.

Case	$\langle v\Sigma_a \rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	649 ± 6	341 550 ± 610	2 814 000 ± 50 000	16 470 000 ± 900 000
(ii)		330 500 ± 2 200	1 933 000 ± 83 000	——

3.5. Moisturized quartz, p = 8 %

The material density is $\rho = 2.518$ g/cm^3.

Table 11. Decay constants λ obtained from the simulated experiment for quartz with the 8 % water content.

R_g [cm]	λ σ(λ) [s^{-1}]	R_g [cm]	λ σ(λ) [s^{-1}]	R_g [cm]	λ σ(λ) [s^{-1}]
4.5	31 978 35	6.5	19 573 19	13.0	7 428 26
5.0	27 900 32	7.0	17 654 30	20.0	4 377 16
5.5	24 628 48	8.0	14 609 16		
6.0	21 870 38	10.0	10 641 13		

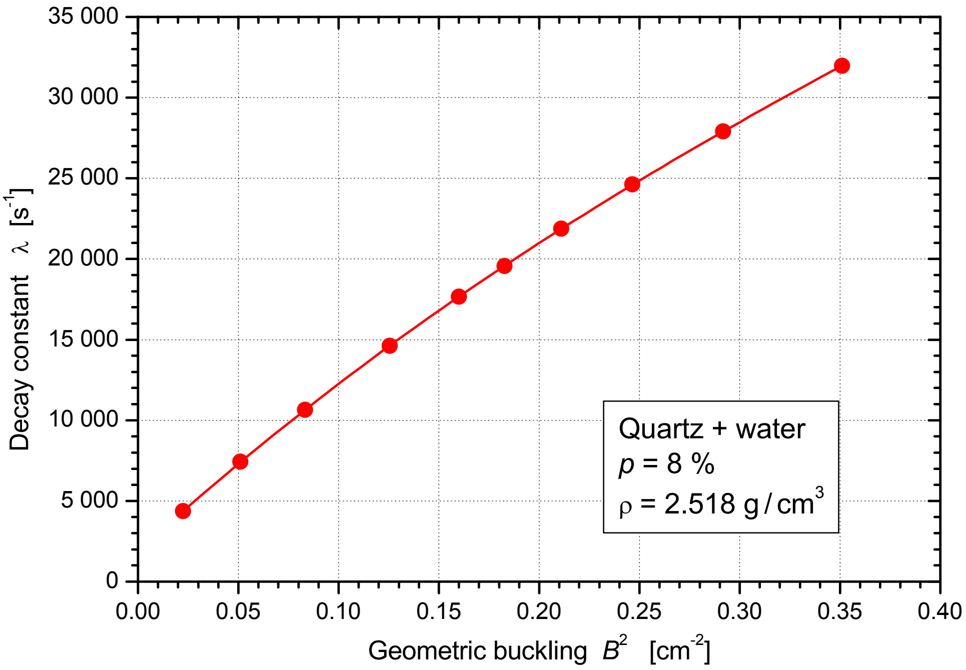

Fig. 5. Results of the simulations of the variable buckling experiment for quartz with the 8 % water content.

Table 12a. Thermal neutron diffusion parameters determined for quartz with the 8 % water content (ρ = 2.518 g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a \rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.023 ÷ 0.351	1861 ± 15	113780 ± 170	105 600 ± 1 700	73 900 ± 3 700
(ii)		0.023 ÷ 0.354		110 120 ± 540	72 300 ± 2 200	——

Table 12b. Density-removed thermal neutron parameters of quartz with the 8 % water content.

Case	$\langle v\Sigma_a \rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	739 ± 6	286 490 ± 430	1 686 000 ± 27 000	7 480 000 ± 370 000
(ii)		277 300 ± 1 300	1 154000 ± 35 000	——

3.6. Moisturized quartz, p = 10 %

The material density is $\rho = 2.485$ g/cm^{-3}.

Table 13. Decay constants λ obtained from the simulated experiment for quartz with the 10 % water content.

