The influence of non-spherical nanoparticles’ shape on sedimentation process

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Abstract. The influence of non-spherical nanoparticles’ shape on sedimentation process was studied. Six different shape of particles were considered. From proposed mathematical model it was shown that for non-spherical nanoparticles the perturbation of Z-component of velocity is slightly lower comparing to spherical particles.

1. Introduction

There is no doubt that the process of sedimentation has important technical applications. Since 1950 when J. Taylor first draw attention to the instability of liquid surface [1], the Rayleigh-Taylor instability (or RT instability) was observed in a various kind of situations including electrodynamics, magnetodynamics and hydrodynamics, nanohydrodynamics [2] in particular. In Glowinski, Pan and Joseph’s study [3] two-dimensional simulation of this phenomena in suspension was created and few years later the three-dimensional simulation was considered in Guda, Bukharina and Mucha's work [4].

The RT-instability induced by particles themselves was studied in work [5]. The single-phase model and Euler-Lagrange two-phase model were used. The impact of Coriolis force for Rayleigh-Taylor instability under rotation was investigated in [6], the critical rotation rate was found for stabilizing the system. Influence of other factors, such as pH, ionic strength, and adsorption of humic acid on the sedimentation process of TiO2 nanoparticles was studied by J. Lu et al. in 2015 [7].

The Rayleigh-Taylor instability of viscous fluids in spherical geometry was first analyzed in 1955 by Chandrasekhar [8] and was later improved by Mikaelian [9].

In several cases the occurring instability is quite similar to RT instability, thus someone can consider it identical. For example, gravitational instability of thin gas layer in liquid was solved for inviscid fluid and viscous gas [10]. In 2008, Saveliev and Rozanov [11] proposed the mathematical model for nanoparticles with fixed size in moving gas. However, there is a lack of research considering the particles with different sizes and shapes.

2. Problem statement

The main goal of this work is to study the influence of nanoparticles’ shape on the sedimentation process of its statistical ensemble. To measure the shape difference from the sphere the coefficient c was used, which is called particle circularity (or surface sphericity). The circularity gives exact the same value in case of two-dimensional and three-dimensional objects, and it ranges between 0 and 1, where 1 corresponds to a perfect circle or sphere.
In this study we are considering a six simple shapes with different value of circularity [12]. The examined shapes are obtained by combining several spherical particles together. The sphericity coefficients are presented in Table 1.

| Particle shape         | Particle circularity, $c$ |
|------------------------|--------------------------|
| Close-to-sphere        | $\frac{\sqrt{2}}{3} \left( 2 + \frac{3\sqrt{3}}{\pi} \right)^{1/2} \approx 0.9011$ |
| Pyramids               | $\frac{1}{5} \left( 5 + \frac{16}{\pi} \right)^{1/2} \approx 0.6354$ |
| Stars                  | $\frac{1}{\sqrt{5}} \approx 0.4472$ |
| H-shaped particle      | $\frac{1}{\sqrt{7}} \approx 0.3779$ |
| Cross-shape particle   | $\frac{1}{\sqrt{7}} \approx 0.3779$ |
| Cylindrical bar        | $\frac{1}{\sqrt{7}} \approx 0.3779$ |

2.1. Mathematical model
The aforementioned process in a gravity field (see the scheme on Figure 1) was modeled, where the upper-half area is the gas dusted with nanoparticles and other half in zero moment of time contains the gas only. System is unbounded in horizontal direction; the nanoparticles are considered as nanosized balls with distribution in sizes. The friction force according to Stokes’ law is $F = 6\pi \mu R \gamma R^2$. 
The scheme of the problem. Z-axis is directed as a gravity force.

