Polydisperse sedimentation processes and transport of cohesive sediment suspensions with different sizes and densities

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Abstract

The process of polydisperse sedimentation, in which particles of different sizes and densities settle in a fluid, is present in countless phenomena that occur every day, such as the sedimentation and entrainment of particles in rivers, estuaries, lakes, oceans, and coastal areas, as well as processes in the mining industry and wastewater treatment in water recovery processes. This study introduces a polydisperse sedimentation model coupled with shallow water equations that not only describes vertical sedimentation but also the horizontal transport and entrainment of sediments. The model and obtained results are suitable for describing and analyzing sand/mud mixtures composed of cohesive particles found in muddy areas within rivers, estuaries, and coastal zones, which often contain mud flocs of different sizes and densities. The mixing theory originally proposed by Fick (1855) and Stefan (1871), and more recently developed by Truesdell and Toupin (1957), allows modeling the process of polydisperse sedimentation as a superposition of continuous media. Following the model derivation, a natural modification of the combined settling velocity, as proposed by Masliyah (1979) and Lockett and Bassoon (1979), is obtained, which provides the basis for introducing the cohesive effects of particles. A numerical method (2D finite volume approach for simplicity) is devised, and multiple numerical simulations (2D) of the polydisperse sedimentation process of cohesive sediment under various scenarios are presented.

Keywords: Polydisperse sedimentation, cohesive sediment, numerical method, Hindered setting

MSC Classification: 76T20 , 86A05 , 86-10

1 Introduction

1.1 Scope

Currently, scientists worldwide are continuously striving to employ numerical methods to predict the evolution of high-impact geophysical and industrial events with social, environmental, and economic consequences. In particular, Chile is a country that has consistently been affected by tsunamis, landslides, and floods that have submerged entire cities in water and mud. Moreover, due to mining activity and its environmental implications, it is of vital importance to predict potential breaches of tailings dams, sedimentation processes in thickeners, and their impact on the environment and urban areas surrounding mining treatment plants. The characterization and study of these phenomena involve mathematical and numerical modeling of complex partial differential equations (PDEs), and having tools that enable numerical simulations of these events would allow us to be one step ahead of their occurrence. Furthermore, such tools would enable us to make decisions that can minimize the environmental and social impact in the event that they unavoidably happen.

From the physical-mathematical perspective, viscous flows such as water or air are modeled using the shallow water equations, also known as the Saint-Venant equations [1–3]. These equations are often coupled with models of polydisperse sedimentation to simulate the processes of transport and deposition of suspended particles in a viscous fluid [4, 5]. These models are suitable for studying and simulating sedimentation processes, sediment transport in rivers and estuaries, as well as certain industrial processes arising from wastewater treatment plants and the mining industry, such as tailings ponds and thickeners [6–8].

In general, these models can be formulated as a system of non-homogeneous conservative hyperbolic partial differential equations (PDEs), which means that we are looking for a vector w of unknown functions satisfying:

$$\partial_t w + \nabla \cdot F(w) = S(w), \tag{1}$$

Where t represents the temporal variable, ∇ is the gradient operator, $F(w)$ is the flux function, and $S(w)$ is the source term. This type of PDEs has the advantage of a wide range of numerical methods available for their solution [9], but it has the difficulty that the solution w is generally discontinuous. This practical implication results in a high computational cost associated with its numerical resolution. Unfortunately, not all models can be written in the form (1), but some can be reformulated in a more general manner as a system of hyperbolic PDEs with non-conservative and non-homogeneous

products.

$$\partial_t w + \mathcal{A}(w) \cdot \nabla w = S(w), \tag{2}$$

Where $\mathcal{A}(w) \cdot \nabla w$ represents a non-conservative product. The non-conservative product in the system of PDEs (2) leads to additional numerical difficulties, precisely associated with the fact that the solution w is discontinuous. This product does not allow for the definition of weak solutions in the classical distributional sense. Therefore, it is necessary to undergo special treatment before designing numerical methods [10].

From the perspective of numerical analysis, both (1) and (2) require dealing with temporal dependence and nonlinearities, as well as with physical properties of the solution that are highly challenging for conventional numerical methods. Particularly, the presence of discontinuities and shock wave formations. In practice, this leads to a high computational cost associated with their numerical resolution, often making it impractical for practical purposes. Studying and developing stable and robust numerical methods capable of providing high-resolution solutions at a low computational cost is crucial.

