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Diffusion Model of Polydisperse Sedimentation

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A novel model for the sedimentation of polydisperse suspensions has been submitted. In the developed model of gravitational sedimentation, an attempt was made to take into account the main known physical features of the process, and a simplified calculation method based on this model has been proposed too. The approach novelty lies in that generalization of the sedimentation model for the case when a polydisperse suspension is specified not as a discrete set of fractions, but with the help of a continuous size distribution function of disperse phase particles, is proposed to do on the basis of a diffusion type equation, supplemented with source terms. Such a model also allows for taking into account the possibility of aggregation of different fractions during sedimentation. A developed model makes it possible to calculate the temporal evolution of the density of the settling suspension, as well as the evolution of the position of sedimentation front and the sediment surface along the reservoir height. The expression for the settling front evolution, which is of fundamental importance for the method of calculating the sedimentation kinetics of polydisperse suspensions, has been obtained.

1. Introduction

Sedimentation processes play an important role in industry (Massah et al., 2020), industrial ecology (Mitchell et al., 2021), and natural phenomena (Garcia, 2007). Such processes take place also in water purification systems from pollution (Chebbi, 2007). Recently, there are more and more investigations demonstrating an increasing interest in sedimentation processes in biology, medicine (Taye, 2020), and pharmacy (Maki et al., 2021). However, despite the widespread use of the phenomenon of suspensions sedimentation, both its experimental study and theoretical description (Bürger et al., 2005) are associated with many difficulties (Pavlenko et al., 2021), that can be explained by complex multicomponent composition. In spite of the long attention of researchers to these processes (Hernando et al., 2014), many issues in this area remain little studied. Calculation problems become even more complex for describing the sedimentation of polydisperse suspensions, which often happens. In the bidisperse sedimentation model (Kondrat'ev and Naumova, 2007), it is assumed that the dispersion can be divided into two fractions: conditionally coarse and conditionally fine.
The kinetic curve of the deposition of a bidisperse suspension in the absence of aggregation of fractions consists of three linear plots (Wallwork et al., 2022). On the first plot, particles of two fractions precipitate simultaneously, the second plot corresponds to the stage when the precipitation of the coarse fraction is completed, but the precipitation of the fine fraction continues (Bürger et al., 2000). The third plot corresponds to the stage of completion of the process of deposition of both fractions. The resistance force of the fluid acting on a spherical particle depends on its size, relative velocity of movement, and viscosity of the medium and is determined by the Reynolds number. Under conditions when such a separation of fractions by dispersity turns out to be too rough, it is necessary to consider another model. Besides, such an approach is acceptable for weakly concentrated suspensions only, in which there is no influence of particles of one fraction on the hydrodynamic conditions for sedimentation of another fraction.
The construction of theoretical models for the sedimentation of polydisperse suspensions (Biggs, 2006), even in the absence of strong interaction between particles, is a nontrivial problem and has not yet been completed (Lippert and Woods, 2020). Some works (Kondrat'ev and Naumova, 2004) consider the hindered (crowded) sedimentation of a polydisperse suspension. The needs of engineering practice force us to look for ways to developing simplified models (Bürger et al., 2005,). The models should adequately reflect the main regularities

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of the sedimentation process (Wallwork et al., 2022), and should give correct estimates of the control parameters for carrying out the optimal calculation of the equipment (Nocoń, 2016).
Although the driving force of the sedimentation process in the general case is not of a stochastic nature, as is the case for diffusion processes, however, the course of the process itself is similar to diffusion processes in a certain way. This similarity is manifested in the fact that in the process of sedimentation, the components of the mixture are separated due to different sedimentation rates depending on the mass and size of the precipitating particles. For a polydisperse mixture characterized by a wide range of masses and particle sizes in the dispersed phase, one can try to build a model that would describe the change in the average density of the suspension based on a diffusion-type equation.
At the same time, the question of the complete procedure for calculating the effective diffusion coefficient in such a model requires further study. In this work, the task is to describe the evolution of the sedimentation front on the basis of the diffusion model. In this case, it becomes possible, based on the analysis of qualitative results, to give a fundamental assessment of the possibility of using the model in methods for calculating the kinetics of polydisperse suspension sedimentation.
In the submitted here paper, an attempt is made to construct a macroscopic sedimentation model based on the distribution function of particles in polydisperse suspension. The introduction of such a generalized parameter is the main novelty and fundamental point of the submitted model, along with the construction of the model in the form of a diffusion equation with a source term. This novel approach has greater generality since it removes the question of the number of fractions.
The model also allows accounting for the possibility of various fractions aggregation during the sedimentation within the description based on the average density of the suspension. The model proposed below is heuristic, and it contains some hypothetical provisions that are based on the analysis of the theoretical results and the long well-known reliable experimental data (Burt, 1987), but that are not derived in detail. In accordance with the logic of the developed model, the method for calculating the effective diffusion coefficient during sedimentation should be based precisely on the kinetics of sedimentation of various fractions, taking into account the constraint of the sedimentation process. There are a lot of studies on this issue in the literature, both old and new (Wallwork et al., 2022). However, the creation of such a technique is the next task of the authors, and it is not included in the goals of this work. Further work is required on the interpretation of the control parameters of the model, as well as on verification of its adequacy on a more extensive and diverse experimental material.
The paper presents a general form of the model, and the model proposed has been analyzed in more detail for the special case of hindered sedimentation, which is not accompanied by the aggregation in the dispersed phase. An analysis of the submitted model in relation to the sedimentation with mutual aggregation of various fractions will be carried out and presented in subsequent publications.

