

Mathematical modeling of sedimentation process of nanoparticles in gradient medium

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Abstract. Mathematical model describing the motion of a light ray in the medium with a varying index of refraction formed by particles settling in a liquid has been built. We have received size distribution of particles settling in a liquid; calculated the light ray's trajectory in the medium; investigated the dependence of the light ray's trajectory on the initial particles concentration; received the solution of the equation of convective diffusion for nanoparticles.

Introduction

The development of nanotechnology has led to creating materials with unique optical properties that are not found in natural environment. Currently research is being carried out to study physical properties of such materials.

New areas of these investigations are connected with phenomena of light propagation in optically inhomogeneous media. In such media the refractive index changes continuously, so a gradient of refractive index serves as a characteristic of the medium. Such phenomena in gradient optics having been studied for a long time and the first educational experiments arising more than a century ago, this area of optics can be attributed to the modern area due to the fact that it is being developed intensively nowadays.

The statement of the problem

Let's consider the gradient medium formed by particles settling in a liquid. To calculate the trajectory of light ray the Fermat principle is used. Sedimentation process of nanoparticles is investigated in detail in the works [1, 2], diffusion is investigated in the work [3].

The purpose of the work is to construct a mathematical model describing the sedimentation process of nanoparticles in the liquid and to calculate the trajectory of ray's motion.

The model

In the experiment a glassful with liquid which contains particles of different sizes is used. Heavy particles settle to the bottom, and light particles stay at the surface, and thus they are distributed over the depth and create a gradient medium. A light ray goes through the medium and its trajectory can be observed.



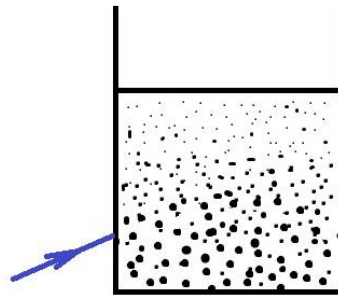


Fig.1. The object of modeling.

The calculation of the motion of the light ray's trajectory

We have investigated the time of ray's propagation through a small section of the route, which has a finite size:

$$dt = \frac{dl}{v} = \frac{n}{c} dl$$

where dt – the time of propagation; dl – part of the way; v – speed of propagation.

Using the formula for calculating particle's trajectory the time of light propagation through the given section has been found:

$$t_{1,2} = \int_{x_1}^{x_2} \frac{n(z)}{c} \sqrt{1 + \left(\frac{dz}{dx}\right)^2} dx, \quad (1)$$

In geometrical optics the approach using Fermat's principle is the most commonly used, i.e. the stationary condition of the integral should be followed:

$$\int_{P_1}^{P_2} n(x, y, z) dz$$

where P_1 and P_2 – the fixed points in space, located on the ray's path; n – the refractive index; dS – element of the trajectory.

According to Fermat's principle a ray has to make its path with zero integral variation, and the function realizing the extremum of the integral has to satisfy the Euler equation:

$$\frac{d}{dx} \frac{\partial F}{\partial z'} = \frac{\partial F}{\partial z}$$

Rewrite this equation, according to (1):

$$\frac{d}{dx} \left(\frac{n}{c} \frac{z'}{\sqrt{1+z'^2}} \right) = \frac{1}{c} \frac{dn}{dz} \sqrt{1+z'^2}, \quad (2)$$

where c – the speed of light.

Let's write refractive index of the medium taking into account the perturbation:

$$n = n_0 (1 + \hat{n}(z)), \quad (3)$$

where $\hat{n}(z)$ – the relative deviation of the refractive index from the constant value.

Let's take for simplifying the relatively small inclination of the ray and small perturbations of the refractive index:

$$\begin{cases} z'^2 \ll 1 \\ \hat{n}(z) \ll 1 \\ z' = \frac{d\hat{n}(z)}{dz} \end{cases}$$

The boundary conditions are:

$$\begin{aligned} z|_{x=0} &= 0 \\ z'|_{x=0} &= z'_0 \end{aligned}$$

We rewrite (2) considering (3), integrating the obtained equation (ranging from 0 to z) with into account boundary conditions and receiving integral form of the equation of the light ray's trajectory:

$$x(z) = \int_0^z \frac{dz'}{\sqrt{z_0'^2 + 2(\hat{n}(z') - \hat{n}(0))}} \quad (4)$$

where $\hat{n}(z')$ – the relative deviation of the refractive index.

