Journal of Physics: Conference Series **643** (2015) 012124 doi:10.1088/1742-6596/643/1/012124

Theoretical investigation of sedimentation process for nanoparticles statistical ensemble

Ksenia Mukhina, Sergey Chivilikhin

ITMO University, 49 Kronverkskiy pr., Saint-Petersburg, 197101, Russia

E-mail: mukhinaks@gmail.com, sergey.chivilikhin@gmail.com

Abstract. In this paper the sedimentation process of nanoparticles which have distribution in sizes was studied. The mathematical model under consideration gives a rise of velocity which resembles Rayleigh-Taylor instability. The numerical solution is consistent with results predicted by the model. The maximum value of concentration, where instability does not occur, was found.

1. Introduction

Sedimentation is the tendency for particles in suspension to settle out of the fluid in which they are entrained and come to rest against a barrier. Sedimentation of particles in a fluid environment is a familiar phenomenon in nature and has important technical applications. In 1950 J. Taylor [1] first paid attention to the problem of instability of liquid surface. But his studies have not dealt with some relevant factors as viscosity and surface tension. Bellman and Pennington [2] developed the problem by adding these factors to mathematical model. The instability occurs in situations between two fluids of different densities where the lighter fluid is pushing the heavier. The Rayleigh-Taylor instability (or RT instability) can be observed in a lot of situations in astrophysics, for instance supernova's explosion, in physics of plasma, also in electro- and magneto- hydrodynamics and nanohydrodynamics [3].

This process in suspension was studied rather well [4-5]. Evolution in time of border of glycerol and suspension was studied by C. Völtz, W. Pesch and I. Rehberg [6]. Experimental data showed existence of instability whish was similar to the RT instability. In Glowinski, Pan and Joseph's work [7] there was created two-dimensional simulation of this phenomenon and the three-dimensional simulation was made by Guda, Bukharina and Mucha [8]. Systems were bounded by walls. In Saveliev and Rozanov's article [9] there was considered the mathematical model of gas with particles of dust with fixed size. There were a number of similarities between results and RT instabilities. The investigations of the dynamics of interfaces between regions in the fluid with different densities might shed some light on the general understanding of interface dynamics in different branches of science.

The major objective of this study was to investigate the process of sedimentation of statistical ensemble of nanoparticles which had some distribution of size. In this paper the term 'nanoparticles' refers to nano-sized balls which don't interact with each other. Statistical ensemble can be defined as probability distribution for the state of the system. And emergence of velocity's instability is expected as result.

2. Methods

The sedimentation process of nanoparticles was modeled in a gravity field (see Figure 1). System is unlimited in horizontal direction and consists of gas and dust. Upper half-space contains mix of gas

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and dust, the lower half-space contains gas only. Particles of dust have some distribution in sizes with density function f_0. Origin point is located on the border of dusted area. Z-axis is directed to the ground. The friction force is $F = 6\pi\mu R\gamma R^2$.

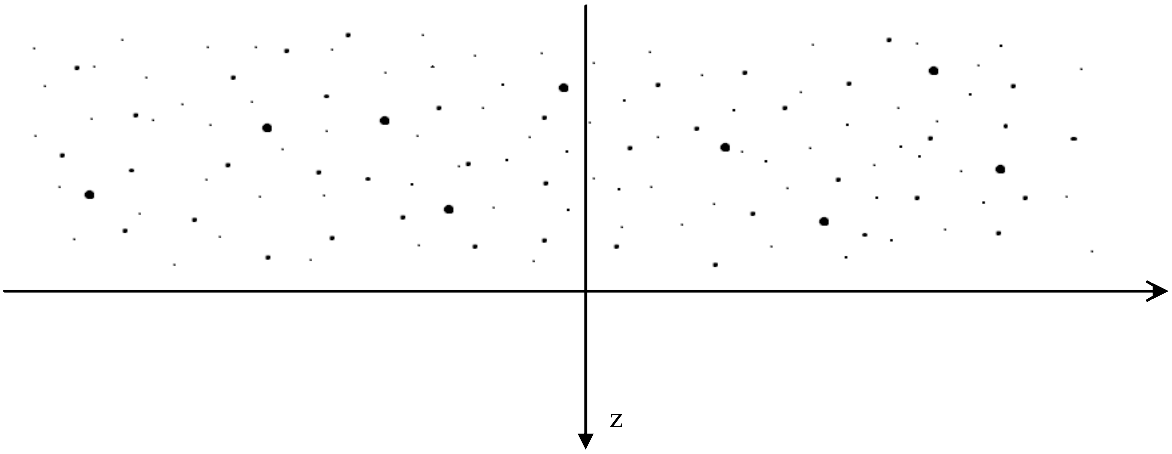

Figure 1. The scheme of the problem. Z-axis is directed as a gravity force.

