Numerical simulations of a model of polydisperse reactive settling in shallow water channels*

Julio Careaga† Víctor Osores‡

Abstract

A multidimensional model of polydisperse reactive sedimentation is approximated using the a multilayer shallow water approach. The model consists of several solid particles of different size and density, and substrates diluted in water, which produce biochemical reactions while settling down.

The model employs the Masliyah–Lockett–Bassoon (MLB) settling velocities of each species.

The final model can be written as a multilayer model with variable density where the unknowns are the average velocities and concentrations in each layer, the transfer terms across each interface, and the total mass. An explicit bound of the minimum and maximum eigenvalues of the transport matrix of the system is utilized to design a Harten–Lax–van Leer (HLL)-type path-conservative numerical method. Numerical simulations illustrate the coupled polydisperse sedimentation and flow fields in various scenarios, including sedimentation in a type of basin that is used in practice in mining industry and in a basin whose bottom topography gives rise to recirculations of the fluid and high solids concentrations.

1 Introduction

Reactive sedimentation is defined as the process in which multiple types of solid particles suspended on a fluid settle due to gravity, while reacting with dilute substrates. The solid phase is then composed by organic or innert matter, including bacteria considered as solid particles, and the fluid phase is constituted by substrates each one completely diluted in water. An example of reactive sedimentation can be found in wastewater industries, when the so-called activated sludge is treated in the Secondary Settling Tank (SST). Activated sludge models (ASMs) have been widely developed in terms of biokinetic reactions and ordinary differential equations (ODEs), see e.g. [34, 29, 35, 36, 32, 31]. Models accounting space variations based on partial differential equations (PDEs) have been studied to a lesser extent. The one-dimensional PDE-based model presented in [8], which has evolved from the previous work [9], constitutes one of the few models including the complexity of nonlinear effects appearing in the sedimentation-consolidation process. Furthermore, this model is tailored to handle mixtures of arbitrary number of solid species and liquid substrates. Extensions to Sequencing Batch Reactors (SBRs), in which the main complication is related to a moving-boundary problem, can be found in [10, 11, 13], and comparisons with experimental data are presented in [12].

In terms of advancements in PDE-based models of mono-dispersed and non-rective sedimentation, including the development of suitable numerical schemes, a variety of works for different space-dimensions and numerical methods can be found in the literature. One-dimensional approaches for batch and continuous sedimentation such as [19, 27, 15, 28, 16, 30, 42] are mainly approximated by finite differences or finite volume schemes, with focus on non-linear flux approximations. The special

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†Departamento de Matemática, Universidad del Bío Bío, Chile, email:jcareaga@ubiobio.cl.

‡Departamento de Matemática, Universidad Católica del Maule, Chile, email:vosores@ucm.cl.

case of quasi-one-dimensional models [1, 23, 6, 7, 14], treat the container geometry as a coefficient function. Already for two space dimensions, most of the models need to be supplemented with momentum balances, increasing the number of equations to be solved and adding a substantial degree of complexity. Different variants appear depending on the velocity field considered: volume-average velocity [20, 21], mass-average velocity [40], and solid-phase velocity [33, 22]. In [20], a multiresolution finite volume scheme is used to approximate the two dimensional model, while a combination of finite volumes and mixed finite element methods is employed in [22]. A sophisticated finite volume element method was tailored in [21] to approximate their developed axisymmetrical model. For suspensions composed by solid species with different densities, an adequate description of the process comes from a polydisperse sedimentation model. In this line, the work in [18] addresses a multilayer Saint-Venant (MSV) polydisperse model in three dimensional domains having a free boundary. This dynamic multilayer approach combines the theory of mixtures with the ideas presented in [2, 4, 3], so that the final model couples a type of multilayer shallow water equations with the polydisperse sedimentation model developed in [5, 41]. The multilayer method provides then an efficient alternative for numerically solving the transport and flow equations by layers, reducing the problem by one space dimension. An additional gain in the formulation proposed in [18] is that the vertical components of the velocity fields are computed by means of a post-processing procedure. The numerical scheme proposed is based on the specialized methods for hyperbolic equations with non-conservative products [26, 25], which employ the theory introduced by Dal Maso et al. [39] to properly approximate the non-conservative products.

The aims of this work is to extend the reactive sedimentation model in [8] to the three-dimensional polydisperse case following the line of [18], this is, employing an MSV approach. In contrast to the one-dimensional scenario, in which only mass balances are required, we need to take into account momentum equations. The latter contemplates the inclusion of the viscous stress tensor of the mixture in terms of a mass-average velocity. Hence, we derive a polydisperse multidimensional reactive sedimentation model, that couples convection-diffusion-reaction transport equations with flow equations. In turn, the MSV approach, which requires the assumption of shallow water, is employed in order to reduce the complexity that three-dimensional evolutionary PDEs mean. With this, we aspire to give a full description of the model equations making distinction beteween the vertical coordinate (pointing in the oposite direction to gravity) and the horizontal ones, so that the equations are written in layers that subdivide the vertical axis. Moreover, we seek to develop a numerical scheme for the approximation of the model equations combining the Harten–Lax–van Leer (HLL)-type path-conservative numerical method from [24] with upwind flux approximations for the substrates.

1.1 Outline of the paper

The organization of the paper is as follows. In Section 2, we introduce derive the general model equations. The multilayer approach is presented in Section 3, and the numerical scheme is described in Section 4. Finally, a selection of numerical results are presented in Section 5 and the concluding remarks are given in Section 6.

2 Model derivation

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Let Ω be a bounded domain in $\mathbb{R}^3$ and $\boldsymbol{x} := (x_1, x_2, z)$ the coordinates of a point in Ω with $\widetilde{\boldsymbol{x}} = (x_1, x_2)$ corresponding to the horizontal coordinates, and $\Omega_T := \Omega \times (0, T]$ for $T > 0$. For ease in notation, for each $k \in \mathbb{N}$, we define the sets $\mathcal{I}(k) := \{1, 2, \ldots, k\}$ and $\mathcal{I}_0(k) := \{0, 1, \ldots, k\}$. We consider $n_{\boldsymbol{c}} \in \mathbb{N}$ species of spherical solid particles dispersed in a viscous fluid whose vector of volume fractions is $\boldsymbol{\phi} := \left(\phi^{(1)}, \phi^{(2)}, \ldots, \phi^{(n_{\boldsymbol{c}})}\right)^{\mathrm{t}}$, where the i-th phase volume fraction is denoted by $\phi^{(i)} := \phi^{(i)}(\boldsymbol{x}, t)$ for

all $(\boldsymbol{x},t)\in\Omega_T$. We assume that each solid phase $i\in\mathcal{I}(n_{\boldsymbol{c}})$ has density $\rho_i>0$ and particle diameter $d_i>0$, such that $d_1\geq d_2\geq\cdots\geq d_N$. The volume fraction and density of the fluid phase is defined by $\phi_{\mathrm{f}}:=\phi_{\mathrm{f}}(\boldsymbol{x},t)$ for all $(\boldsymbol{x},t)\in\Omega_T$ and ρ_{f}, resepectively. The velocity field of the phase i is denoted by $\boldsymbol{v}_i:=(u_i,v_i,w_i)\in\mathbb{R}^3$, being $\widetilde{\boldsymbol{v}}_i:=(u_i,v_i)\in\mathbb{R}^2$ its horizontal component for all $i\in\mathcal{I}(n_{\boldsymbol{c}})$, we will also write $\boldsymbol{v}_i=(\widetilde{\boldsymbol{v}}_i,w_i)$. We denote the fluid velocity by $\boldsymbol{v}_{\mathrm{f}}$ and define the vector of solid concentrations by $\boldsymbol{c}:=\big(c^{(1)},c^{(2)},\dots,c^{(n_{\boldsymbol{c}})}\big)^{\mathtt{t}}\in\mathbb{R}^{n_{\boldsymbol{c}}}$ such that $c^{(i)}(\boldsymbol{x},t):=\rho_i\phi^{(i)}(\boldsymbol{x},t)$ for all $i\in\mathcal{I}(n_{\boldsymbol{c}})$. The total concentration at each point $(\boldsymbol{x},t)\in\Omega_T$ is given by

$$\rho:=\rho(\boldsymbol{\Phi}(\boldsymbol{x},t))=\rho_{\mathrm{f}}\phi_{\mathrm{f}}(\boldsymbol{x},t)+\sum_{i=1}^{n_{\boldsymbol{c}}}c^{(i)}(\boldsymbol{x},t)\,, \tag{1}$$?def:rho?