The trajectory chart of the light ray indicates the ray's path and its deviation from more dense part of the medium:

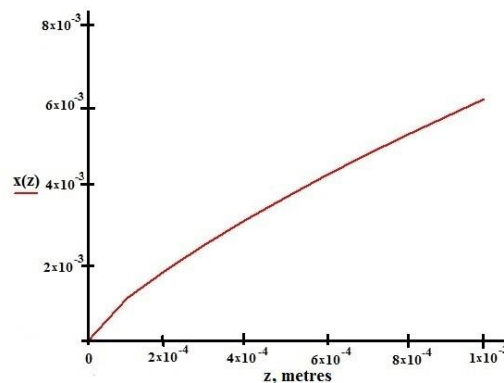


Fig.2. The trajectory of the light ray .

The calculation of the sedimentation process of particles in a liquid.

Let's consider a particle that settles at the constant speed and turns out to be at the depth z in the time t .

The attractive force (mg), the friction force (F_{fr}) and the buoyancy force (F_a) act on the particle.



Fig.3. The particle and the forces applied to it .

The condition of equilibrium of forces applied to the settling particles is:

$$6\pi\mu Rv = \frac{4}{3}\pi R^3(\rho - \rho_p)g,$$

where $v = \gamma R^2$ – velocity of the particle's settling.

This implies that:

$$\gamma = \frac{2(\rho - \rho_p)g}{9\mu}$$

Let's consider $f(R, z, t)$ – the density of function of particle size distribution in the time t at the depth z . The equation for its calculation is written as:

$$\frac{df}{dt} + v \frac{df}{dz} = 0$$

The initial condition is:

$$f|_{t=0} = f_0(R, z)\Theta(z)$$

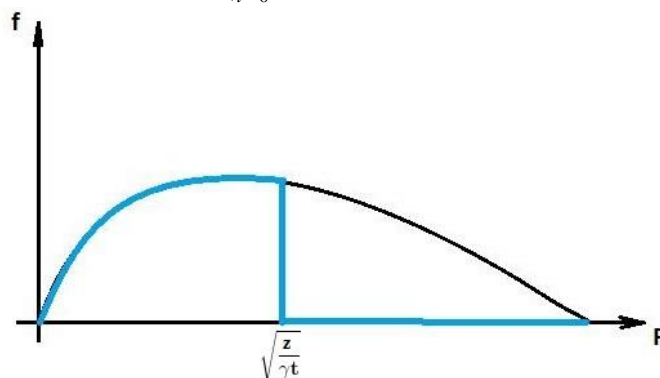


Fig.4. The function of particle size distribution.

Also we calculated the radius of particle, which was at the depth z in the time t :

$$R_z(z, t) = \sqrt{\frac{z}{\gamma t}}$$

The specific volume (volume of particles per unit volume):

$$V_p(z, t) = \frac{4}{3}\alpha^2 n \pi \left(\frac{24}{\alpha^4} - \frac{24e^{-\alpha R}}{\alpha^4} - \frac{24R e^{-\alpha R}}{\alpha^4} - \frac{12R^2 e^{-\alpha R}}{\alpha^3} - \frac{4R^3 e^{-\alpha R}}{\alpha^2} - \frac{R^4 e^{-\alpha R}}{\alpha} \right)$$

$$\hat{n}(z) = \left(\frac{n_p}{n_0} - 1 \right) V_p(z, t)$$

where n_0 – refractive index at the initial time, n_p – refractive index medium formed settling particles.

Next we consider settling particles taking into account the Brownian diffusion.