R_g [cm]	λ σ(λ) [s^{-1}]
4.5	30 633 50
5.0	26 575 45
5.5	23 330 45
6.0	20 664 43
6.5	18 444 27
7.0	16 588 21
8.0	13 719 22
10.0	10 023 26
13.0	7 039 18
20.0	4 290 16

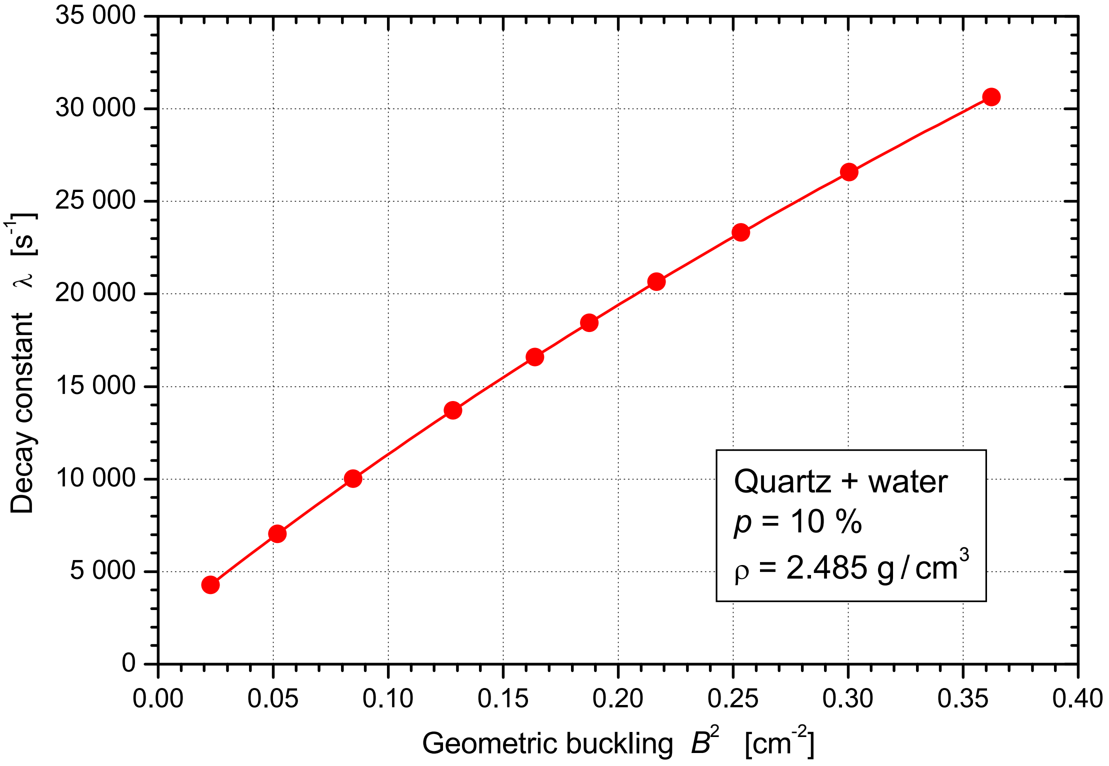

Fig. 6. Results of the simulations of the variable buckling experiment for quartz with the 10 % water content.

Table 14a. Thermal neutron diffusion parameters determined for quartz with the 10 % water content ($\rho = 2.485$ g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a\rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.023 ÷ 0.362	2061 ± 15	99 730 ± 150	74 600 ± 1 400	47 000 ± 2 900
(ii)		0.023 ÷ 0.364		97 280 ± 390	53 000 ± 1 600	——

Table 14b. Density-removed thermal neutron parameters of quartz with the 10 % water content.

Case	$\langle v\Sigma_a\rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	829 ± 6	247 820 ± 360	1 144 000 ± 21 000	4 450 000 ± 270 000
(ii)		241 740 ± 960	814 000 ± 25 000	——

3.7. Moisturized quartz, *p* = 20 %

The material density is $\rho = 2.320$ g/cm^3.

Table 15. Decay constants λ obtained from the simulated experiment for quartz with the 20 % water content.