where $\boldsymbol{\Phi}:=\big(\phi_{\mathrm{f}},\phi^{(1)},\dots,\phi^{(n_{\boldsymbol{c}})}\big)^{\mathtt{t}}$ is the vector of volume fractions including the fluid volume fraction. We also define the total solids volume fraction as $\phi:=\phi^{(1)}+\cdots+\phi^{(n_{\boldsymbol{c}})}$. Using the constitutive assumption that $\phi_{\mathrm{f}}+\phi=1$, we can express ϕ_{f} in terms of $\boldsymbol{c}$ as follows

$$\phi_{\mathrm{f}}(\boldsymbol{c})=1-\sum_{i=1}^{n_{\boldsymbol{c}}}\frac{1}{\rho_i}c^{(i)}\,,$$

so that we can write $\boldsymbol{\Phi}$ in terms of $\boldsymbol{c}$, therefore $\boldsymbol{\Phi}=\boldsymbol{\Phi}(\boldsymbol{c})$. In turn, we assume that the fluid phase is composed by $n_{\boldsymbol{s}}\in\mathbb{N}$ soluble substrate diluted in water, and define the vector of substrate concentrations by $\boldsymbol{s}:=\big(s^{(1)},s^{(2)},\dots,s^{(n_{\boldsymbol{s}})}\big)^{\mathtt{t}}\in\mathbb{R}^{n_{\boldsymbol{s}}}$, where each component is a function of $(\boldsymbol{x},t)\in\Omega_T$. Taking into account that the solid phase may react with the fluid phase, each solid component satisfies the continuity equation or mass conservation

$$\frac{\partial c^{(i)}}{\partial t}+\operatorname{div}\big(c^{(i)}\boldsymbol{v}_i\big)=\mathcal{R}_{\boldsymbol{c}}^{(i)}(\boldsymbol{c},\boldsymbol{s})\qquad\forall i\in\mathcal{I}(n_{\boldsymbol{c}})\,, \tag{2}$$ eq:mass:c

where $\mathcal{R}_{\boldsymbol{c}}^{(i)}:=\mathcal{R}_{\boldsymbol{c}}^{(i)}(\boldsymbol{c},\boldsymbol{s})$ is a (nonlinear) function involving the kinetic reactions between solid and fluid components. The fluid phase, on the other hand, is composed by $n_{\boldsymbol{s}}$ substrates and water, whose concentration is denoted by $\mathcal{W}:=\mathcal{W}(\boldsymbol{x},t)$, so that the following equation holds

$$\rho_{\mathrm{f}}\phi_{\mathrm{f}}=s^{(1)}+\cdots+s^{(n_{\boldsymbol{s}})}+\mathcal{W}\,.$$

Similarly to (2), the fluid phase fulfills the mass conservation equation

$$\rho_{\mathrm{f}}\frac{\partial\phi_{\mathrm{f}}}{\partial t}+\operatorname{div}(\rho_{\mathrm{f}}\phi_{\mathrm{f}}\boldsymbol{v}_{\mathrm{f}})=\widetilde{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c},\boldsymbol{s})\qquad\forall i\in\mathcal{I}(n_{\boldsymbol{s}}) \tag{3}$$ eq:mass:phif

where the function $\widetilde{\mathcal{R}}_{\boldsymbol{s}}:=\widetilde{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c},\boldsymbol{s})$ corresponds to sum of the functions describing the reactions of each substrate component, defined by $\mathcal{R}_{\boldsymbol{s}}^{(i)}:=\mathcal{R}_{\boldsymbol{s}}(\boldsymbol{c},\boldsymbol{s})$ for $i\in\mathcal{I}(n_{\boldsymbol{s}})$, therefore $\widetilde{\mathcal{R}}_{\boldsymbol{s}}:=\mathcal{R}_{\boldsymbol{s}}^{(1)}+\mathcal{R}_{\boldsymbol{s}}^{(2)}+\cdots+\mathcal{R}_{\boldsymbol{s}}^{(n_{\boldsymbol{s}})}$. In addition, using the vector of percentages corresponding to each substrate $\boldsymbol{p}:=\big(p^{(1)},p^{(2)},\dots,p^{(n_{\boldsymbol{s}})}\big)\in\mathbb{R}^{n_{\boldsymbol{s}}}$, where $\boldsymbol{p}(\boldsymbol{x},t):=\boldsymbol{s}(\boldsymbol{x},t)/(\rho_{\mathrm{f}}\phi_{\mathrm{f}}(\boldsymbol{x},t))$, and assuming that the substrate components move with the same velocity $\boldsymbol{v}_{\mathrm{f}}$, we can establish from (3) the continuity equation for each substrate component and water concentration

$$\frac{\partial s^{(i)}}{\partial t}+\operatorname{div}(s^{(i)}\boldsymbol{v}_{\mathrm{f}})=\mathcal{R}_{\boldsymbol{s}}^{(i)}(\boldsymbol{c},\boldsymbol{s})\qquad\forall i\in\mathcal{I}(n_{\boldsymbol{s}})\,, \tag{4a}$$ eq:mass:s

$$\frac{\partial\mathcal{W}}{\partial t}+\operatorname{div}\left(\mathcal{W}\boldsymbol{v}_{\mathrm{f}}\right)=0\,, \tag{4b}$$ eq:mass:w

$$s^{(1)}+\cdots+s^{(n_{\boldsymbol{s}})}+\mathcal{W}=\rho_{\mathrm{f}}\phi_{\mathrm{f}}\,. \tag{4c}$$?eq:sum:s?

We observe that Equation (4b), which determines $\mathcal{W}$, does not need to be solved since this variable can be recovered directly from the third equation as $\mathcal{W} = \rho_{\mathrm{f}}\phi_{\mathrm{f}}(\boldsymbol{c}) - \big(s^{(1)} + \cdots + s^{(n_{\boldsymbol{s}})}\big)$. Now we are going to introduce constitutive assumptions over the velocity terms in equations (2) and (4a) such that we can reformulate these equations in terms of the slip velocities $\boldsymbol{u}_i := \boldsymbol{v}_i - \boldsymbol{v}_{\mathrm{f}}$ for $i \in \mathcal{I}(n_{\boldsymbol{c}})$ and the so-called mass-average velocity, defined by

$$\boldsymbol{v} := \frac{1}{\rho(\boldsymbol{\Phi})}\left(\rho_{\mathrm{f}}\phi_{\mathrm{f}}\boldsymbol{v}_{\mathrm{f}} + \sum_{j=1}^{n_{\boldsymbol{s}}} c^{(j)}\boldsymbol{v}_j\right). \tag{5}$$?def:mass-avera

Then, straightforwardly from the definition of the slip and mass-average velocities, we can obtain the following expressions for the velocity of the solid and fluid phase

$$\boldsymbol{v}_i = \boldsymbol{v} + \boldsymbol{u}_i - \frac{1}{\rho}\sum_{j=1}^{n_{\boldsymbol{c}}} c^{(j)}\boldsymbol{u}_j \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,, \tag{6}$$ eq:relmassv

$$\boldsymbol{v}_{\mathrm{f}} = \boldsymbol{v} - \frac{1}{\rho_{\mathrm{f}}\phi_{\mathrm{f}}}\sum_{i=1}^{n_{\boldsymbol{c}}} c^{(i)}\left(\boldsymbol{u}_i - \frac{1}{\rho}\sum_{j=1}^{n_{\boldsymbol{c}}} c^{(j)}\boldsymbol{u}_j\right). \tag{7}$$ eq:relslipv