In [11], the authors study the shallow water equations with variable bathymetry in space and bottom friction. It is known that these hyperbolic PDE systems degenerate and discontinuities appear in the solution after a critical time. Such discontinuities are well approximated by the Discontinuous Galerkin (DG) methods. For times during which the solution remains smooth, the authors observe that DG methods are a good choice when seeking high-order methods to solve hyperbolic systems [11]. Similarly, shallow water models applied to erosion, sediment transport, and avalanches are addressed in [1, 2, 12]. Such models can be compactly formulated as a system of conservative hyperbolic PDEs. The authors design numerical schemes using strategies of the finite volume method type.

Some systems of non-conservative hyperbolic PDEs are addressed in [13–16], where the authors utilize the theory introduced by Dal Maso et al. [10] to define these products appropriately based on a family of paths that satisfy certain consistency and regularity properties. This approach opens up the possibility of designing suitable numerical methods for this type of PDEs.

2 The modified MLB function

In this section, using the mixing theory developed more recently by Truesdell and Toupin [17], a mathematical model is obtained that describes the polydisperse sedimentation process, which in turn leads to obtaining a modification of the MLB velocity function proposed by Masliyah [18]. This approach allows considering a mixture as a superposition of continuous media. Then, each of the solid spherical species and the fluid satisfy a mass balance and linear momentum law given by

$$\partial_t(\rho_j \phi_j) + \nabla \cdot (\rho_j \phi_j \boldsymbol{v}_j) = 0, \quad j = 0, \ldots, N. \tag{3}$$

$$\partial_t(\rho_j \phi_j \boldsymbol{v}_j) + \nabla \cdot (\rho_j \phi_j \boldsymbol{v}_j \otimes \boldsymbol{v}_j) = \nabla \cdot \boldsymbol{T}_j - \rho_j \phi_j g \boldsymbol{k} + \boldsymbol{m}_i^{\mathrm{f}}, \quad j = 1, \ldots, N, \tag{4}$$

$$\partial_t(\rho_0\phi_0\boldsymbol{v}_0) + \nabla\cdot(\rho_0\phi_0\boldsymbol{v}_0\otimes\boldsymbol{v}_0) = \nabla\cdot\boldsymbol{T}_0 - \rho_0\phi_0 g\boldsymbol{k} - (\boldsymbol{m}_1^{\mathrm{f}} + \cdots + \boldsymbol{m}_N^{\mathrm{f}}). \tag{5}$$

where for each species of spherical solid particles dispersed in a viscous fluid j, $j = 1,\ldots,N$, ϕ_j, ρ_j, and d_j denote volumetric concentration, density, and diameter, respectively. Furthermore, $\boldsymbol{v}_j = (u_j, v_j, w_j)^{\mathrm{T}} \in \mathbb{R}^3$ its phase velocity. The fluid velocity is indexed by $j = 0$. The stress tensor (without viscous stress tensor) is given by $\boldsymbol{T}_j = -p_j\boldsymbol{I}$ ($\boldsymbol{T}_0$ for the fluid), and $p_j = \phi_j p$ is the pressure of phase j for $j = 1,\ldots,N$. The interaction forces per unit volume between solid species j and the fluid is given by $\boldsymbol{m}_i^{\mathrm{f}} = \alpha_j(\Phi)\boldsymbol{u}_j + p\nabla\phi_j$, where α_j is the resistance coefficient for the transfer of momentum between the fluid and solid phase species j satisfying $\phi_j/\alpha_j(\Phi) = -d_j^2 V(\phi)/18\mu_{\mathrm{f}}$, where μ_{f} is the viscosity of the fluid, $V(\phi)$ is the well-known hindered settling factor which is given by the Richardson-Zaki expression [19]

$$V(\phi) = \begin{cases} (1-\phi)^{n-2} & \text{for } \phi \le 1, \\ 0 & \text{for } \phi > 1, \end{cases} \quad n > 2. \tag{6}$$

that satisfy $V(\phi) > 0$ and $V'(\phi) < 0$ for $0 < \phi < \phi_{\max}$ [18, 20–23].