R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]	R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]	R_g [cm]	λ $\sigma(\lambda)$ [s^{-1}]
4.5	25 353 60	6.5	14 929 14	13.0	6 336 18
5.0	21 764 33	7.0	13 480 24	20.0	4 430 12
5.5	18 942 23	8.0	11 238 20		
6.0	16 728 22	10.0	8 471 25		

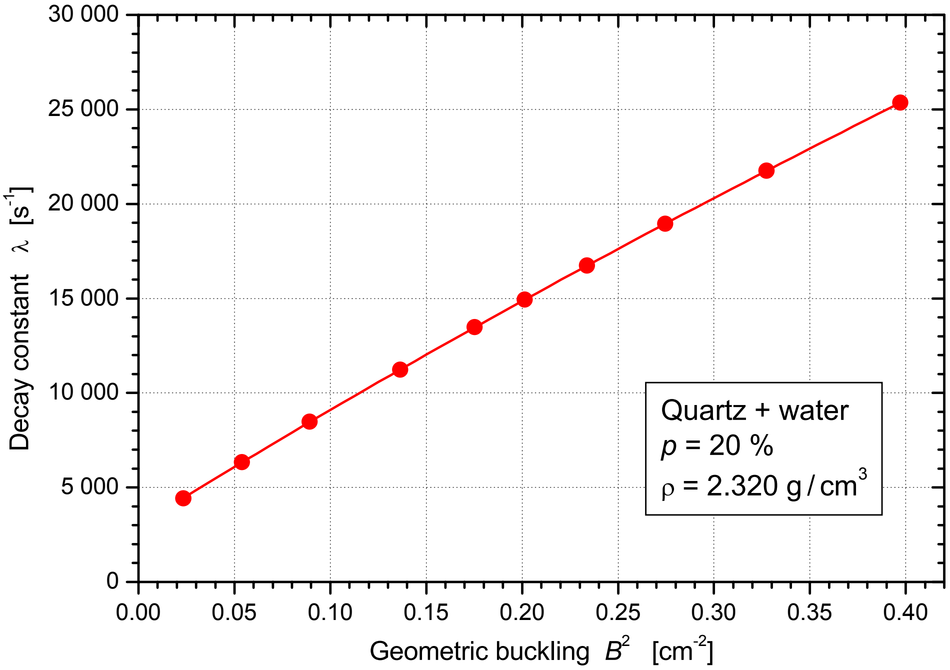

Fig. 7. Results of the simulations of the variable buckling experiment for quartz with the 20 % water content.

Table 16a. Thermal neutron diffusion parameters determined for quartz with the 20 % water content ($\rho = 2.320$ g/cm^3).

Case	Range of R_g [cm]	Range of B^2 [cm^{-2}]	Fixed	Fitted		
			$\langle v\Sigma_a\rangle$ [s^{-1}]	D_0 [cm^{2}s^{-1}]	C [cm^{4}s^{-1}]	F [cm^{6}s^{-1}]
(i)	4.5 ÷ 20	0.023 ÷ 0.397	2972 ± 13	63 360 ± 170	21 600 ± 1 400	10 000 ± 2 700
(ii)		0.023 ÷ 0.398		62 770 ± 120	16 820 ± 480	——

Table 16b. Density-removed thermal neutron parameters of quartz with the 20 % water content.

Case	$\langle v\Sigma_a\rangle^M$ [s^{-1}/(g/cm^3)]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
(i)	1281 ± 6	146 990 ± 390	270 000 ± 17 000	670 000 ± 180 000
(ii)		145 620 ± 280	210 000 ± 6 000	——

4. Dependence of the thermal neutron diffusion coefficients on the water content in quartz

4.1. The diffusion constant D_0 and the diffusion coefficient D

A dependence of the thermal neutron diffusion constant on the water content in quartz, $D_0(w)$, obtained from the simulations performed, is shown in Table 17 and in Fig. 8. The corresponding values of the diffusion coefficient, D, can be found from the relation:

$$\langle D(E)\rangle(w) = \left\langle \frac{1}{v} \right\rangle D_0(w) = \frac{\sqrt{\pi}}{2 v_0} D_0(w) \ . \tag{5}$$

The diffusion constants D_{0C} have been independently calculated from an approximate theoretical formula for homogeneous mixtures of the hydrogenous and non-hydrogenous components [2], [14]. The data in Table 17 and the plot in Fig. 8 show that values of the diffusion constant obtained from the simulations, D_0, and from the approximate calculation, D_{0C}, are very close.