Next, introducing the consitutive assumption given in [18, Equation 2.9], we can describe each slip velocity as a function of the of the vector of solid concentrations and its gradient, i.e., $\boldsymbol{u}_i = \boldsymbol{u}_i(\boldsymbol{c}, \nabla\boldsymbol{c})$ for $i \in \mathcal{I}(n_{\boldsymbol{c}})$, so that we have

$$c^{(i)}\left(\boldsymbol{u}_i - \frac{1}{\rho}\sum_{j=1}^{n_{\boldsymbol{c}}} c^{(j)}\boldsymbol{u}_j\right) = f_i(\boldsymbol{c})\boldsymbol{k} - \boldsymbol{a}_i(\boldsymbol{c}, \nabla\boldsymbol{c}) \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,, \tag{8}$$ eq:sliprel

where $f_i(\boldsymbol{c}) := c^{(i)}v_i^{\mathrm{MLB}}(\boldsymbol{c})$ is the batch flux function of the solid componet $i \in \mathcal{I}(n_{\boldsymbol{c}})$, with $v_i^{\mathrm{MLB}}(\boldsymbol{c})$ the i-th Masliyah–Lockett–Bassoon (MLB) settling velocity function [38, 37], and $\boldsymbol{a}_i := \boldsymbol{a}_i(\boldsymbol{c}, \nabla\boldsymbol{c})$ is the compression term corresponding to the i-th solid specie. For each solid component $i \in \mathcal{I}(n_{\boldsymbol{c}})$, the MLB settling velocity and compression functions are given by

$$v_i^{\mathrm{MLB}}(\boldsymbol{c}) := \mu v_{\mathrm{hs}}(c_{\mathrm{tot}})\vartheta_i(\boldsymbol{c})\,, \tag{9}$$?def:vLMB?

$$\begin{aligned}\boldsymbol{a}_i(\boldsymbol{c}, \nabla\boldsymbol{c}) := -\frac{\mu}{g}v_{\mathrm{hs}}(c_{\mathrm{tot}})\Bigg\{&\frac{(1-\phi(\boldsymbol{c}))c^{(i)}}{\phi(\boldsymbol{c})}\big(\delta_i - \boldsymbol{\delta}^{\mathrm{T}}\boldsymbol{c}/\rho(\boldsymbol{c})\big)\nabla\sigma_{\mathrm{e}}(c_{\mathrm{tot}}) \\ &+ \sigma_{\mathrm{e}}(c_{\mathrm{tot}})\left[\delta_i\nabla\left(\frac{c^{(i)}}{\phi(\boldsymbol{c})}\right) - c^{(i)}\sum_{j=1}^{N}\frac{\delta_j}{\rho(\boldsymbol{c})}\nabla\left(\frac{c^{(j)}}{\phi(\boldsymbol{c})}\right)\right]\Bigg\},\end{aligned} \tag{10}$$ def:a_i

where $c_{\mathrm{tot}} := c^{(1)} + \cdots + c^{n_{\boldsymbol{c}}}$ is the total solids concentration, $v_{\mathrm{hs}} := v_{\mathrm{hs}}(c_{\mathrm{tot}})$ is the hindered settling velocity, $\sigma_{\mathrm{e}} := \sigma_{\mathrm{e}}(c_{\mathrm{tot}}) \geq 0$ is the effective solid stress function with compact contained in $[0, c_{\max}]$, and for each $i \in \mathcal{I}(n_{\boldsymbol{c}})$, the function ϑ_i is given by

$$\vartheta_i(\boldsymbol{c}) := \delta_i\big(\rho_i + \phi_{\mathrm{f}}(\boldsymbol{c})\rho_{\mathrm{f}} - c_{\mathrm{tot}}\big) - \sum_{k=1}^{n_{\boldsymbol{c}}}\frac{c^{(k)}}{\rho(\boldsymbol{c})}\delta_k\big(\rho_k + \phi_{\mathrm{f}}(\boldsymbol{c})\rho_{\mathrm{f}} - c_{\mathrm{tot}}\big)\,.$$

Then, replacing the relation for the slip velocities (8) into the expressions for the solid and fluid velocities, (6) and (7), respectively, we can finally write the fluxes corresponding to (2) and (4a) in terms of $\boldsymbol{v}$, $\boldsymbol{c}$ and $\nabla\boldsymbol{c}$, as follows

$$c^{(i)}\boldsymbol{v}_i = c^{(i)}\boldsymbol{v} + f_i(\boldsymbol{c})\boldsymbol{k} - \boldsymbol{a}_i(\boldsymbol{c}, \nabla\boldsymbol{c}) \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,,$$

$$s^{(i)}\boldsymbol{v}_{\mathrm{f}} = s^{(i)}\boldsymbol{v} - \frac{s^{(i)}}{\rho_{\mathrm{f}}\phi_{\mathrm{f}}(\boldsymbol{c})}\sum_{j=1}^{n_{\boldsymbol{c}}}\Big(f_j(\boldsymbol{c})\boldsymbol{k} - \boldsymbol{a}_j(\boldsymbol{c}, \nabla\boldsymbol{c})\Big) \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{s}})\,,$$

where $\boldsymbol{k}$ is the unit vector pointing in the opposite direction of gravity, i.e., $\boldsymbol{k} = (0, 0, -1)$, or simply $\boldsymbol{k} = (\boldsymbol{0}, -1)$. Adding up (2) and (4a), we get an equation for mass conservation of the mixture

$$\frac{\partial \rho}{\partial t} + \operatorname{div}\big(\rho \boldsymbol{v}\big) = \widetilde{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}, \boldsymbol{s}) + \widetilde{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c}, \boldsymbol{s})\,. \tag{11}$$?eq:mass:mixtur

Note that ρ is also a function of $\boldsymbol{c}$. To determine the mass-average velocity $\boldsymbol{v}$, we introduce the momentum balance equation of the mixture (see for instance [17])

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \mathbf{div}\big(\rho \boldsymbol{v} \otimes \boldsymbol{v} - \mu \boldsymbol{e}(\boldsymbol{v})\big) + \nabla p = -\rho g \boldsymbol{k}\,, \tag{12}$$?eq:momentum:mi

where p is the pressure (excess pore pressure maybe), μ is the viscosity of the mixture, and $\boldsymbol{e}(\boldsymbol{v}) := \frac{1}{2}\big(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\mathsf{t}}\big)$ is the symmetric part of the gradient. Then, the final PDE system of equations is the following: Find $(\boldsymbol{c}, \boldsymbol{s}, (\boldsymbol{v}, p))$ such that for each $\boldsymbol{x} \in \Omega$ and $t > 0$

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$$\frac{\partial \rho}{\partial t} + \operatorname{div}\big(\rho \boldsymbol{v}\big) = \widetilde{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}, \boldsymbol{s}) + \widetilde{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c}, \boldsymbol{s})\,, \tag{13a}$$ eq:fm:mass:mixt

$$\frac{\partial}{\partial t}(\rho \boldsymbol{v}) + \mathbf{div}\big(\rho \boldsymbol{v} \otimes \boldsymbol{v} - \mu \boldsymbol{e}(\boldsymbol{v})\big) + \nabla p = -\rho g \boldsymbol{k}\,, \tag{13b}$$ eq:fm:momentum:

$$\frac{\partial c^{(i)}}{\partial t} + \operatorname{div}\big(c^{(i)} \boldsymbol{v} + f_i(\boldsymbol{c}) \boldsymbol{k} - \boldsymbol{a}_i(\boldsymbol{c}, \nabla \boldsymbol{c})\big) = \mathcal{R}_{\boldsymbol{c}}^{(i)}(\boldsymbol{c}, \boldsymbol{s}) \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,. \tag{13c}$$ eq:fm:mass:c

$$\frac{\partial s^{(i)}}{\partial t} + \operatorname{div}\left(s^{(i)} \boldsymbol{v} - s^{(i)} \sum_{j=1}^{n_{\boldsymbol{c}}} \frac{f_j(\boldsymbol{c}) \boldsymbol{k} - \boldsymbol{a}_j(\boldsymbol{c}, \nabla \boldsymbol{c})}{\rho_{\mathrm{f}} \phi_{\mathrm{f}}(\boldsymbol{c})}\right) = \mathcal{R}_{\boldsymbol{s}}^{(i)}(\boldsymbol{c}, \boldsymbol{s}) \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,. \tag{13d}$$ eq:fm:mass:s