To get the joint sedimentation velocity v^{MLB}, the mass balance equation for species j is used, and the product $\rho_j\phi_j\boldsymbol{v}_i$ is rewritten. Defining the slip velocities $\boldsymbol{u}_j := \boldsymbol{v}_j - \boldsymbol{v}_0$ and $\lambda_j := \rho_j\phi_j/\rho$ for $j = 1,\ldots,N$, with $\rho = \rho_0\phi_0 + \rho_1\phi_1 + \cdots + \rho_N\phi_N$ yields

$$\rho_j\phi_j\boldsymbol{v}_j = \rho_j\phi_j\big(\boldsymbol{u}_j + \boldsymbol{v} - (\lambda_1\boldsymbol{u}_1 + \cdots + \lambda_N\boldsymbol{u}_N)\big), \quad j = 1,\ldots,N; \tag{7}$$

where $\boldsymbol{v}$ is the mixture velocity given by $\boldsymbol{v} = \sum_{k=0}^{N}\lambda_k\boldsymbol{v}_k$. Analogously to the work carried out by the authors in [20], an expression for the slip velocity is obtained using the linear momentum equations for the solid species and the fluid, (4) and (5), respectively.

$$\begin{aligned} \boldsymbol{u}_j &= g\frac{\phi_j}{\alpha_j(\Phi)}(\bar{\rho}_j - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi)\boldsymbol{k} \\ &= \mu\delta_j V(\phi)(\bar{\rho}_j - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi)\boldsymbol{k} \end{aligned} \quad j = 1,\ldots,N, \tag{8}$$

where we introduce the vector of reduced densities $\bar{\boldsymbol{\rho}} = (\bar{\rho}_1,\ldots,\bar{\rho}_N)^{\mathrm{T}}$ with $\bar{\rho}_i = \rho_i - \rho_0$, $i = 1,\ldots,N$, $\mu := -gd_1^2/(18\mu_{\mathrm{f}})$, $\delta_i := d_i^2/d_1^2$, $i = 1,\ldots,N$ and $\Phi = (\phi_1,\ldots,\phi_N)$.

Introducing equation (8) into (9) we get for $j = 1,\ldots,N$

$$\begin{aligned} \rho_j\phi_j\boldsymbol{v}_j &= \rho_j\phi_j\boldsymbol{v} + \rho_j\phi_j\mu V(\phi)\big(\delta_j(\bar{\rho}_j - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi) - \sum_{i=1}^{N}\lambda_i\delta_i(\bar{\rho}_i - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi)\big)\boldsymbol{k} \\ &= \rho_j\phi_j\boldsymbol{v} + \rho_j f_j^{\mathrm{M}}(\Phi)\boldsymbol{k}. \end{aligned} \tag{9}$$

where $f_j^{\mathrm{M}}(\Phi)$ is a vertical flux function that contain the modified MLB velocity and is given by

$$f_j^{\mathrm{M}}(\Phi) = \phi_j v_j^{MLB} = \phi_j \mu V(\phi)\left(\delta_j(\bar{\rho}_j - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi) - \sum_{k=1}^{N} \lambda_k \delta_k(\bar{\rho}_k - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi)\right), \tag{10}$$

for $j = 1, \ldots, N$. In this case the MLB velocity v_j^{MLB} for $j = 1, \ldots, N$ is

$$v_j^{\mathrm{MLB}} = \mu V(\phi)\left(\delta_j(\bar{\rho}_j - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi) - \sum_{k=1}^{N} \lambda_k \delta_k(\bar{\rho}_k - \bar{\boldsymbol{\rho}}^{\mathrm{T}}\Phi)\right). \tag{11}$$

Equivalently, after some algebraic manipulations, we obtain

$$v_j^{\mathrm{MLB}} = V(\phi)\left(w_{s,0}^j \frac{\rho_j - \rho}{\rho_j - \rho_0} - \sum_{i=1}^{N} \frac{\rho_i - \rho}{\rho_i - \rho_0} \lambda_i w_{s,0}^i\right), \tag{12}$$

where $w_{s,0}^j = \mu\delta_j(\rho_j - \rho_0)$ for $j = 1, \ldots, N$. Finally, it is possible to note the difference between (12) and the classical model observed in equation (28) in [24] and in the [18].

