Theoretical Study of Sedimentation of Particles Submerging in Homogenized Fluid

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Abstract: This study focused on exploring sedimentation phenomena by developing a simplified theoretical model to analyze the mechanics of high-density spherical particles, specifically those with submicrometric sizes, as they deposit in homogeneous liquids. A theoretical equation was derived to quantify the relationship between the terminal velocity of these particles and their diameters. Simulation results revealed significant variations in terminal velocities among the examined particles. Specifically, particles with diameters of D1 = 10^{-9} m, D2 = 10^{-8} m, and D3 = 5×10^{-8} m demonstrated terminal velocities of 0.073 m/s, 0.738 m/s, and 3.691 m/s, respectively. These findings suggest that even minor changes in particle size can lead to substantial differences in sedimentation rates, highlighting the critical role of particle diameter in sedimentation dynamics. This research contributes to a deeper understanding of sedimentation mechanisms at the nanoscale and has potential implications for various fields, including environmental science, materials engineering, and nanotechnology. The developed model not only quantifies sedimentation behavior but also serves as a foundational tool for future research aimed at optimizing the deposition processes of submicrometric particles in liquid mediums.

Keywords: Resistance force, terminal velocity, sedimentation, solid particles.

1- Introduction

The phenomenon of sedimentation refers to the process by which solid particles fall and accumulate within a liquid medium. Understanding this process is crucial for various applications, as theoretical, experimental, and computational studies have significantly contributed to optimizing industrial operations, predicting pollutant behavior in aquatic environments, and developing innovative materials [1-4]. The mechanics of spherical particle deposition in liquids is of particular interest across multiple sectors, given its relevance to both industrial and environmental contexts.

A notable example of this is the interaction between microplastics and microalgae. This interaction includes processes such as colonization and heteroaggregation, which can substantially influence particle sedimentation dynamics in surface waters. Such alterations not only affect the sedimentation processes themselves but also disrupt the ecological balance of microalgae, inhibiting their growth and overall health [2.5].

This work introduces the theoretical development of a simplified model for the mechanics of spherical particles with submicrometric dimensions during their deposition process in homogeneous liquids.

2- Theoretical model of particle sedimentation in fluid medium

When nonporous particles are immersed in an aqueous medium, they are subjected to three distinct forces: gravitational force, fluid drag (or resistance force), and buoyancy force. In this context, we examine a scenario involving low velocities, allowing the fluid drag force to be approximately represented by Eq. (01):

$$\overrightarrow{F_r} = a \overrightarrow{v} + b \overrightarrow{v}^2 \tag{01}$$

Where $(\overrightarrow{F_r})$ represents the resistance force exerted by the medium, (\overrightarrow{v}) is the velocity of the particles, and (a) and (b) are coefficients that depend on the geometry of the particles and the properties of the fluid [8]. The terms (av) and $(bv)^2$ correspond to the linear and quadratic contributions, respectively. The linear term arises from the viscous drag of the medium, while the quadratic term is associated with the mass of fluid accelerated due to collisions with the moving particle [9].

Assuming that the particles exhibit spherical symmetry, the coefficients (a) and (b) can be expressed as: a = yD; $b = \xi D^2$ (02)

In Eq. (02), (D) denotes the diameter of the particles, while (γ) and (ζ), are coefficients that depend on the characteristics of the medium. Given that the particle size distribution in micrometric powders can range from 10^{-6} to 10^{-9} m, we can reasonably approximate that (b), influenced by the square of (D), becomes negligible. Consequently, we will consider only the linear term presented in Eq. (01). Therefore, the dynamics of particle sedimentation is described by Newton's second law:

$$\vec{P} - \vec{F_r} - \vec{B} = m\vec{z} \tag{03}$$

Where (\overrightarrow{P}) represents the gravitational force, $(\overrightarrow{F_r})$ is the drag force, (\overrightarrow{B}) is the buoyancy force, (m) is the mass of the particles in the fluid, and (\overrightarrow{z}) denotes their acceleration. We define the positive direction of the (z) axis as downward, such that both $(\overrightarrow{F_r})$ and (\overrightarrow{B}) act upwards and are therefore considered negative in this reference frame, as illustrated in Fig. 1."