In Section 3, we are going to introduce the multilayer approach of (13), where an extra unknown corresponding to the height of each layer is included. Nevertheless, an additional assumption on the pressure p will allow us maintaining the same number of equations as in system (13). We end this section by posting the assumptions that the reaction terms need to fulfill. We assume that there exist stoichiometric matries $\boldsymbol{\sigma}_{\boldsymbol{c}} \in \mathbb{R}^{\ell \times n_{\boldsymbol{c}}}$ and $\boldsymbol{\sigma}_{\boldsymbol{s}} \in \mathbb{R}^{\ell \times n_{\boldsymbol{s}}}$, where $\ell > 0$ is the number of non-negative reaction rates. Considering that the ℓ reaction rates are given by the vector function $\boldsymbol{\kappa} := \boldsymbol{\kappa}(\boldsymbol{c}, \boldsymbol{s}) \in \mathbb{R}^{\ell}$, the reaction terms are defined as

$$\boldsymbol{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}, \boldsymbol{s}) = \boldsymbol{\sigma}_{\boldsymbol{c}} \boldsymbol{\kappa}(\boldsymbol{c}, \boldsymbol{s})\,, \qquad \boldsymbol{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c}, \boldsymbol{s}) = \boldsymbol{\sigma}_{\boldsymbol{s}} \boldsymbol{\kappa}(\boldsymbol{c}, \boldsymbol{s})\,.$$

We also define the following sets

$$J^{-}_{\boldsymbol{\eta},l} := \Big\{ j \in \mathbb{N} : \sigma_{\boldsymbol{\eta}}^{(l,j)} < 0 \Big\}\,, \qquad J^{+}_{\boldsymbol{\eta},l} := \Big\{ j \in \mathbb{N} : \sigma_{\boldsymbol{\eta}}^{(l,j)} > 0 \Big\}\,, \qquad \boldsymbol{\eta} \in \{\boldsymbol{c}, \boldsymbol{s}\}\,, \quad l \in \mathcal{I}(\ell)\,,$$

and make the next assumption for $\boldsymbol{\kappa}$: Given $k \in \mathcal{I}(\ell)$, if $j \in J^{-}_{\boldsymbol{c},k}$, then there exists a bounded function $\bar{\kappa}^{(j)}$ such that

$$\kappa^{(j)}(\boldsymbol{c}, \boldsymbol{s}) = \bar{\kappa}^{(j)}(\boldsymbol{c}, \boldsymbol{s}) c^{(k)}\,. \tag{14}$$?eq:kappacond?

In addition, to guarantee that the numerical solutions of each component of $\boldsymbol{c}$ do not exceed $c_{\max}$, we require the reactive terms tending to zero as c_{tot} approaches $c_{\max}$: There exists an $\varepsilon > 0$ such that $\boldsymbol{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}, \boldsymbol{s}) = \boldsymbol{0}$ for all $c_{\mathrm{tot}} \geq c_{\max} - \varepsilon$.

For the hindered settling velocity v_{hs}, we assume that $v_{\mathrm{hs}}'(u) \leq 0$ for all $u \in [0, u_{\max}]$ and $v_{\mathrm{hs}}(u) = 0$, for $u \geq u_{\max}$. The function $\mathcal{D}$ depends on v_{hs} and the effective solids stress $\sigma_{\mathrm{e}} := \sigma_{\mathrm{e}}(u)$, which is positive only when $u > u_{\mathrm{c}}$ and $\sigma_{\mathrm{e}}(u) = 0$ for $u \leq u_{\mathrm{c}}$. The compression function is then defined by the integral

$$\mathcal{D}(u) := \int_{u_{\mathrm{c}}}^{u} a(s) \mathrm{d}s \qquad \text{with} \qquad a(u) := \frac{\rho}{g(\rho - \rho_{\mathrm{L}})} v_{\mathrm{hs}}(u) \sigma_{\mathrm{e}}'(u)\,,$$

where $0 < \rho_{\mathrm{L}} < \rho$ is the density of the liquid phase.

3 Multilayer model equations

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3.1 Preliminaries

From now on, we consider that for each $t \in [0,T]$, the domain varies with time, this is $\Omega := \Omega(t)$. In order to implement a multilayer approach of (13) we divide the domain $\Omega(t)$ along the vertical direction $-\boldsymbol{k}$ into $M \in \mathbb{N}$ different layers. More precisely, for each $\alpha \in \mathcal{I}(M)$, we consider surfaces $z := z_{\alpha+1/2}(\widetilde{\boldsymbol{x}},t)$ with $\widetilde{\boldsymbol{x}} \in \mathbb{R}^2$, such that layer α at time t corresponds to the set comprehended between the curves $z = z_{\alpha-1/2}(\widetilde{\boldsymbol{x}},t)$ and $z = z_{\alpha+1/2}(\widetilde{\boldsymbol{x}},t)$, i.e. z lies in the interval

$$I_\alpha(\widetilde{\boldsymbol{x}},t) := \big(z_{\alpha-1/2}(\widetilde{\boldsymbol{x}},t), z_{\alpha+1/2}(\widetilde{\boldsymbol{x}},t) \big) \subset \mathbb{R}\,.$$

Then, the layer and interfaces are defined by the sets

$$\Omega_\alpha(t) := \Big\{ (\widetilde{\boldsymbol{x}},z) : \quad z \in I_\alpha(\widetilde{\boldsymbol{x}},t), \quad \widetilde{\boldsymbol{x}} \in \boldsymbol{\Pi}(t) \Big\}, \qquad \forall \alpha \in \mathcal{I}(M)\,, \tag{15}$$ {?}

$$\Gamma_{\alpha+1/2}(t) := \Big\{ (\widetilde{\boldsymbol{x}},z) : \quad z = z_{\alpha+1/2}(\widetilde{\boldsymbol{x}},t), \quad \widetilde{\boldsymbol{x}} \in \boldsymbol{\Pi}(t) \Big\}, \qquad \forall \alpha \in \mathcal{I}_0(M)\,, \tag{16}$$ {?}

where $\boldsymbol{\Pi}(t)$ maps the points in $\Omega(t)$ to their projection in the horizontal plane, i.e., $\widetilde{\boldsymbol{x}} \in \boldsymbol{\Pi}(t)$ if only if there exists $z \in \mathbb{R}$ such that $(\widetilde{\boldsymbol{x}},z) \in \Omega(t)$. The set of layers $\{\Omega_\alpha(t)\}_{\alpha\in\mathcal{I}(M)}$ fulfill the following identities

$$\overline{\Omega(t)} = \bigcup_{\alpha=1}^{M} \overline{\Omega_\alpha(t)} \quad \text{and} \quad \partial\Omega_\alpha(t) = \Gamma_{\alpha-1/2}(t) \cup \Gamma_{\alpha+1/2}(t) \cup \Theta_\alpha(t)\,,$$

where

$$\Theta_\alpha(t) := \Big\{ (\widetilde{\boldsymbol{x}},z) : \quad \widetilde{\boldsymbol{x}} \in \partial\boldsymbol{\Pi}(t), \quad z \in I_\alpha(\widetilde{\boldsymbol{x}},t) \Big\}\,.$$

In addition, we assume that the interfaces are of class C^1 in time and space. The thickness of layer α is defined by the function $h_\alpha := h_\alpha(\widetilde{\boldsymbol{x}},t) := z_{\alpha+1/2}(\widetilde{\boldsymbol{x}},t) - z_{\alpha-1/2}(\widetilde{\boldsymbol{x}},t)$ which will vary with respect to the horizontal position $\widetilde{\boldsymbol{x}}$ and time t, see Figure 1. The top and bottom surfaces are denoted by $z_{\mathrm{B}} := z_{1/2}$ and $z_{\mathrm{S}} := z_{M+1/2}$, and the height of the fluid is $h := z_{\mathrm{S}} - z_{\mathrm{B}}$, and there hold

$$h = \sum_{\alpha=1}^{M} h_\alpha\,, \quad z_{M+1/2} = z_{\mathrm{B}} + h \quad \text{and} \quad z_{\alpha+1/2} = z_{\mathrm{B}} + \sum_{j=1}^{\alpha} h_j\,, \quad \forall \alpha = \mathcal{I}(M)\,,$$

Furthermore, we assume that the layer thicknesses are small enough to neglect the dependence of the horizontal velocities and the concentrations on the vertical variable inside each layer. Finally, for each $\alpha \in \mathcal{I}(M)$ and function $\varphi : \Omega \to \mathbb{R}$, we define the one-sided limits

$$\varphi^-_{\alpha+1/2} := (\varphi|_{\Omega_\alpha})|_{\Gamma_{\alpha+1/2}}, \qquad \varphi^+_{\alpha+1/2} := (\varphi|_{\Omega_{\alpha+1}})|_{\Gamma_{\alpha+1/2}}\,.$$

If φ is continuous across $\Gamma_{\alpha+1/2}(t)$, we simply set $\varphi_{\alpha+1/2} := \varphi|_{\Gamma_{\alpha+1/2}}$.