The equation (12) will allow us to introduce all the necessary modifications to model the polydisperse sedimentation process where the mixture in question consists of cohesive and non-cohesive particles, thus obtaining an appropriate model to simulate coastal areas and other muddy environments. Another important point here is that this combined sedimentation velocity v^{MLB} is penalized in those areas where the density of the mixture is high. A particular case, for $N = 1$ the MLB velocity is given by

$$v^{\mathrm{MLB}} = -\frac{gd^2\bar{\rho}}{18\mu_{\mathrm{f}}} V(\phi)(1-\phi)^2 \frac{\rho_0}{\rho},$$

in contrast to the monodisperse sedimentation model presented by Tory et al. [25].

2.1 Hindered settling velocity for mixtures with cohesive and noncohesive particles

Within this section, we present the expressions that will be used to describe hindered settling velocity, among which we will distinguish between hindered settling velocity for cohesive and non-cohesive particles. We will also differentiate between the model for bidisperse suspensions (sand and mud suspension) and a more general model for polydisperse sedimentation.

From the equation (12) defining $w_s^j = (1-\phi)^n w_{s,0}^j$ we get

$$v_j^{\mathrm{MLB}} = \frac{1}{(1-\phi)^2}\left(\frac{\rho_j - \rho}{\rho_j - \rho_0} w_s^j - \sum_{i=1}^{N} \lambda_i \frac{\rho_i - \rho}{\rho_i - \rho_0} w_s^i\right), \tag{13}$$

This last equality allows for the introduction of all velocity models for both cohesive and non-cohesive particles that arise from the deconstruction of the Richardson-Zaki equation explored in [24] for mixtures in which all species have equal density. Here, the model (13) is more comprehensive and suitable to describe mixtures comprising different solid particle species (both cohesive and non-cohesive) with different sizes and densities.

Following the results obtained by Spearman et al. [24], for polydisperse mixtures we define for cohesive particles $j \in \{1, \ldots, N\}$,

$$w_s^j = w_{s,0}^j (1-\phi) \left(1 - \frac{\phi_{max}}{\phi_{gel}}\phi\right) \left(1 - \frac{\phi}{\phi_{gel}}\right)^{1.5} \tag{14}$$

and for the noncohesive particles we propose

$$w_s^j = \max(w1_s^j, w2_s^j) \tag{15}$$

where

$$w1_s^j = w_{s,0}^j (1-\phi)^m \left(1 - \frac{\phi}{\phi_{max}}\right)^{n'} \text{ and } w2_s^j = (1-\phi)^n w_{s,0}^j,$$

respectively, with $n' = 0.62n - 1.46$ and $m = 2.7 - 0.15n$. In (14) ϕ_{max}, is a maximum packing volume and ϕ_{gel} the volume concentration at which gelling occurs.

3 Numerical method

3.1 Mathematical model

The polydisperse sedimentation model for mixtures of cohesive and non-cohesive particulate material dispersed in a viscous fluid that we propose is given by the mass conservation and linear momentum balance equations for the solids species and the global linear momentum of the mixture

$$\partial_t(\rho_j \phi_j) + \nabla \cdot (\rho_j \phi_j \boldsymbol{v} + \rho_j f_j^{\mathrm{M}}(\Phi)\boldsymbol{k}) = 0, \quad j = 1, \ldots, N, \tag{16}$$

$$\rho_j(\partial_t(\phi_j \boldsymbol{v}_j) + \nabla \cdot (\phi_j \boldsymbol{v}_j \otimes \boldsymbol{v}_j)) = -\phi_j \nabla p - \phi_j \rho g \boldsymbol{k}, \quad j = 1, \ldots, N. \tag{17}$$

$$\partial_t \left(\sum_{j=0}^{N} \rho_j \phi_j \boldsymbol{v}_j\right) + \nabla \cdot \left(\sum_{j=0}^{N} \rho_j \phi_j \boldsymbol{v}_j \otimes \boldsymbol{v}_j\right) = -p\boldsymbol{I} - \rho g \boldsymbol{k}. \tag{18}$$

plus the vertical flux function (10) with the modified Masliyah Lockett and Basson velocity given by (13), (14) and (15).