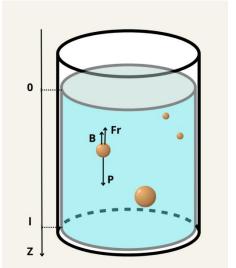


Figure 1 – Schematic representation of the forces acting during the sedimentation of particles in a fluid.

Considering the vertical movement with linear drag, Eq. (03) is one-dimensional, and we can work only with the magnitudes of the quantities that compose it. Therefore, it assumes the form of Eq. (04):

$$mg - a\dot{z} - \rho Vg = m\ddot{z} \tag{04}$$

Where (g) is the acceleration due to gravity, (\dot{z}) is the velocity of the particles, (V) is the volume of fluid displaced by them, and (ρ) is the density of this medium.

Note that the weight and buoyant forces are constant, but the drag force depends linearly on velocity, which may increase or decrease during the settling of the powder. This depends on the relationship between the initial velocity (\dot{z}_0) and the terminal velocity (\dot{z}_t) : if $(\dot{z}_0 < \dot{z}_t)$, the particle is accelerated until equilibrium is reached; if $(\dot{z}_0 > \dot{z}_t)$, the particle is decelerated before this occurs[10]. In both cases, there is a moment when the sum of the drag force and the buoyant force equals the weight of the particles, and the motion becomes uniform. When this occurs, the particles are said to have reached the terminal velocity (\dot{z}_t) , which can be obtained by taking $(\ddot{z} = 0; z = 0)$ in Eq. (04).

Equation (04) is a linear, inhomogeneous second-order ordinary differential equation (ODE). Its general solution is well described in the literature and represents velocity as a function of time in the sedimentation of particles in a fluid, of the form [6]:

$$\dot{z}(t) = \dot{z}_0 e^{-\frac{\gamma \mathcal{D}}{m}t} + \frac{(m - \rho V)g}{\gamma \mathcal{D}} \left(1 - e^{-\frac{\gamma \mathcal{D}}{m}t}\right) \tag{05}$$

It is noteworthy that if we take the limit as $(t \to \infty)$ in Eq. (05), we recover the terminal velocity. This means that after a relatively long settling time, we obtain $(\dot{z}(t) = \dot{z}_t)$, which is consistent with the preceding analysis. Furthermore, to find the position of the particles as a function of time during the discussed motion, we need to integrate Eq. (05) with respect to the variable (t), remembering that, for convenience, we initially set (z(0) = 0). Doing this yields:

$$z(t) = \frac{1}{\gamma D} \left[(m - \rho V) g \left(t + \frac{m}{\gamma D} e^{-\frac{\gamma D}{m} t} \right) - \dot{z}_0 m e^{-\frac{\gamma D}{m} t} \right]$$
(06)

This function describes the position in the sedimentation of particles in a fluid with linear drag. However, Eq. (06) presents a problem: it diverges as ($t \to \infty$). To address this, we must consider that the particles settle in a container of depth (l) such that, after a limit time (l), they reach the coordinate (l) l). Thus, the limit time is given by:

$$t_{\infty} \approx \frac{\gamma Dl}{(m - \rho V)g} \tag{07}$$

This results from applying the boundary condition in Eq. (06)."

3- Model simulation results of the deposition.

For this purpose, we express the volume (V) of the grain, which is equivalent to the volume displaced from the solution due to its submersion, as $(4/3)\pi(D/2)^3$.

We define the following constants: the standard acceleration due to gravity, ($g = 9.81 \text{ m/s}^2$) (NIST Reference on Constants, Units, and Uncertainty, 2022); the dynamic drag coefficient of water at 25 °C, ($\gamma = 8.903 \times 10^{-4} \text{ N.s/m}^2 \equiv 8.903 \times 10^{-4} \text{ Pa.s}$) [7]; and the density of water, ($\rho = 10^3 \text{ kg/m}^3$) [11].