3.2 Multilayer equations

In what follows, we are going to derive a multilayer approach of system (13), so that the balance equations are established on each layer $\Omega_\alpha(t)$ for all $\alpha \in \mathcal{I}(M)$. In this regard, to properly write the equations in (13) over each α-layer, we need to take into account the flux transmisions at the interfaces

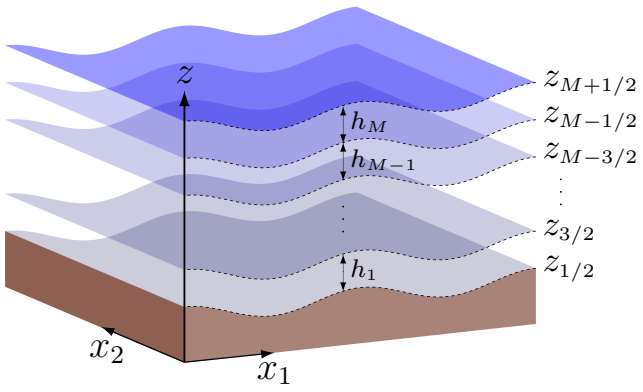

Figure 1: Illustration of the domain subdivision by layers.

$\Gamma_{\alpha+1/2}$. Before delving deeper, we introduce the divergence and gradient operators in the horizontal coordinates as $\mathrm{div}_{\boldsymbol{x}}$ and $\nabla_{\boldsymbol{x}}$, this is

$$\mathrm{div}_{\boldsymbol{x}} := \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}, \qquad \nabla_{\boldsymbol{x}} := (\partial_{x_1}, \partial_{x_2})^{\mathtt{t}},$$

and define $\mathbf{div}_{\boldsymbol{x}}$ as the row-wise tensorial version of the divergence $\mathrm{div}_{\boldsymbol{x}}$. For all $\alpha \in \mathcal{I}(M)$, we employ the subscript α to denote the restriction of each function to the layer α, i.e. $\boldsymbol{c}_\alpha = \boldsymbol{c}|_{\Omega_\alpha(t)}$, $\boldsymbol{s}_\alpha = \boldsymbol{s}|_{\Omega_\alpha(t)}$ and $\boldsymbol{v}_\alpha = \boldsymbol{v}|_{\Omega_\alpha(t)}$, and similarly with the rest of scalar, vector and tensor variables. In addition, we split the volume-average velocity at the α-layer into its horizontal component $\widetilde{\boldsymbol{v}}_\alpha$ and vertical velocity w_α, this is $\boldsymbol{v}_\alpha := (\widetilde{\boldsymbol{v}}_\alpha, w_\alpha)$. Among the assumptions required for this approach, we assume the layer thicknesses are small enough to neglect the dependence of the horizontal velocities and the concentration of each species on the vertical coordinate within each layer. This means that

$$\partial_z \widetilde{\boldsymbol{v}}_\alpha = \mathbf{0} \quad \text{and} \quad \partial_z \boldsymbol{c}_\alpha = \partial_z \boldsymbol{s}_\alpha = \mathbf{0} \qquad \forall \alpha \in \mathcal{I}(M)\,. \tag{17}$$

?u_constant?

In addition, we assume that the vertical volume-average velocity w_α is piecewise linear in z, and possibly discontinuous. Under this assumption the vertical velocity and (hydrostatic) pressure are piecewise linear in z, i.e.,

$$\partial_z w_\alpha = (\partial_z w_\alpha)(\boldsymbol{x}, t) \quad \text{and} \quad \partial_z p_\alpha = (\partial_z p_\alpha)(\boldsymbol{x}, t) \qquad \forall \alpha \in \mathcal{I}(M)\,. \tag{18}$$

?strucvp?

More precisely, the assumption of a hydrostatic pressure means that

$$p_\alpha(\boldsymbol{x}, z, t) = p_{\alpha+1/2}(\boldsymbol{x}, t) + \rho_\alpha g (z_{\alpha+1/2} - z), \qquad p_{\alpha+1/2}(\boldsymbol{x}, t) := p_{\mathrm{S}}(\boldsymbol{x}, t) + g \sum_{\beta=\alpha+1}^{M} \rho_\beta h_\beta(\boldsymbol{x}, t)\,,$$

where p_{S} denotes the pressure at the free surface. We begin by describing the multilayer version of equation (13a) for the total density of the mixture, which is obtained by integrating this equation on the vertical coordinate over the interval I_α, this is

$$\partial_t(\rho_\alpha h_\alpha) + \mathrm{div}_{\boldsymbol{x}}(\rho_\alpha h_\alpha \widetilde{\boldsymbol{v}}_\alpha) = \mathcal{G}^-_{\alpha+1/2} - \mathcal{G}^+_{\alpha-1/2} + h_\alpha\big(\widetilde{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}_\alpha, \boldsymbol{s}_\alpha) + \widetilde{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c}_\alpha, \boldsymbol{s}_\alpha)\big)\,, \tag{19}$$

eq:PDErho

where the flux difference on the right-hand side involves the normal mass fluxes $\mathcal{G}^-_{\alpha+1/2}$ and $\mathcal{G}^+_{\alpha-1/2}$ across the interfaces $\Gamma_{\alpha+1/2}(t)$ and $\Gamma_{\alpha-1/2}(t)$, which we will assume satisfy the continuity condition $\mathcal{G}^-_{\alpha+1/2} = \mathcal{G}^+_{\alpha+1/2} = \mathcal{G}_{\alpha+1/2}$ for each $\alpha \in \mathcal{I}(M)$, so that they are given by

$$\mathcal{G}_{\alpha+1/2} := \rho_\alpha\big(\partial_t z_{\alpha+1/2} + \widetilde{\boldsymbol{v}}_\alpha \cdot \nabla_{\boldsymbol{x}} z_{\alpha+1/2} - w_\alpha\big) \qquad \forall \alpha \in \mathcal{I}(M)\,. \tag{20}$$

def:flux:G

Similarly, the multilayer version of (13c) is obtained by integration on the vertical axis

$$\partial_t(c_\alpha^{(i)}h_\alpha) + \mathrm{div}_{\boldsymbol{x}}(c_\alpha^{(i)}h_\alpha\widetilde{\boldsymbol{v}}_\alpha) = \mathcal{G}_{\alpha+1/2}^{(i)} - \mathcal{G}_{\alpha-1/2}^{(i)} + h_\alpha\mathcal{R}_{\boldsymbol{c}}^{(i)}(\boldsymbol{c}_\alpha, \boldsymbol{s}_\alpha)\,, \tag{21}$$ eq:PDEc

where the normal mass flux $\mathcal{G}_{\alpha+1/2}^{(i)}$ of each i-specie is defined in the same way as in [17] so that they are continuous accross the interface $\Gamma_{\alpha+/2}$, so that adding up $\mathcal{G}_{\alpha+1/2}^{(i)}$ from $i=1$ to $i=n_{\boldsymbol{c}}$, we recover $\mathcal{G}_{\alpha+1/2}$, therefore we have

$$\mathcal{G}_{\alpha+1/2}^{(i)} = \tilde{c}_{\alpha+1/2}^{(i)}\mathcal{G}_{\alpha+1/2} - \tilde{f}_{\alpha+1/2}^{(i)} + \tilde{a}_{3,\alpha+1/2}^{(i)}\,,$$

where the averages $\tilde{c}_{\alpha+1/2}^{(i)}$, $\tilde{f}_{\alpha+1/2}^{(i)}$, and $\tilde{a}_{3,\alpha+1/2}^{(i)}$ are defined by

$$\tilde{c}_{\alpha+1/2}^{(i)} := \frac{1}{2}\left(\frac{c_{\alpha+1}^{(i)}}{\rho_{\alpha+1}} + \frac{c_\alpha^{(i)}}{\rho_\alpha}\right), \quad \tilde{f}_{\alpha+1/2}^{(i)} := \frac{1}{2}\big(f_{\alpha+1/2}^{(i),+} + f_{\alpha+1/2}^{(i),-}\big), \quad \tilde{a}_{3,\alpha+1/2}^{(i)} := \frac{1}{2}\big(\boldsymbol{a}_{\alpha+1/2}^{(i),+} + \boldsymbol{a}_{\alpha+1/2}^{(i),-}\big).$$