Table 17. Dependence of the fitted, D_0, and calculated, D_{0C}, diffusion constants of moisturized quartz on the water content.

w	ρ [g/cm^3]	D_0 [cm^{2}s^{-1}]	D_{0C} [cm^{2}s^{-1}]
0.00	2.65	308 500 ± 2 400	~ 333 030 ± 430
0.01	2.633	249 000 ± 2 400	~ 267 100 ± 2 300
0.02	2.617	210 100 ± 1 500	~ 223 400 ± 3 200
0.04	2.584	163 210 ± 450	~ 169 200 ± 3 600
0.06	2.551	133 890 ± 240	~ 136 800 ± 3 500
0.08	2.518	113 780 ± 170	~ 115 400 ± 3 300
0.10	2.485	99 730 ± 150	~ 100 100 ± 3 100
0.20	2.320	63 360 ± 170	~ 62 400 ± 2 200
1.00	0.99762	35 450 ± 150	~ 33 400 ± 1 400

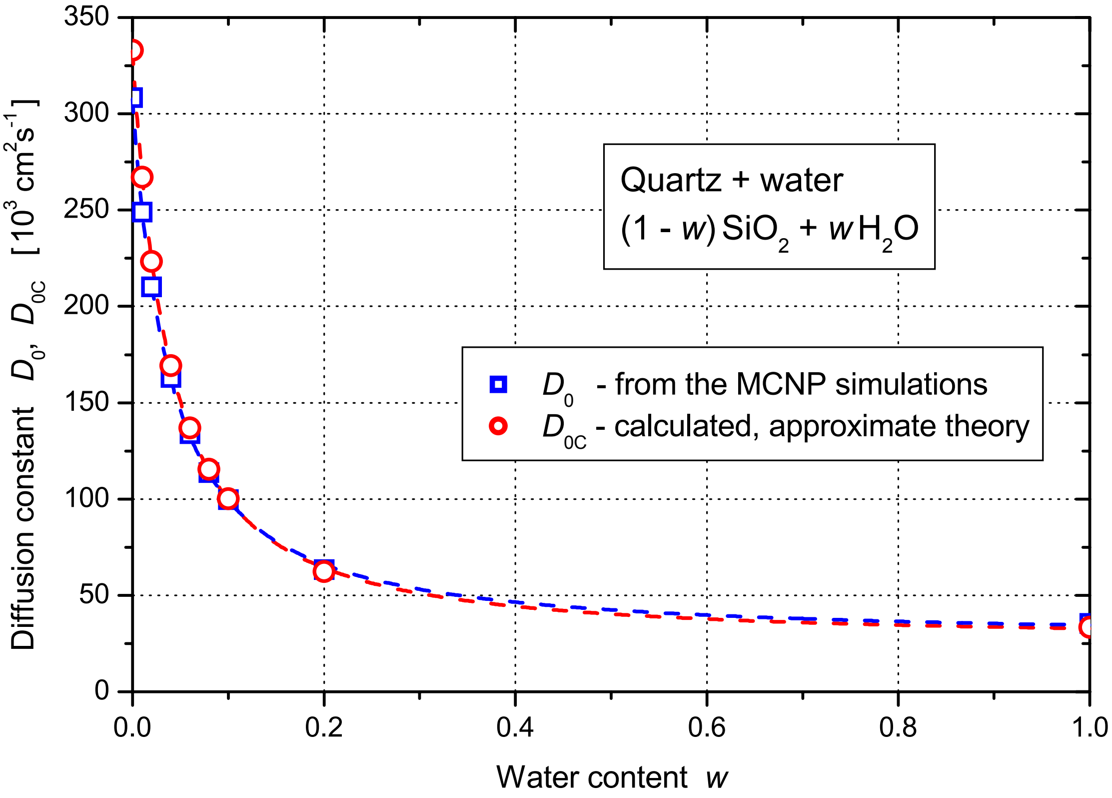

Fig. 8. Thermal neutron diffusion constant of moisturized quartz as a function of the water content.

4.1. The diffusion cooling coefficient C with its correction F

The dependence of the density-removed thermal neutron diffusion parameters, D_0^M, C^M, F^M, on water content w, obtained from the performed Monte Carlo simulations, is presented in Table 18.

The density-removed diffusion cooling coefficient C^M as a function of the water content in moisturized quartz is plotted in Fig. 9.