The Navier–Stokes equations and kinetic equation were used to describe the system of spherical nanoparticles:

\[
\begin{align*}
\frac{\partial v_j}{\partial t} + \gamma R^2 \frac{\partial}{\partial z} v_j &= 0 \\
\rho \frac{\partial v_j}{\partial t} &= \mu \left( \frac{\partial^2 v_j}{\partial z^2} + \frac{\partial^2 v_j}{\partial y^2} + \frac{\partial^2 v_j}{\partial x^2} \right) - \frac{\partial^2 p}{\partial z^2} + \int_0^\infty 6\pi \eta R^2 \hat{z} dR \\
\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} &= \int_0^\infty 6\pi \eta R^2 \hat{z} dR 
\end{align*}
\]

After solving this system, the mathematical expression for Z-component of velocity was obtained previously in case of spherical nanoparticles [13]. Its numerical solution represented below:

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

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

Figure 2. Comparing Fourier transform of velocity’s Z-component with and without perturbation depending on different shape of particles; \(\nu = 10^{-6};\) \(\gamma = 2.173 \cdot 10^6;\) \(n_0 = 10^{16}\)

Figure 3. Comparing Fourier transform of velocity’s Z-component with and without perturbation with different value of \(c;\) \(\nu = 10^{-6};\) \(\gamma = 2.173 \cdot 10^6;\) \(n_0 = 10^{16}\)
3. Results and Discussions
The influence of particle shape on its velocity is presented on figures 2 and 3. As we can see from the charts with growing of coefficient $c$ the velocity of nanoparticle increases. Comparing given values with obtained velocity without perturbation (Figure 3) we can conclude that the shape of particle has significant influence on the value of Z-component of velocity. Thus, the highest value of velocity corresponds to shape which is the closest to sphere. It should be noticed that for spherical nanoparticles the limit value of concentration is $n_0 = 3 \cdot 10^{10} \text{m}^{-3}$, for the higher concentration the instability is appearing. However, the influence of shape on concentration for non-spherical particles requires further investigations.

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References
[1] Taylor G.I. 1950 The instability of liquid surfaces when accelerated in a direction perpendicular to their planes Proc. Roy. Soc. A. 201 p 192–196
[2] Chandrasekhar S. 1981 Hydrodynamic and Hydromagnetic Stability NY.: Dover 652
[3] Völtz C, Pesch W and I Rehberg 2001 Rayleigh-Taylor instability in a sedimenting suspension Phys. Rev. E. 65 p 1–7.
[4] Mucha, P., & Guda, S. 2007 Rayleigh-Taylor Instability in a Sedimenting Suspension. In APS Division of Fluid Dynamics Meeting Abstracts 1
[5] Chou, Y. J., & Shao, Y. C. 2016 Numerical study of particle-induced Rayleigh-Taylor instability: Effects of particle settling and entrainment. Physics of Fluids (1994-present) 28(4) p 043302.
[6] Baldwin, K. A., Scase, M. M., & Hill, R. J. 2015 The inhibition of the Rayleigh-Taylor instability by rotation. Scientific reports, 5.
[7] Lu, J. et al. 2015 Sedimentation of TiO2 nanoparticles in aqueous solutions: influence of pH, ionic strength, and adsorption of humic acid. Desalination and Water Treatment, p 1-8.
[8] Chandrasekhar, S. 1955 The character of the equilibrium of an incompressible fluid sphere of variable density and viscosity subject to radial acceleration. The Quarterly Journal of Mechanics and Applied Mathematics, 8(1) p 1-21.
[9] Mikaelian, K. O. 2016 Viscous Rayleigh-Taylor instability in spherical geometry. Physical Review E, 93(2) p 023104.
[10] Pimenova A.V. and Goldobin D.S. 2015 Gravitational instability of thin gas layer between two thick liquid layers
[11] Saveliev R.S., Rozanov N.N., Sochilin G.B., Chivilikhin S.A. Rayleigh-taylor instability of a dusty gas (in Russian) Scientific and Technical Journal of Information Technologies, Mechanics and Optics 3(73) p 18-21
[12] Tran-Cong, S., Gay, M., & Michaelides, E. E. 2004 Drag coefficients of irregularly shaped particles. Powder Technology, 139(1) p 21-32.
[13] Mukhina, K., & Chivilikhin, S. 2015 Theoretical investigation of sedimentation process for nanoparticles statistical ensemble. In Journal of Physics: Conference Series 643(1) p 012124 IOP Publishing.