The vector of normal mass fluxes for the solid phase is defined as $\boldsymbol{\mathcal{G}}_{\alpha+1/2} := \big(\mathcal{G}_{\alpha+1/2}^{(i)}\big)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}$ and we also define the vectors of the average variables

$$\tilde{\boldsymbol{c}}_{\alpha+1/2} := \big(\tilde{c}_{\alpha+1/2}^{(i)}\big)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}\,, \qquad \tilde{\boldsymbol{f}}_{\alpha+1/2} := \big(\tilde{f}_{\alpha+1/2}^{(i)}\big)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}, \qquad \tilde{\boldsymbol{a}}_{3,\alpha+1/2} := \big(\tilde{a}_{3,\alpha+1/2}^{(i)}\big)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}\,.$$

For the substrate equations (13d), we first observe that (asumir al igual que con los solidos que la componente horizontal de la velocidad de los sustratos coincide con $\widetilde{\boldsymbol{v}}_\alpha$)

$$\partial_t(s_\alpha^{(i)}h_\alpha) + \mathrm{div}_{\boldsymbol{x}}(s_\alpha^{(i)}h_\alpha\widetilde{\boldsymbol{v}}_\alpha) = \mathcal{S}_{\alpha+1/2}^{(i)} - \mathcal{S}_{\alpha-1/2}^{(i)} + h_\alpha\mathcal{R}_{\boldsymbol{s}}^{(i)}(\boldsymbol{c}_\alpha, \boldsymbol{s}_\alpha) \qquad \forall i\in\mathcal{I}(n_{\boldsymbol{s}})\,, \tag{22}$$ eq:PDEs

where the normal mass fluxes for the liquid phase $\mathcal{S}_{\alpha+1/2}^{(i)}$ for each $i\in\mathcal{I}(n_{\boldsymbol{s}})$ substrate are defined as

$$\mathcal{S}_{\alpha+1/2}^{(i)} := \frac{1}{2}\left(\frac{s_\alpha^{(i)}}{\rho_\alpha} + \frac{s_{\alpha+1}^{(i)}}{\rho_{\alpha+1}}\right)\mathcal{G}_{\alpha+1/2} + \frac{1}{2\rho_{\mathrm{f}}}\left(\frac{s_\alpha^{(i)}}{\phi_{\mathrm{f},\alpha}} + \frac{s_{\alpha+1}^{(i)}}{\phi_{\mathrm{f},\alpha+1}}\right)\sum_{j=1}^{n_{\boldsymbol{c}}}\big(\tilde{f}_{\alpha+1/2}^{(j)} - \tilde{a}_{3,\alpha+1/2}^{(j)}\big)\,,$$

and as for the solid phase, we also the vector $\boldsymbol{\mathcal{S}}_{\alpha+1/2} := \big(\mathcal{S}_{\alpha+1/2}^{(i)}\big)_{i\in\mathcal{I}(n_{\boldsymbol{s}})}$. For the multilayer version of the momentum equation (13b), we observe that such a formulation can be obtained in the same way as in [17], so that we skip its derivation and directly introduce it as follows

$$\begin{aligned}&\partial_t(h_\alpha\rho_\alpha\widetilde{\boldsymbol{v}}_\alpha) + \nabla_{\boldsymbol{x}}\cdot\big(h_\alpha\rho_\alpha\widetilde{\boldsymbol{v}}_\alpha\otimes\widetilde{\boldsymbol{v}}_\alpha\big) + h_\alpha\big(\nabla_{\boldsymbol{x}}\bar{p}_\alpha + g\rho_\alpha\nabla_{\boldsymbol{x}}\bar{z}_\alpha\big)\\ &\quad= \frac{1}{2}\mathcal{G}_{\alpha+1/2}\big(\widetilde{\boldsymbol{v}}_{\alpha+1} - \widetilde{\boldsymbol{v}}_\alpha\big) - \frac{1}{2}\mathcal{G}_{\alpha-1/2}\big(\widetilde{\boldsymbol{v}}_\alpha - \widetilde{\boldsymbol{v}}_{\alpha-1}\big) + \boldsymbol{K}_{\alpha+1/2} - \boldsymbol{K}_{\alpha-1/2}\,,\end{aligned} \tag{23}$$ eq:PDEv

where the vector $\boldsymbol{K}_{\alpha+1/2}$ is given by

$$\boldsymbol{K}_{\alpha+1/2} := \frac{\mu}{2}\widetilde{\boldsymbol{Q}}_{\alpha+1/2}$$

and $\tilde{\boldsymbol{Q}}_{\alpha+1/2}$ is an approximation of $\partial_z\boldsymbol{u}$ at the interface $\Gamma_{\alpha+1/2}$ in the multilayer framework. To approximate $\boldsymbol{Q}$, the solution of the equation $\boldsymbol{Q} = \partial_z\boldsymbol{u}$, we approximate $\boldsymbol{u}$ by a linear interpolation in z, denoted by $\boldsymbol{u}$, such that

$$\boldsymbol{u}|_{z=\frac{1}{2}(z_{\alpha-1/2}+z_{\alpha+1/2})} = \tilde{\boldsymbol{v}}_\alpha,$$

then

$$\widetilde{\boldsymbol{Q}}_{\alpha+1/2} = \frac{\tilde{\boldsymbol{v}}_{\alpha+1} - \tilde{\boldsymbol{v}}_\alpha}{h_{\alpha+1/2}}$$

with $h_{\alpha+1/2}$ the distance between the midpoints of layers α and $\alpha+1/2$. On the other hand $\bar{p}_\alpha$ and $\bar{z}_\alpha$ are defined by (25) and (26), respectively.

Next, to close the system, we further assume that the thickness of each layer h_α is a fixed fraction of the total height h, such that $h_\alpha = l_\alpha h$ for $\alpha \in \mathcal{I}(M)$, where $l_1, \dots, l_M$ are positive numbers that add up to 1. Then, defining new variables $m_\alpha := \rho_\alpha h$, $\boldsymbol{q}_\alpha := \rho_\alpha h \widetilde{\boldsymbol{v}}_\alpha$, $\boldsymbol{r}_\alpha := \boldsymbol{c}_\alpha h$ and $\boldsymbol{\zeta}_\alpha := \boldsymbol{s}_\alpha h$ for $\alpha \in \mathcal{I}(M)$ and replacing them into (19), (23), (21) and (22), we can writte the multilayer formulation of (13) as

nalmodel_ml⟩

$$\partial_t m_\alpha + \operatorname{div}_{\boldsymbol{x}}(\boldsymbol{q}_\alpha) = \frac{1}{l_\alpha}\big(\mathcal{G}_{\alpha+1/2} - \mathcal{G}_{\alpha-1/2}\big) + h\Big(\widetilde{\mathcal{R}}_{\boldsymbol{s},\alpha} + \widetilde{\mathcal{R}}_{\boldsymbol{c},\alpha}\Big)\,, \tag{24a}$$ eq:ml:m