Table 18. Dependence of the density-removed thermal neutron diffusion parameters of moisturized quartz on the water content.

w	ρ [g/cm^3]	D_0^M [cm^{2}s^{-1} (g/cm^3)]	C^M [cm^{4}s^{-1} (g/cm^3)^3]	F^M [cm^{6}s^{-1} (g/cm^3)^5]
0.00	2.65	817 500 ± 6 400	39 400 000 ± 1 360 000	922 000 000 ± 68 000 000
0.01	2.633	655 500 ± 6 400	18 320 000 ± 720 000	243 000 000 ± 19 000 000
0.02	2.617	549 700 ± 3 900	10 620 000 ± 380 000	103 100 000 ± 7 900 000
0.04	2.584	421 700 ± 1 200	5 045 000 ± 90 000	36 400 000 ± 1 600 000
0.06	2.551	341 550 ± 610	2 814 000 ± 50 000	16 470 000 ± 900 000
0.08	2.518	286 490 ± 430	1 686 000 ± 27 000	7 480 000 ± 370 000
0.10	2.485	247 820 ± 360	1 144 000 ± 21 000	4 450 000 ± 270 000
0.20	2.320	146 990 ± 390	270 000 ± 17 000	670 000 ± 180 000
1.00	0.99762	35 360 ± 150	4 940 ± 570	1 510 ± 510

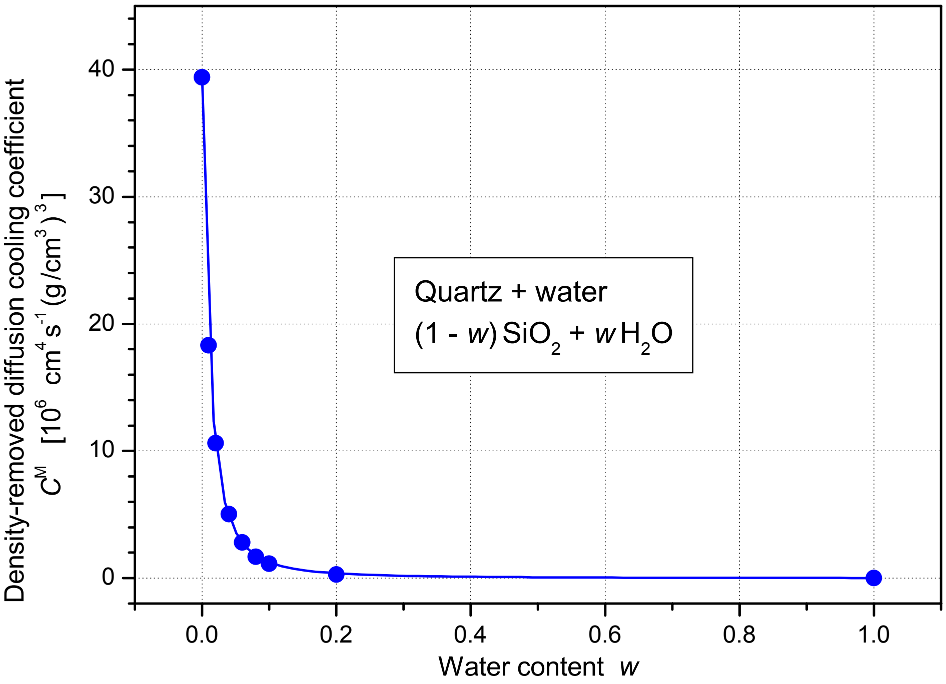

Fig. 9. Density-removed diffusion cooling coefficient C^M of moisturized quartz as a function of the water content.

The dependence $C^{\mathrm{M}}(w)$ has a hyperbolic shape, as found in [7]. The function

$$C^{\mathrm{M}}(w) = a\,(w + w_0)^{b} \tag{6}$$

has been fitted to the 'experimental' data C_i^{M} and the following parameters have been obtained:

$$\left.\begin{aligned} w_0 &= 0.02125 \pm 0.00090 \\ a &= 19\,500 \pm 2\,900 \ \mathrm{cm^4 s^{-1} (g/cm^3)^3} \\ b &= -1.977 \pm 0.060 \end{aligned}\right\} . \tag{6a}$$

Formula (6) is slightly different than that reported in [7] for dolomite. When additional simulations for moisturized dolomite were made for very low water contents, the function (6) was found to be better and, therefore, it has been also used for moisturized quartz here.