In case of moving gas, dust gets gas velocity immediately. In vertical direction velocity contains velocity of gas and velocity of dust in zeroth-order approximation. Kinetic equation keeps same form as form one-dimension case.

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial x}(v_x f) + \frac{\partial}{\partial y}(v_y f) + \frac{\partial}{\partial z}(v_z f) = 0$$

Probability density function will be found as sum of density function in zeroth-order approximation and perturbation function which is considering rather small.

$$f = f^{(0)} + \hat{f}$$

$$\frac{\partial f^{(0)}}{\partial t} + \frac{\partial \hat{f}}{\partial t} + \frac{\partial}{\partial x}\left[\hat{v}_x(f^{(0)} + \hat{f})\right] + \frac{\partial}{\partial y}\left[\hat{v}_y(f^{(0)} + \hat{f})\right] + \frac{\partial}{\partial z}\left[(\hat{v}_z + \gamma R^2)(f^{(0)} + \hat{f})\right] = 0$$

Dusted gas is considered as continuous medium, thus we can use Navier-Stokes equations for describing our model.

$$\begin{cases} \rho\dfrac{\partial \hat{v}_z}{\partial t} = \mu(\dfrac{\partial^2 \hat{v}_z}{\partial x^2} + \dfrac{\partial^2 \hat{v}_z}{\partial y^2} + \dfrac{\partial^2 \hat{v}_z}{\partial z^2}) - \dfrac{\partial \hat{p}}{\partial z} + \displaystyle\int_0^\infty 6\pi\mu R\gamma R^2 \hat{f} dR \\ \rho\dfrac{\partial \hat{v}_x}{\partial t} = \mu(\dfrac{\partial^2 \hat{v}_z}{\partial x^2} + \dfrac{\partial^2 \hat{v}_z}{\partial y^2} + \dfrac{\partial^2 \hat{v}_z}{\partial z^2}) - \dfrac{\partial \hat{p}}{\partial x} \\ \rho\dfrac{\partial \hat{v}_y}{\partial t} = \mu(\dfrac{\partial^2 \hat{v}_z}{\partial x^2} + \dfrac{\partial^2 \hat{v}_z}{\partial y^2} + \dfrac{\partial^2 \hat{v}_z}{\partial z^2}) - \dfrac{\partial \hat{p}}{\partial y} \\ \dfrac{\partial \hat{v}_x}{\partial x} + \dfrac{\partial \hat{v}_y}{\partial y} + \dfrac{\partial \hat{v}_z}{\partial z} = 0 \end{cases}$$

Using Navier–Stokes equations and kinetic equation, the system of equations describing the given model was completed:

$$\begin{cases} \dfrac{\partial \hat{f}}{\partial t} + \gamma R^2 \dfrac{\partial \hat{f}}{\partial z} + \hat{v}_z \dfrac{\partial f^{(0)}}{\partial z} = 0 \\ \rho \dfrac{\partial \hat{v}_z}{\partial t} = \mu(\dfrac{\partial^2 \hat{v}_z}{\partial z^2} + \dfrac{\partial^2 \hat{v}_z}{\partial y^2} + \dfrac{\partial^2 \hat{v}_z}{\partial x^2}) - \dfrac{\partial \hat{p}}{\partial z} + \int_0^\infty 6\pi\mu R\gamma R^2 \hat{f} dR \\ \dfrac{\partial^2 \hat{p}}{\partial x^2} + \dfrac{\partial^2 \hat{p}}{\partial y^2} + \dfrac{\partial^2 \hat{p}}{\partial z^2} = \int_0^\infty 6\pi\mu R\gamma R^2 \dfrac{\partial \hat{f}_{\hat{k}}}{\partial z} dR \end{cases}$$

Solving this system we get mathematical expression for Z-component of velocity.

$$\frac{\partial \hat{v}_{zk}}{\partial t} = \frac{\mu}{\rho}(\frac{\partial^2 \hat{v}_{zk}}{\partial z^2} - k^2 \hat{v}_{zk}) + k\frac{e^{kz}}{2\rho}\int_z^\infty e^{-kz'} J(z')dz' + k\frac{e^{-kz}}{2\rho}\int_0^z e^{kz'} J(z')dz'$$

The concentration value can be found by using this numerical solution:

$$V_{j,n+1} = V_{j,n} + \nu\Delta t\left(\frac{V_{j+1,n} + V_{j-1,n} - 2V_{j,n}}{(\Delta z)^2} - k^2 V_{j,n}\right) + \frac{k\Delta t}{2} e^{k\cdot j\Delta z} \sum_{j'=j}^{\infty} e^{-k\cdot j'\Delta z} \frac{J(j')}{\rho}\Delta z + \frac{k\Delta t}{2} e^{-k\cdot j\Delta z} \sum_{j'=0}^{j} e^{k\cdot j'\Delta z} \frac{J(j')}{\rho}\Delta z$$

3. Results and Discussion

If we assume that integral summands are equal to zero, we get the system which has some similarity with system which describes diffusion problem. It means that with growth of viscosity the velocity of particles will be decline (Fig. 2).