Let us write the refractive indices of the medium at the initial time and at the moment when the particle has reached a depth of z by the time t :

$$n_0 = \int_0^{\infty} f(R) dR$$

$$n = \int_0^{\infty} f(R, z, t) dR = \int_0^{\infty} f_0(R) \Theta\left(\sqrt{\frac{z}{\pi t}} - R\right) dR = \int_0^{\sqrt{\frac{z}{\pi t}}} f_0(R) dR$$

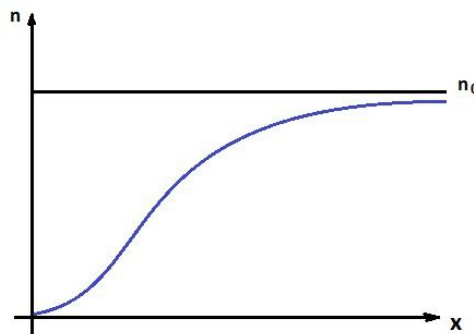


Fig.5. The refractive index distribution.

The equation for the density of function of the particle size distribution is:

$$\frac{\partial f}{\partial z} + v(R) \frac{\partial}{\partial z} (v(R)f) = 0$$

$$\frac{\partial f}{\partial t} + \frac{\partial j}{\partial z} = 0$$

where j – the particle flux density:

$$j = v(R)f - D \frac{\partial f}{\partial z}, \quad (5)$$

Taking advantage of (4) we obtain the equation of convective diffusion:

$$\frac{df}{dt} + v(R) \frac{\partial f}{\partial z} = D(R) \frac{\partial^2 f}{\partial z^2}, \quad (6)$$

The boundary conditions are

$$f|_{t=0} = f_0(R, z) \Theta(z)$$

$$j|_{x=0} = 0$$

$$f|_{x \rightarrow \infty} = f_0(R)$$

Then, using the image of the Laplace for f we have had the solution of equation (6):

$$f(z, t) = f_0 - 2vf_0 \int_0^t \left(\frac{1}{\sqrt{\pi t'}} e^{-\frac{1}{4D} \left(v^2 \sqrt{t'} + \frac{z^2}{t'} \right)} - \frac{v}{\sqrt{D}} e^{\frac{zv}{2D}} \operatorname{Erfc} \left(\frac{z}{2\sqrt{Dt'}} + \frac{v\sqrt{t'}}{2\sqrt{D}} \right) \right) dt', \quad (7)$$

where v – velocity of sedimentation, f_0 – the cumulative distribution function at the initial time, D – diffusion, z – coordinate, t – time of sedimentation.

To sum up, analytical study was carried out. The graphs showing the change in the particle distribution function that depends on changing the sedimentation time were plotted:

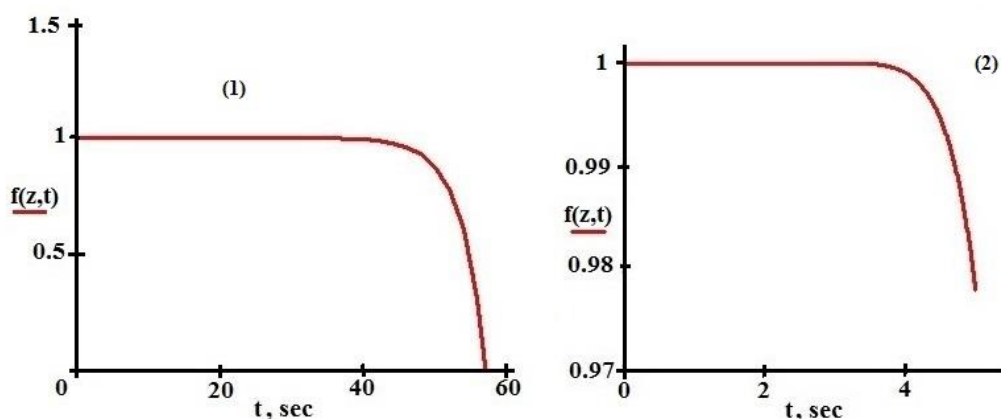


Fig.6. The density of the particle distribution function at large (1) and small times (2).

Acknowledgments

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