Additionally, we assign values to three variable parameters: sedimentation time (t) (s); initial velocity of particles (\dot{z}_0) (m/s); and particle mass ($m = \rho_{on} \cdot V$ (kg), where ($\rho_{on} = 6.7 \times 10^3 \, \text{kg/m}^3$) is a is a typical plausible density value. The results of this simulation can be observed in Figure -2 the simulation results of Eq. (04) for various particle diameters (D).

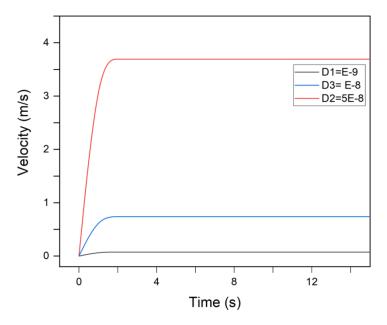


Figure 2 – Simulation of the temporal evolution of velocity curve for particles with different diameters (D).

For large values of time, the particle velocity approaches the terminal velocity, such that Eq. (06) yields $(\dot{z}(\mathcal{D}) \approx \dot{z}_t)$, where (\dot{z}_t) is defined by Eq. (05). Consequently, Graph 2 indicates that as the diameter of the particles increases, the terminal velocity they attain also increases, that particles with diameters D1 = 10^{-9} m, D2 = 10^{-8} m, and D3 = 5×10^{-8} m exhibited terminal velocities of 0.073 m/s, 0.738 m/s, and 3.691 m/s, respectively. However, a more detailed analysis reveals that while the drag force is directly proportional to the diameter (D), the weight force ($m \cdot g = \rho_{on} \cdot V \cdot g$) and the buoyant force ($B = \rho \cdot V \cdot g$) are directly proportional to (\mathcal{D}^3). See Figure 3.

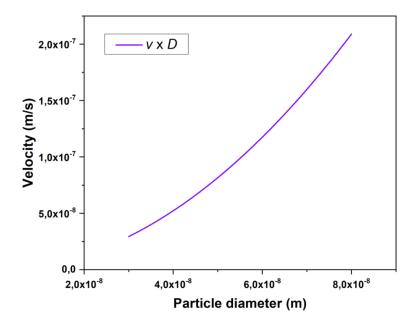


Figure 3 – Simulation of the particle velocity curve (\dot{z}) as a function of diameter (D) for an initial velocity ($\dot{z}_0 = 1 \text{ mm/s}$) and a sedimentation time (t = 300 s).

It is important to emphasize that under the condition $(\dot{z}(D) \approx \dot{z}_t)$, we obtain $(\dot{z}(D) \approx \frac{(\rho_{om} - \rho).\pi g}{6\gamma})$. Which indicates that the terminal velocity depends on the square of the diameter. Since the density of the solid used in the simulation is greater than that of water, this relationship is increasing, consistent with the trends shown in Figure 2.

4- Conclusion

This work aimed to develop a simplified model for the mechanics of spherical particles with submicrometric dimensions during their deposition process in homogeneous liquids. The simulations of the derived equations incorporated a resistance force proportional to velocity while disregarding thermal effects, surface charge interactions, van der Waals forces, magnetic forces, and any other factors that may lead to particle agglomeration. The results indicated that terminal velocity depends on the square of the particle diameter, while the buoyant force (B = $\rho \cdot V \cdot g$) is directly proportional to the cube of the diameter (D³). Moreover, larger particles reach their terminal velocity more quickly and, consequently, settle at the bottom of the container at a faster rate

In future theoretical studies, we intend to investigate how sedimentation rates are influenced by variations in particle density, allowing for the consideration of van der Waals forces and thermal agitation.

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5- References

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