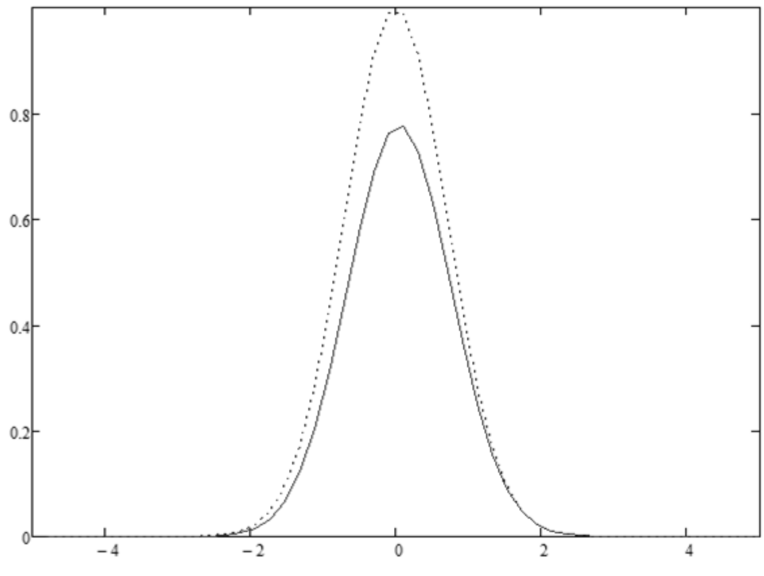

Figure 2. The dependencies of Fourier transform of velocity's Z-component from coordinate in first moment of time (dotted line) and after n iterations

Then let's the probability density function in first moment of time be $f_0 = n_0\alpha^2 Re^{-\alpha R}$, where n_0 is the particles of dust concentration. The charts below show velocity's behaviour with different concentration of particles. It is clear that after certain level of concentration was reached, velocity has a sudden rise which can be explained by the instability similar to RT instability. The minimum value of concentration, where instability is appearing, is $n_0 = 3 \cdot 10^{10}\ m^{-3}$.

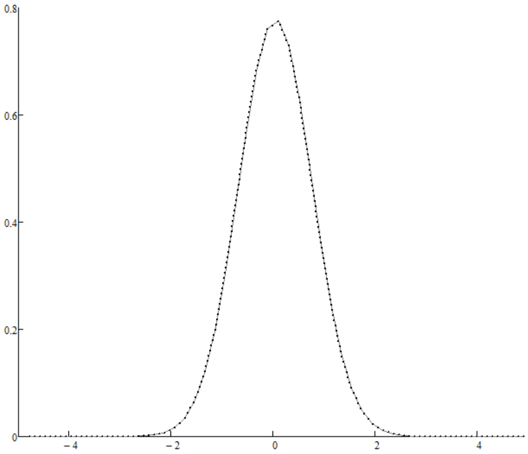

Figure 3. Comparison Fourier transform of velocity's Z-component dependence from coordinate with and without perturbation; $\nu = 10^{-6}; \gamma = 2.173 \cdot 10^6; n_0 = 10^{10}$

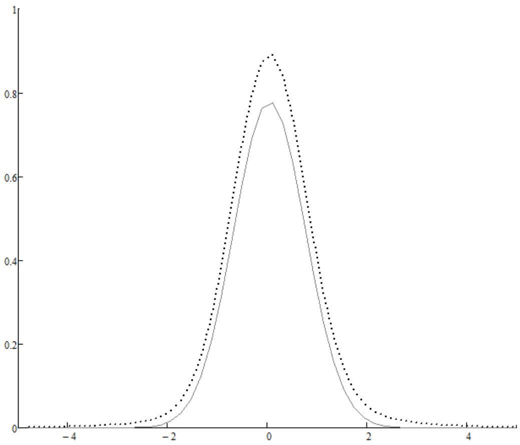

Figure 4. Comparison Fourier transform of velocity's Z-component dependence from coordinate with and without perturbation; $\nu = 10^{-6}; \gamma = 2.173 \cdot 10^6; n_0 = 10^{16}$

Thus, there was discovered a phenomenon which is close to process taking place during the Rayleigh-Taylor instability and the predicted rise of velocity was found. However, for better understanding of particles' behaviour the further investigations are required.

Acknowledgments

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

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