Finding the distribution density of settling nanoparticles in a liquid with regard to their Brownian diffusion using the boundary layer theory

Ezhenkova S.I., Chivilikhin S.A.
sveta.ejenkova@yandex.ru

Abstract

The sedimentation process of nanoparticles in a liquid considering their Brownian diffusion was investigated with the methods of mathematical modeling. We have received solution of the equation of convective diffusion of nanoparticles in the case of the boundary layer formed at the bottom of the glassful.

1 Introduction

The problem of the influence of Brownian diffusion occurring between the nanoparticles on their deposition is still remain relevant [1].
Since the times of the experiment about the movement of pollen particles in a liquid drop, which was open by Scottish physicist Robert Brown in 1827, many scientists have studied the behavior of particles in different types of environments. For example, in works [2]-[3] studied the theoretical aspects of the sedimentation of nanoparticles and their characteristics, and in the works [4]-[6] - Brownian motion of nanoparticles in specific environments.
The examples of the elementary colloidal systems (a mixture in which small particles of the substance are distributed in another substance) are "Indian ink" (coal particles in water), smoke (particulate matter in the air) and butterfat (tiny balls of fat in a water).
In this paper, we investigate the sedimentation of spherical nanoparticles in a liquid. As object of research we take glassful with liquid, which contains particles of different sizes. More heavy particles settle to the bottom, a lighter particles stay at the surface, and thus it is distributed over the depth and creating a gradient medium.

2 A mathematical model

In this work we deals with the sedimentation process of spherical nanoparticles occurring under the influence of gravity in a glassful with liquid taking into account

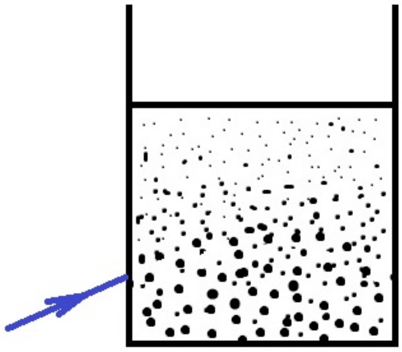

Figure 1: The object of research

the Brownian diffusion between them; where $f(x,t,R)$ - the density of function of particle size distribution in the time t at the depth x. The equation of convective diffusion:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = D(R)\frac{\partial^2 f}{\partial x^2} \tag{1}$$

where $v(R)$ - velocity of sedimentation, f - the particle distribution function, D - diffusion, x - coordinate, t- time of sedimentation.
The initial condition:

$$f\mid_{t=0} = f_0(R,x)\Theta(x) \tag{2}$$

where $\Theta(x)$ - the Heaviside step function.
The boundary conditions:

$$j\mid_{x=0} = 0 \tag{3}$$

$$f\mid_{x=L} = 0 \tag{4}$$

where $j = v(R)f - D\frac{\partial f}{\partial x}$ вЃҰ the particles flux density, L - a boundary layer.
Let suppose formally $D = 0$ in the equation (1). Then we get a first order differential equation:

$$v(R)\frac{\partial f}{\partial x} + \frac{\partial f}{\partial t} = 0 \tag{5}$$

The solution of this equation (see [5]) The solution of this equation (which we describe in [5]) contain only one arbitrary constant, whereby it is impossible to satisfy two boundary conditions (3) and (4).The second boundary condition manifested in a rather small coordinate interval (a boundary layer) adjacent to the coordinate $x = L$.
To find the solution inside the boundary layer we are reduce (5) to a dimensionless form. For this we introduce the dimensionless parameters for variables x Рч t:

$$x = L\bar{x}$$
$$t = T\bar{t} \tag{6}$$
$$\epsilon = \frac{L}{\gamma R^2}\frac{D(R)}{L^2} = \frac{D(R)}{\gamma R^2 L}, \tag{7}$$

where $T = \frac{L}{v(R)}$, L – height of liquid in the glass, $v(R) = \gamma R^2$ – velocity of sedimentation.
Rewrite the the equation in the new notation:

$$\epsilon^{1-2\lambda}\frac{\partial^2 f}{\partial \xi^2} + \epsilon^{-\lambda}\frac{\partial f}{\partial \xi} - \epsilon^0\frac{\partial f}{\partial \bar{t}} = 0, \tag{8}$$

where $\xi = \epsilon^{-\lambda}(L - \bar{x}) = \epsilon^{-\lambda}\bar{z}$ – another dimensionless parameter.
For cross-linking the solution $\bar{f}^p(\xi)$ of the equation (8) inside the boundary layer, with the solution $f^0 = Ae^{-\alpha R}$ outside the boundary layer (see. [7]), the next asymptotic equality is must perform:

$$\lim_{\bar{x}\to 1} f^0(\bar{x},\bar{t}) = \lim_{\xi\to\infty} f^p(\xi) \tag{9}$$