$$\begin{aligned}\partial_t \boldsymbol{q}_\alpha + \operatorname{div}_{\boldsymbol{x}}\left(\frac{\boldsymbol{q}_\alpha \otimes \boldsymbol{q}_\alpha}{m_\alpha}\right) + h\big(\nabla_{\boldsymbol{x}}\bar{p}_\alpha + g\rho_\alpha \nabla_{\boldsymbol{x}}\bar{z}_\alpha\big) \\ = \frac{1}{l_\alpha}\big(\tilde{\boldsymbol{q}}_{\alpha+1/2}\mathcal{G}_{\alpha+1/2} - \tilde{\boldsymbol{q}}_{\alpha-1/2}\mathcal{G}_{\alpha-1/2}\big) + \frac{1}{l_\alpha}\big(\boldsymbol{K}_{\alpha+1/2} - \boldsymbol{K}_{\alpha-1/2}\big)\,,\end{aligned} \tag{24b}$$ eq:ml:v

$$\partial_t r_\alpha^{(i)} + \operatorname{div}_{\boldsymbol{x}}\left(\frac{r_\alpha^{(i)}\boldsymbol{q}_\alpha}{m_\alpha}\right) = \frac{1}{l_\alpha}\big(\mathcal{G}^{(i)}_{\alpha+1/2} - \mathcal{G}^{(i)}_{\alpha-1/2}\big) + h\mathcal{R}^{(i)}_{\boldsymbol{c},\alpha} \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{c}})\,, \tag{24c}$$ eq:ml:c

$$\partial_t \zeta_\alpha^{(i)} + \operatorname{div}_{\boldsymbol{x}}\left(\frac{\zeta_\alpha^{(i)}\boldsymbol{q}_\alpha}{m_\alpha}\right) = \frac{1}{l_\alpha}\big(\mathcal{S}^{(i)}_{\alpha+1/2} - \mathcal{S}^{(i)}_{\alpha-1/2}\big) + h\mathcal{R}^{(i)}_{\boldsymbol{s},\alpha} \qquad \forall i \in \mathcal{I}(n_{\boldsymbol{s}})\,, \tag{24d}$$ eq:ml:s

where $\bar{p}_\alpha$, $\bar{z}_\alpha$, and the average $\tilde{\boldsymbol{q}}_{\alpha+1/2}$ are defined by

$$\bar{p}_\alpha := p_{\mathrm{S}} + \frac{1}{2}g l_\alpha m_\alpha + \sum_{\beta=\alpha+1}^{M} g l_\beta m_\beta\,, \tag{25}$$ def:pbar

$$\bar{z}_\alpha := z_{\mathrm{B}} + \frac{1}{2}l_\alpha h + \sum_{\beta=1}^{\alpha-1} l_\beta h\,, \tag{26}$$ def:zbar

$$\tilde{\boldsymbol{q}}_{\alpha+1/2} := \frac{1}{2}\left(\frac{\boldsymbol{q}_{\alpha+1}}{m_{\alpha+1}} + \frac{\boldsymbol{q}_\alpha}{m_\alpha}\right). \tag{27}$$?def:vbar?

Using the definitions (25) and (26), together with $l_1 + \cdots + l_M = 1$ and $m_\alpha = \rho_\alpha h$, the third term on the left-hand side of (24b), accounting for the gradient of pressure, can be written as

$$\begin{aligned}h\big(\nabla_{\boldsymbol{x}}\bar{p}_\alpha + g\rho_\alpha\nabla_{\boldsymbol{x}}\bar{z}_\alpha\big) = g m_\alpha \nabla_{\boldsymbol{x}}(z_{\mathrm{B}} + h) + g h^2\left(\frac{1}{2}l_\alpha + \sum_{\beta=\alpha+1}^{M} l_\beta\right)\nabla_{\boldsymbol{x}}\rho_\alpha \\ + g h \sum_{\beta=\alpha+1}^{M} l_\beta \nabla_{\boldsymbol{x}}\big(m_\beta - m_\alpha\big)\,.\end{aligned} \tag{28}$$ eq:expresionP

The conservation equation for the total mass of the solid phase is obtained by adding up equation (24a) (after multiplying by l_α in both sides of the equation) from $\alpha = 0$ to $\alpha = M$, this is

$$\partial_t \bar{m} + \nabla_{\boldsymbol{x}} \cdot \left(\sum_{\beta=1}^{M} l_\beta \boldsymbol{q}_\beta\right) = \mathcal{G}_{M+1/2} - \mathcal{G}_{1/2}\,, \tag{29}$$?eq:ml:mtot?

where $\bar{m} := \sum_{\beta=1}^{M} l_\beta m_\beta$ is the total mass of the solid phase, and $\mathcal{G}_{M+1/2}$ and $\mathcal{G}_{1/2}$ represent the mass transfer on the bottom and at the free surface, respectively. For each $\alpha \in \mathcal{I}(M)$, the normal mass flux $\mathcal{G}_{\alpha+1/2}$, as it was defined in (20), depends explicitly on the vertical velocities w_α, which we are going

to be determined on a post processing procedure. To avoid this dependency, we reformulate these fluxes in the same way as in [18]. First, we define the following vector and scalar variables

$$\boldsymbol{R}_\alpha := \boldsymbol{q}_\alpha - \sum_{j=1}^{N} r_\alpha^{(j)} \frac{\boldsymbol{q}_\alpha}{m_\alpha} \frac{\rho_j - \rho_{\mathrm{f}}}{\rho_j}, \quad \bar{\boldsymbol{R}} := \sum_{\beta=1}^{M} l_\beta \boldsymbol{R}_\beta, \quad \tilde{\rho}_{\alpha+1/2} := \frac{2\rho_\alpha \rho_{\alpha+1}}{\rho_\alpha + \rho_{\alpha+1}}, \quad L_\alpha := \sum_{\beta=1}^{\alpha} h_\beta \,,$$

for all $\alpha \in \mathcal{I}(M)$. Then, [18, Equation (5.19)] gives

$$\mathcal{G}_{\alpha+1/2} = \frac{\tilde{\rho}_{\alpha+1/2}}{\rho_{\mathrm{f}}} \sum_{\beta=1}^{\alpha} l_\beta \mathrm{div}_{\boldsymbol{x}}(\boldsymbol{R}_\beta - \bar{\boldsymbol{R}}) + \tilde{\mathcal{G}}_{\alpha+1/2} \qquad \forall \alpha \in \mathcal{I}_0(M)\,, \tag{30}$$?eq:fluxGnew?

where

$$\begin{aligned}\tilde{\mathcal{G}}_{\alpha+1/2} := \sum_{j=1}^{N} \frac{(\rho_j - \rho_{\mathrm{f}})\tilde{\rho}_{\alpha+1/2}}{\rho_j \rho_{\mathrm{f}}} \Big(&- \left(\tilde{f}^{(j)}_{\alpha+1/2} - \tilde{a}^{(j)}_{3,\alpha+1/2}\right) + (1 - L_\alpha)\left(\tilde{f}^{(j)}_{1/2} - \tilde{a}^{(j)}_{3,1/2}\right) \\ &+ L_\alpha \left(\tilde{f}^{(j)}_{M+1/2} - \tilde{a}^{(j)}_{3,M+1/2}\right)\Big) + (1 - L_\alpha)\frac{\tilde{\rho}_{\alpha+1/2}}{\tilde{\rho}_{1/2}}\mathcal{G}_{1/2} + L_\alpha \frac{\tilde{\rho}_{\alpha+1/2}}{\tilde{\rho}_{M+1/2}}\mathcal{G}_{M+1/2}\,.\end{aligned}$$

3.3 Vertical velocity of the mixture

The vertical velocities of the mixture in each layer are computed recursively as follows. First, the vertical velocity $w^+_{1/2}$ is computed using mass transference condition at the bottom by

$$w^+_{1/2} = \partial_t z_{\mathrm{B}} + \widetilde{\boldsymbol{v}}_1 \cdot \nabla_{\boldsymbol{x}} z_{\mathrm{B}} - \frac{G_{1/2}}{\rho_1}. \tag{31}$$?v:1?

