SUPPLEMENT

to the manuscript: Maria Trukhina, Sergey Tkachenko, Anastasia Ryabova, Maxim Oshchepkov, Anatoly Redchuk and Konstantin Popov "Calcium sulfate crystallization in presence of fluorescent-tagged polyacrylate and some refinement of scale inhibition mechanism", Minerals, 2023 .

Calculation of an average distance to the nearest suspended particle for free-floating particles in solution

Initial assumptions:

a) There is no interaction between particles at a distance;
b) Particles move chaotically;
c) The size of the particles can be neglected compared to the distance between them, i.e. the particles can be considered as material points;
d) The influence of gravity can be neglected;
e) The number of particles is sufficiently large to assume that the law of large numbers is satisfied.

The mean value of *a*, which is a function of the distance to the nearest particle *l*, can be calculated using the probability density function for *l* - *f(l)*. The probability that a random variable *l* is greater than or equal to *l* but less than *l+dl* is *f(l)dl*. The density of the distribution is the first derivative of the integral distribution function *F(l): f(l) = F'(l)*. The integral distribution function is the probability that a random variable *l* lies between 0 and *l*.

The average value of *a(l)* is calculated according to the formula (1)

$$\overline{a(l)} = \int_{0}^{\infty} a(l)f(l)dl \quad (1)$$

To determine the distribution density *f(l)*, isolate any particle in the suspension and describe two spheres of radius *l* and *l+dl* whose centers coincide with the position of the isolated particle (Fig. S1).

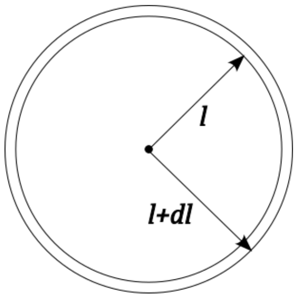

Fig.S1. The spheres of radius *l* and *l+dl*

The probability, that the particle located closest to the one selected, falls in a spherical layer between spheres of radius *l* and radius *l+dl* is expressed on the one hand by the distribution density as above, and on the other hand it can be considered as the multiplication of the probabilities of two independent events: there is no particle in a sphere of radius *l* and there is only one particle in a spherical layer of the same radius and thickness *dl*. The probability of the first event, according to the definition of the distribution function, is *1-F(l)*. The probability of the second event is equal to the ratio of the volume of the spherical layer to the volume of the system multiplied by the number of particles in the system (2), i.e.

$$f(l)dl = \left(1 - F(l)\right)\frac{4\pi l^2 dl}{V}N, \quad (2)$$

where N is the number of particles in the system of volume V.

Combining all quantities independent of l into a single multiplier $A = 4\pi N/V$, reduce dl and, given the relation of the distribution function to the probability density function, a differential equation (3) for finding $F(l)$ is obtained:

$$\frac{dF}{dl} = A(1-F)l^2 \, . \tag{3}$$

Equation (3) is conveniently solved by the method of separation of variables [68], the integration constant being defined on the assumption that F(0) = 0. Hence, we obtain (4):

$$F(l) = 1 - e^{-\frac{Al^3}{3}} \;\; u \; f(l) = \frac{dF}{dl} = Al^2 e^{-\frac{Al^3}{3}}. \tag{4}$$

By substituting the original values for A, we obtain the final expression for the probability density of the distance to the nearest neighbor (5), as follows:

$$f(l) = 4\pi \frac{N}{V} l^2 e^{-4\pi \frac{N}{3V} l^3} \, . \tag{5}$$

The average value of the distance to the nearest neighbor particle is found as above:

$$\bar{l} = \int_0^\infty l f(l) dl, \tag{6}$$

or, by substituting the expression for the density of the distribution (in a more compact form from the equation (4)):

$$\bar{l} = \int_0^\infty Al^3 e^{-\frac{Al^3}{3}} dl. \tag{7}$$

Simplify the integrand by replacing the variables:

$$x = \sqrt[3]{A/3}\, l \qquad \bar{l} = \sqrt[3]{81/A} \int_0^\infty x^3 e^{-x^3} dx. \tag{8}$$

where $A = 4\pi N/V$ and for $V = 1$ cm^3 = $1 \cdot 10^{21}$ nm^3 and $N = 5 \cdot 10^{15}$ $A = 6{,}283 \cdot 10^{-5}$ nm^3.

The integral in (8) was calculated using the Wolfram Alpha online calculator [69] and was found to be 0.29766. Substituting these values into formula (8) we obtain:

$$\bar{l} = 32{,}4 \; nm.$$

Then, the mean number of nanoimpurities in a cubic volume 100x100x100 nm of aqueous solution, can be estimated as 5 units, Fig.S2:

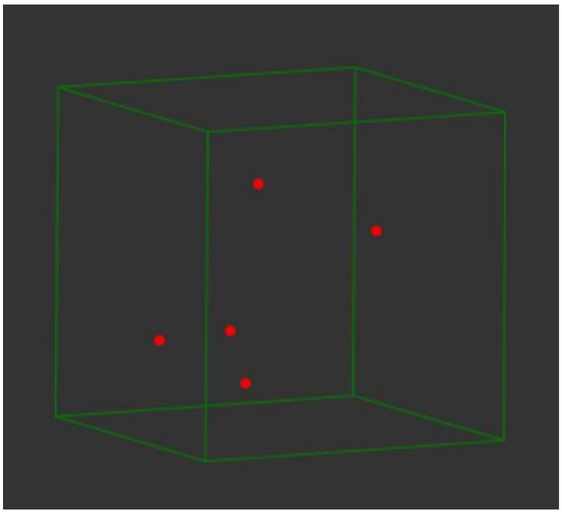

Fig. S2. Approximate location of particles in a volume 100x100x100 nm

References

[68] Korn, G.A. and Korn, T.M. Mathematical Handbook for Scientists and Engineers. Definitions, Theorems, and Formulas for Reference and Review. Dover Publications, Inc., New York, 2000

[69] Wolfram Alpha LLC. 2023. Wolfram|Alpha. https://www.wolframalpha.com/input?i2d=true&i=Integrate%5BPower%5Bx%2C3%5DExp%5B-Power%5Bx%2C3%5D%5D%2C%7Bx%2C0%2C%E2%88%9E%7D%5D (access February 21, 2023).