Let consider the behavior of individual members of the equation for $\epsilon \to 0$. Each term in (8) has form $\epsilon^{P(\lambda)}$, where $P(\lambda)$ – the linear function.

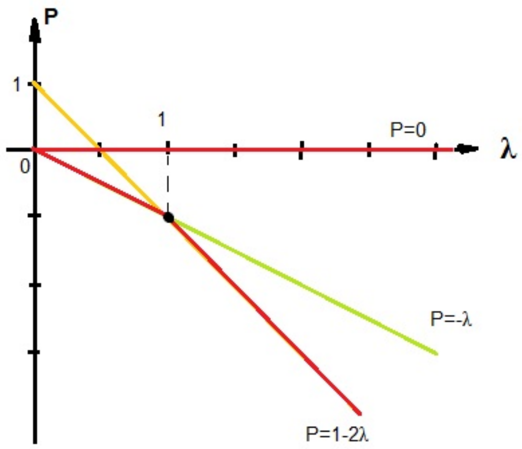

Figure 2: the Newton polygon

The asymptotic of (8) for $\epsilon \to 0$ is determined by the term with the lowest degree of ϵ, ie the bottom of the curve the family of lines. This curve which allocated a thick line is called the Newton polygon.
The solution of this equation outside the boundary layer:

$$f^0(\bar{x},\bar{t}) = ARe^{-\lambda R^2}\Theta(\bar{x}-\bar{t}) \quad (10)$$

The solution of this equation intside the boundary layer:

$$f = A + Be^{-\xi} \quad (11)$$

Let substitute this solutions into (9) and then find the required coefficients. Finally we find the final formula for the particle size distribution:

$$f = f_0(R)\Theta(1-\frac{tv(R)}{L})(1+\frac{D(R)}{D(R)+v(R)L}e^{-\frac{v(R)}{D(R)}(L-x)}) \quad (12)$$

This equation is investigated analytically at the moment.

Acknowledgements

This work was financially supported by the Government of Russian Federation, Grant 074-U01.

References

[1] H. Vahedi Tafreshi, P. Piseri, E. Barborini , G. Benedek and P. Milani Simulation on the effect of Brownian motion on nanoparticle trajectories in a pulsed microplasma cluster source Journal of Nanoparticle Research 4: 511-524, 2002

[2] Suvankar Gangulya, Suman Chakrabortyb, Sedimentation of nanoparticles in nanoscale colloidal suspensions. Physics Letters A 375 (2011) 2394-2399

[3] B. Demeler, Tich-Lam Nguyen, G. E. Gorbet, V. Schirf, E. H. Brookes, P. Mulvaney, A. O. El-Ballouli, J. Pan, O. M. Bakr, A. K. Demeler, B. I. Hernandez Uribe, N. Bhattarai, R. L. Whetten, Characterization of Size, Anisotropy, and Density Heterogeneity of Nanoparticles by Sedimentation Velocity. Anal. Chem. 2014, 86, 7688вЏЎ7695

[4] Eun Chul Cho, Qiang Zhang, Younan Xia The effect of sedimentation and diffusion on cellular uptake of gold nanoparticles. DOI: 10.1038/NNANO.2011.58

[5] Ezhenkova S.I., Chivilikhin S.A. Mathematical modeling of sedimentation process of nanoparticles in gradient medium. Journal of Physics: Conference Series 643 (2015) 012111

[6] Fisenko S.P., Shnip A.I. Physics, Chemistry and Applications of Nanoctructures. Singapore, 2003. P. 291вЏЎ293

[7] Nayfeh A.H. Perturbation Methods. New York: J. Wiley, 1973

Ezhenkova S.I., ITMO University, Saint-Petersburg, Russia
Chivilikhin S. A., ITMO University, Saint-Petersburg, Russia