5. Conclusions

The formulae $C^{\mathrm{M}}(w)$ obtained for moisturized quartz and dolomite [7] are accurate for $w \in [0, 0.1]$, and can be used approximately up to $w = 0.2$. At higher water contents (which are not interested for geophysical interpretation of neutron log measurements) the formulae would be inaccurate as the simulations for $w \in (0.2, 1.0)$ have not been done. The revised parameters for dolomite, according to the fit (6), are

$$\left.\begin{aligned} w_0 &= 0.0356 \pm 0.0050 \\ a &= 11\,900 \pm 5500 \ \mathrm{cm^4 s^{-1} (g/cm^3)^3} \\ b &= -2.20 \pm 0.23 \end{aligned}\right\} . \tag{6b}$$

The dependences $C^{\mathrm{M}}(w)$ obtained for quartz and dolomite are, as expected, similar but the values at a particular water content are significantly different. Moreover, the quartz-to-dolomite diffusion cooling ratio, $C_{\mathrm{Q}}{}^{\mathrm{M}}(w)/C_{\mathrm{D}}{}^{\mathrm{M}}(w)$, is not constant as a function of the water content. The ratio is plotted in Fig. 10.

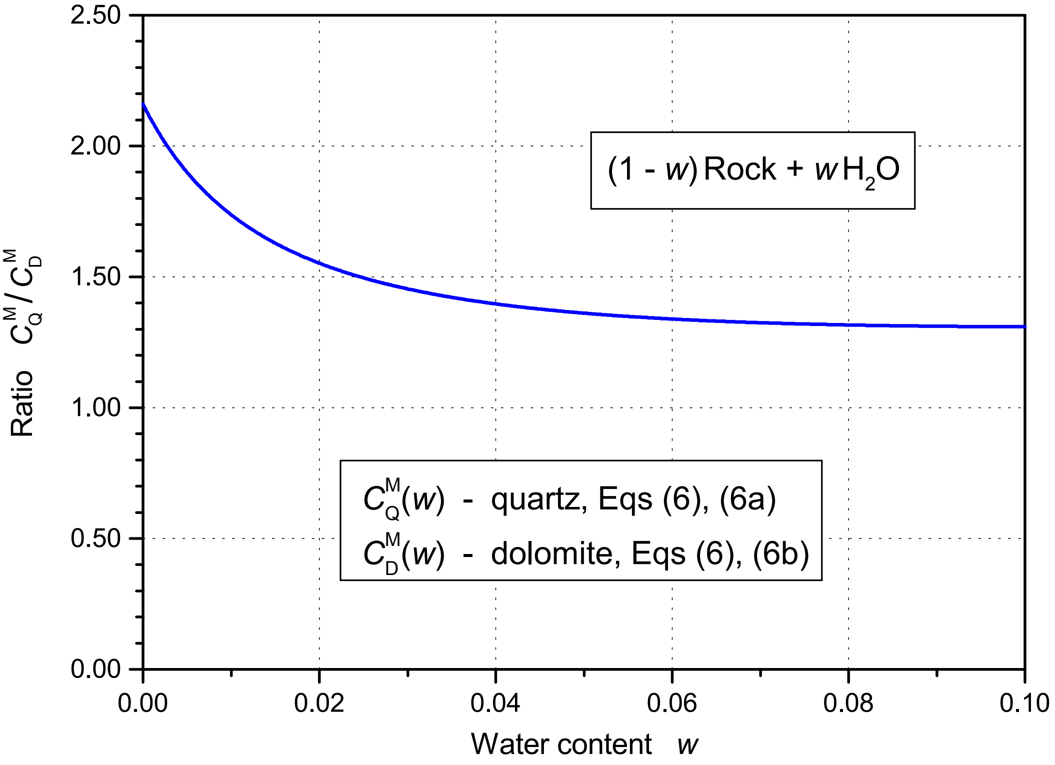

Fig. 10. Ratio of the diffusion cooling coefficients C^M of moisturized quartz (Q) and dolomite (D) as a function of the water content w.

The obtained results show that the influence of the water content in the rock on the thermal neutron diffusion cooling properties is individual for different rocks. Therefore, similar simulations as performed here for quartz and in [7] for dolomite are also desired at least for the third basic rock mineral, calcite – $CaCO_3$.

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