2. Model description

If the solid phase of the suspension consists of several fractions (numbered by indices i) with different settling rates for each, then several fronts of the suspension settling fronts are formed in the suspension. These fronts separate regions depleted in fractions with particles having higher settling rates. But the system has two main moving free boundaries: the sedimentation front S and the sediment surface H^*. At any moment they are related by the balance ratio:

$$H\sum\rho_i(0)=\rho^*H^*+\int_{H^*}^{S}\sum\rho_i dy \tag{1}$$

A generalization of the model for describing the sedimentation of polydisperse suspensions with a given particle size distribution function of the solid phase can be constructed on the basis of a diffusion-type equation. A similar equation for each *i*-th conditional fraction reads:

$$\frac{\partial\rho_i}{\partial t}=D_{eff(i)}\frac{\partial^2\rho_i}{\partial y^2}+I(\rho_i) \tag{2}$$

Here $D_{eff(i)}$ is the effective fractional diffusion coefficient, determined taking into account the deposition rate of each fraction; $I(\rho_i)$ is the source function due to the transition of particles from one conditional phase to another, namely, from suspension to sediment. For the effective fractional diffusion coefficient, a formula similar to the formula for calculating the average diffusion coefficient of a multicomponent impurity can be proposed as follows:

$$D_{eff} = \sum_i D_{eff(i)} \frac{\rho_i}{\overline{\rho}} \tag{3}$$

Similarly, for a suspension with a continuous particle size distribution function, the function of averaged suspension density $\rho(y,t)$ reads

$$\frac{\partial \rho}{\partial t} = D_{eff} \frac{\partial^2 \rho}{\partial y^2} + I(\rho) \tag{4}$$

By that, when modeling the process using a continuous particle size distribution function $f(d)$ the average diffusion coefficient reads

$$D_{eff} = \frac{1}{\overline{\rho}} \int_d D_{eff}(d) \rho(d) f(d) d(d) \tag{5}$$

According to the logic of this model, the conditional driving force of the sedimentation process can be represented in the form of a gradient law so that it becomes equal to zero at zero density of solid phase in suspension and a density equal to the sediment one, i.e.:

$$F_{sed} \sim \frac{\partial \rho}{\partial y} = k\rho\left(\rho - \rho^*\right) \tag{6}$$

Then the source function in Eq. (4) also vanishes at $\rho = 0$ and $\rho = \rho^*$. In addition, to match the gradient law with the diffusion relation, as well as from physical considerations, we assume additionally that the source function $I(\rho)$ becomes close to zero also at some hypothetical intermediate suspension density $0 < \rho_s < \rho^*$ corresponding to the hindered sedimentation near the interface between suspension and sediment. The meaning of this assumption is that in this zone the rate of different fractions sedimentation is almost the same (Bürger et al., 2000). It can be written as follows:

$$I(\rho) = -\gamma\rho(\rho - \rho_s)\left(\rho - \rho^*\right) \tag{7}$$

The distribution function changes along the reservoir height both due to different settling rates of different fractions and due to the possible aggregation of particles in the dispersed phase. In this case, it is necessary to take into account the competition between the characteristic aggregation times and the characteristic drift times, which depend on the rate of fraction settling (Brener et al., 2017). During aggregation, the parameters of the distribution function change, which affects the average fractional diffusion coefficient. Aggregation of particles of the dispersed phase also leads to a change in the degree of crowding during sedimentation. Enlargement of particles can lead to both a decrease in the degree of crowding and its increase, which is also determined by the ratio of the characteristic drift times in the process of sedimentation and the characteristic aggregation time. The kinetic equation for the dispersed phase distribution function $f(d)$ in continuous form during the aggregation is usually written on the basis of probabilistic considerations similar to those adopted in the derivation of the Smoluchowski equation for binary coagulation (Lee et al., 2008).