In [23], a model with sediment compression and vertical viscosity is introduced. The authors develop two-dimensional and three-dimensional coupled models (Navier-Stokes + sedimentation models) that consider horizontal motions along with vertical

particle segregation processes. Numerically solving the resulting full 3D model is highly complicated (three spatial dimensions plus time). One of the strategies that has been recently used is the introduction of the multilayer framework, which allows for a reduction in both equation analysis costs and computational expenses. In [26–29], the authors obtain multilayer versions of more complex models whose most notable advantage is the reduction in the number of spatial coordinates. Following the introduction of the multilayer framework, efficient numerical methods are designed to simulate the phenomenon under study across different scenarios. The direction in the following sections is to obtain the multilayer version of the obtained model and then design a suitable numerical method to simulate mixtures with cohesive and non-cohesive material, varying in sizes and densities.

3.2 Layers, interfaces, and boundaries

We shall consider a d-dimensional space ($d = 2, 3$). For a given final time $T > 0$ and each time $t \in [0, T]$ we denote by $\Omega_{\mathrm{F}}(t)$ the fluid domain and by $I_{\mathrm{F}}(t)$ its projection onto the horizontal plane. In order to introduce a multilayer system, the fluid domain is divided along the vertical direction into $M \in \mathbb{N}^*$ pre-set layers of thickness $h_\alpha(t, \boldsymbol{x})$ with $M + 1$ interfaces

$$\Gamma_{\alpha+1/2}(t) = \big\{(\boldsymbol{x}, z) \in \mathbb{R}^d : z = z_{\alpha+1/2}(t, \boldsymbol{x}),\, \boldsymbol{x} \in I_{\mathrm{F}}(t)\big\}, \quad \alpha = 0, 1, \ldots, M$$

(see Figure **??**). We assume that the interfaces $\Gamma_{\alpha+1/2}(t)$ are smooth, concretely at least of class C^1 in time and space. We denote by $z_{\mathrm{B}} = z_{1/2}$ and $z_{\mathrm{S}} = z_{M+1/2}$ the equations of the bottom and the free surface interfaces $\Gamma_{\mathrm{B}}(t)$ and $\Gamma_{\mathrm{S}}(t)$, respectively. The thickness of layer α at time t and horizontal position $\boldsymbol{x}$ is

$$h_\alpha = h_\alpha(t, \boldsymbol{x}) = z_{\alpha+1/2}(t, \boldsymbol{x}) - z_{\alpha-1/2}(t, \boldsymbol{x}), \quad \alpha = 1, \ldots, M,$$

such that $z_{\alpha+1/2} = z_{\mathrm{B}} + h_1 + \cdots + h_\alpha$ for $\alpha = 1, \ldots, M$. Then the height of the fluid is $h := z_{\mathrm{S}} - z_{\mathrm{B}} = h_1 + \cdots + h_M$.

The boundary $\partial\Omega_{\mathrm{F}}(t)$ of $\Omega_{\mathrm{F}}(t)$ can be represented as $\partial\Omega_{\mathrm{F}}(t) = \Gamma_{\mathrm{B}}(t) \cup \Gamma_{\mathrm{S}}(t) \cup \Theta(t)$, where $\Theta(t)$ is the inflow/outflow boundary which we assume here to be vertical. The fluid domain is split as $\overline{\Omega_{\mathrm{F}}(t)} = \cup_{\alpha=1}^{M} \overline{\Omega_\alpha(t)}$, where we define the layers and their boundaries as

$$\Omega_\alpha(t) := \big\{(\boldsymbol{x}, z) : \boldsymbol{x} \in I_{\mathrm{F}}(t) \text{ and } z_{\alpha-1/2} < z < z_{\alpha+1/2}\big\},$$

such that

$$\partial\Omega_\alpha(t) := \Gamma_{\alpha-1/2}(t) \cup \Gamma_{\alpha+1/2}(t) \cup \Theta_\alpha(t), \quad \Theta_\alpha(t) := \big\{(\boldsymbol{x}, z) : \boldsymbol{x} \in \partial I_{\mathrm{F}}(t) \text{ and } z_{\alpha-1/2} < z < z_{\alpha+1/2}\big\}.$$

Hence the inflow/outflow boundary is split as $\overline{\Theta(t)} = \cup_{\alpha=1}^{M} \overline{\Theta_\alpha(t)}$.

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