$$\frac{\partial f}{\partial t} = \frac{1}{2} \int_0^d f(d - d') f(d') K(d - d', d) \mathrm{d}d' - \int_0^\infty f(d') f(d) K(d', d) \mathrm{d}d' \tag{8}$$

Eqs(4), (5), (7), and (8) should be solved in the system. It should also be noted that the hindered sedimentation assumption (8) may not be entirely correct and should be transformed according to the work (Brener, 2014). The question of the influence of the accuracy while determining the parameters of the distribution function on the errors in calculating the kinetics of sedimentation and the dynamics of the sedimentation front should be studied more carefully. This is where more research is needed. Let us analyze below the diffusion model in more detail for the case of no aggregating fractions.

3. Model analysis and discussion

In the absence of fractions aggregation a solution to the problem can be looked for in the form of a traveling front with a certain speed W_f :

$$W_f = \frac{ds}{dt} = -\frac{(\partial\rho/\partial t)_s}{(\partial\rho/\partial s)_t} \tag{9}$$

where s is the position of the suspension front.
Introducing a moving coordinate system with variable $\eta = s - W_f t$, Eq(5) can be rewritten as:

$$D_{eff}\frac{d^2\rho}{d\eta^2} + W_f\frac{d\rho}{\partial\eta} + I(\rho) = 0 \tag{10}$$

Then instead of Eq(6) the following equation can be obtained

$$\frac{d^2\rho}{d\eta^2} = 2k\rho\frac{d\rho}{d\eta} - k\rho^*\frac{d\rho}{d\eta} \tag{11}$$

From (6), (7), it follows

$$\frac{d^2\rho}{d\eta^2} = k^2\rho(\rho-\rho^*)(2\rho-\rho^*) \tag{12}$$

Since ρ is a variable, from the compatibility conditions of relations Eqs(4), (6) and (7) it can be obtained (Zaslavskii et al, 1992):

$$k = \sqrt{\gamma/(2D_{eff})} \tag{13}$$

This also implies the relationship between the velocity of the moving front of the clarified slurry and the intermediate density:

$$W_f = \sqrt{2D_{eff}\gamma}\left(\frac{\rho^*}{2} - \rho_s\right) \tag{14}$$

Now the following relation can be written in moving coordinate system

$$\frac{d\rho}{d\eta} = \sqrt{\frac{\gamma}{2D_{eff}}}\rho(\rho-\rho^*) \tag{15}$$

With constant values of the effective diffusion coefficient and parameter γ , Eq(15) can be integrated, which gives:

$$\rho = \frac{\rho^*}{2}\left[1\text{-}\operatorname{th}\left(\frac{1}{2}k\rho^*\eta + \ln\left(\frac{\rho_0}{\rho^*}\right)\right)\right] \tag{16}$$

Replacing the self-similar variable η , (16) takes the form

$$\rho = \frac{\rho^*}{2}\left[1\text{-}\operatorname{th}\left(\frac{1}{2}\sqrt{\frac{\gamma}{2D_{eff}}}\rho^*(s - W_f t) + \ln\left(\frac{\rho_0}{\rho^*}\right)\right)\right] \tag{17}$$

From here, using Eq(14), the main novel and principal result of the submitted diffusion model reads

$$\rho = \frac{\rho^*}{2}\left[1\text{-}\operatorname{th}\left(\frac{1}{2}\sqrt{\frac{\gamma}{2D_{eff}}}\rho^*\left(s - \sqrt{2\gamma D_{eff}}\left(\frac{\rho^*}{2} - \rho_s\right)t\right) + \ln\left(\frac{\rho_0}{\rho^*}\right)\right)\right] \tag{18}$$

Figure 1 shows some results of numerical experiments carried out using the obtained formulas.

The initial state of the suspension is represented as a density $\rho_0/\rho^* = 0.65$ uniformly distributed along the height. Numerical experiment and plotting have been carried out using the MATLAB 6.5 package. The patterns observed in the course of the numerical experiment are in good qualitative agreement with although old, but the well confirmed and reliable experimental data (Burt, 1987). The experimental data qualitatively confirm the suitability of the model. However, to assess the practical effectiveness of the proposed model, additional experimental studies may be required to develop a methodology for calculating the effective diffusion coefficient in the diffusion model of sedimentation of polydispersed suspensions.

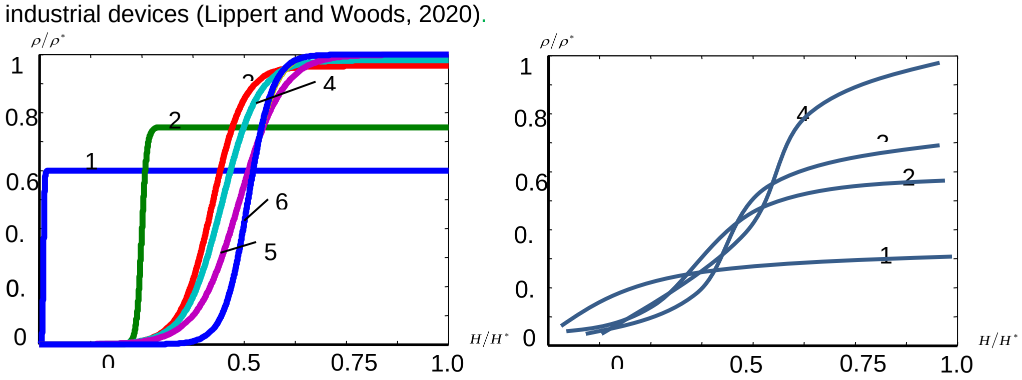
To assess the error of a quantitative description, the authors do not have enough at their disposal because it is difficult to accurately estimate the effective diffusion coefficient on the base of known experimental data.

The carried-out analysis and numerical experiment make it possible to highlight both the advantages and disadvantages of the considered macroscopic model.

The advantages include obtaining a dependence for describing the moving free boundaries dynamics of the system: "clarified liquid-suspension-sediment". The numerical experiment quite convincingly shows a qualitatively correct picture of long-known patterns in the described system dynamics (Burt,1987).

At the same time, the model contains a number of control parameters, the theoretical calculation of which, based on the known physical properties of the components of the polydisperse system (Schleiss et al., 2016), is not clarified enough.

This can be seen as the main drawback of the model. However, the introduced control parameters can be experimentally investigated on laboratory benches and then used while scaling when designing industrial devices and processes. The model under consideration also does not take into account the effect of reservoir walls on hindered sedimentation. This assumption is acceptable for reservoirs with a diameter significantly exceeding the size of the coarse fraction of dispersion particles, and it is acceptable for a significant part of industrial devices (Lippert and Woods, 2020).



A B

Figure 1: Typical time evolution plots of suspension density with height. A- according to Eq.(18); dimensionless time variable $\tau = tD_{eff}/H^2$: 1- $\tau=5$; 2- $\tau=10$; 3- $\tau=15$; 4- $\tau=20$; 5- $\tau=25$; 6- $\tau=35$; B- some experimental data for water suspension of wolframite particles with medium diameter of 2 mm (Burt, 1987).

4. Conclusions

The presented model makes it possible to calculate all the important practice dynamical characteristics of the sedimentation of polydisperse suspensions. The analysis of the obtained dependences and the type of graphs is in good agreement with the known, studied patterns of sedimentation. In particular, as a result of the numerical experiment, it was shown that at the initial state of the uniformly distributed over the height suspension in the reservoir with a density of 0.65 from the sediment density, the formed sediment layer height is approximately 0.25 from the height of the tank. An estimate of the deposition time in a dimensionless form has also been given. Similar accelerated calculations using this model can be carried out with different initial data. For reliable, practical application, this model requires the identification of control parameters for specific physicochemical systems. Only after that, it will be possible to recommend a reliable step-by-step algorithm for using the model in practice.

Nomenclature

d – characteristic particle size, m

D_{eff} – effective diffusion coefficient, m^2/s

W_f – velocity of sedimentation front, m/s

γ – proportional coefficient in Eq. (7), m^6/kg^2s

H – reservoir height, m

H^* – sediment height, m

k – proportional coefficient in Eq. (6), m^2/kg

t – time, s

ρ – average suspension density, kg/m^3

ρ_s – intermediate suspension density, kg/m

ρ^* – sediment density, kg/m^3

ρ_0 – initial average suspension density, kg/m^3

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