Then, for $\alpha \in \mathcal{I}(M)$ and $z \in (z_{\alpha-1/2}, z_{\alpha+1/2})$ we obtain the vertical velocities of the mixture in each layer successively as

$$\begin{aligned} w_\alpha(\boldsymbol{x}, z, t) &= w^+_{\alpha-1/2} - \frac{1}{\rho_\alpha}\big(\partial_t \rho_\alpha + \nabla_{\boldsymbol{x}} \cdot (\rho_\alpha \widetilde{\boldsymbol{v}}_\alpha)\big)(z - z_{\alpha-1/2}), \\ w^-_{\alpha+1/2} &= w^+_{\alpha-1/2} - \frac{h_\alpha}{\rho_\alpha}\big(\partial_t \rho_\alpha + \nabla_{\boldsymbol{x}} \cdot (\rho_\alpha \widetilde{\boldsymbol{v}}_\alpha)\big), \\ w^+_{\alpha+1/2} &= \frac{1}{\rho_\alpha}\Big((\rho_\alpha - \rho_{\alpha-1})\partial_t z_{\alpha-1/2} + (\rho_\alpha \widetilde{\boldsymbol{v}}_\alpha - \rho_\alpha \widetilde{\boldsymbol{v}}_\alpha) \cdot \nabla_{\boldsymbol{x}} z_{\alpha-1/2} + \rho_{\alpha-1} w^-_{\alpha-1/2}\Big). \end{aligned} \tag{32}$$?v:2?

Ver hiperbolicidad, y alguna otra propiedad.

4 Numerical scheme

ec:numschem⟩

In this section, we describe the numerical method designed to approximate system (24) for the case of $\Omega \subset \mathbb{R}^3$ and two-dimensional horizontal domain projections. In order to employ the numerical scheme developed in [17] for our model, which computes the viscous terms in (24b) separately, we start by writing system (24) in compact form, without including the term $\boldsymbol{K}_{\alpha+1/2} - \boldsymbol{K}_{\alpha-1/2}$. Considering that for each $\alpha \in \mathcal{I}(M)$, $\boldsymbol{q}_\alpha \in \mathbb{R}^2$, $\boldsymbol{r}_\alpha \in \mathbb{R}^{n_{\boldsymbol{c}}}$ and $\boldsymbol{\zeta}_\alpha \in \mathbb{R}^{n_{\boldsymbol{s}}}$, we define the vector of unknowns of (24) on each α-layer as $\tilde{\mathbf{w}}_\alpha := (m_\alpha, \boldsymbol{q}_\alpha, \boldsymbol{r}_\alpha, \boldsymbol{\zeta}_\alpha)^{\mathtt{t}} \in \mathbb{R}^N$, where $N := 3 + n_{\boldsymbol{c}} + n_{\boldsymbol{s}}$ and $\mathbf{w}_\alpha := (\boldsymbol{q}_\alpha, \boldsymbol{r}_\alpha, \boldsymbol{\zeta}_\alpha) \in \mathbb{R}^{N-1}$. The vector solution gathering the M layers is defined by $\tilde{\mathbf{W}} := (\tilde{\mathbf{w}}_1, \ldots, \tilde{\mathbf{w}}_M) \in \mathbb{R}^{NM}$, and the transformed vector taking into account the total mass $\bar{m}$ is

$$\mathbf{W} := (\bar{m}, \mathbf{w}_1, \ldots, \mathbf{w}_M) \in \mathbb{R}^{(N-1)M+1}\,.$$

The connection between both vectors, $\mathbf{W}$ and $\tilde{\mathbf{W}}$, is provided by the linear system

$$\mathbf{W} = \mathbf{C}\tilde{\mathbf{W}}, \tag{33}$$?eq:relWhatW?

where the matrix $\mathbf{C} \in \mathbb{R}^{((N-1)M+1)\times NM}$ is defined as follows. We define $\mathbf{e}_i$ as the i-th N-dimensional unit vector ($i = 1, \dots, N$), $\mathbf{0}_d$ as the zero vector of size d, and $\mathbf{0}$ (without index) as a zero matrix of unspecified size. Then, the matrix $\mathbf{C}$ is defined by

$$\mathbf{C} = \begin{bmatrix} l_1\mathbf{e}_1^\mathsf{t} & l_2\mathbf{e}_1^\mathsf{t} & \cdots & l_M\mathbf{e}_1^\mathsf{t} \\ \mathbf{J} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{J} \end{bmatrix} \quad \text{where} \quad \mathbf{J} := \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ 0 & 0 & \cdots & 0 & 1 \end{bmatrix} \in \mathbb{R}^{(N-1)\times N}.$$

The convective fluxes corresponding to each equation (24a), (24c), (24d) and (24b), for $\alpha \in \mathcal{I}(M)$ are denoted by the single matrix $\boldsymbol{F} := (\boldsymbol{F}_1^\mathsf{t}, \dots, \boldsymbol{F}_M^\mathsf{t})^\mathsf{t} \in \mathbb{R}^{NM\times 2}$ where

$$\boldsymbol{F}_\alpha := \left[\boldsymbol{q}_\alpha, \frac{1}{m_\alpha}\boldsymbol{q}_\alpha \otimes \boldsymbol{q}_\alpha, \frac{r_\alpha^{(1)}}{m_\alpha}\boldsymbol{q}_\alpha, \dots, \frac{r_\alpha^{(n_c)}}{m_\alpha}\boldsymbol{q}_\alpha, \frac{\zeta_\alpha^{(1)}}{m_\alpha}\boldsymbol{q}_\alpha, \dots, \frac{\zeta_\alpha^{(n_s)}}{m_\alpha}\boldsymbol{q}_\alpha\right]^\mathsf{t} \in \mathbb{R}^{N\times 2} \qquad \forall \alpha \in \mathcal{I}(M).$$

For the third term on the left-hand side of Equation (24b), we define the vector $\boldsymbol{P} := (\boldsymbol{P}_1^\mathsf{t}, \dots, \boldsymbol{P}_M^\mathsf{t})^\mathsf{t} \in \mathbb{R}^{NM}$, where $\boldsymbol{P}_\alpha := \left[0\,, \boldsymbol{\psi}_\alpha^\mathsf{t}\,, \mathbf{0}_{n_c}\,, \mathbf{0}_{n_s}\right]^\mathsf{t} \in \mathbb{R}^N$ for all $\alpha \in \mathcal{I}(M)$, with $\boldsymbol{\psi}_\alpha \in \mathbb{R}^2$ given by (28), this is

$$\boldsymbol{\psi}_\alpha := gm_\alpha\nabla_{\boldsymbol{x}}(z_\mathrm{B} + h) + gh^2\left(\frac{1}{2}l_\alpha + \sum_{\beta=\alpha+1}^{M} l_\beta\right)\nabla_{\boldsymbol{x}}\rho_\alpha + gh\sum_{\beta=\alpha+1}^{M} l_\beta\nabla_{\boldsymbol{x}}(m_\beta - m_\alpha). \tag{34}$$ def:psi

For the right-hand sides of (24) we introduce the following vectors $\boldsymbol{\mathcal{J}}_\mathrm{L} := (\boldsymbol{\mathcal{J}}_{1-1/2}^\mathsf{t}, \dots, \boldsymbol{\mathcal{J}}_{M-1/2}^\mathsf{t})^\mathsf{t}$, $\boldsymbol{\mathcal{J}}_\mathrm{R} := (\boldsymbol{\mathcal{J}}_{1+1/2}^\mathsf{t}, \dots, \boldsymbol{\mathcal{J}}_{M+1/2}^\mathsf{t})^\mathsf{t}$ and $\boldsymbol{\mathcal{R}} := (\boldsymbol{\mathcal{R}}_1^\mathsf{t}, \dots, \boldsymbol{\mathcal{R}}_M^\mathsf{t})^\mathsf{t}$ in $\mathbb{R}^{NM}$ where for $\alpha \in \mathcal{I}_0(M)$ and $\beta \in \mathcal{I}(M)$:

$$\boldsymbol{\mathcal{J}}_{\alpha+1/2} := \frac{1}{l_\alpha}\begin{bmatrix} \mathcal{G}_{\alpha+1/2} \\ \tilde{\boldsymbol{q}}_{\alpha+1/2}\mathcal{G}_{\alpha+1/2} \\ \boldsymbol{\mathcal{G}}_{\alpha+1/2} \\ \boldsymbol{\mathcal{S}}_{\alpha+1/2} \end{bmatrix}, \qquad \boldsymbol{\mathcal{R}}_\beta := h\begin{bmatrix} \widetilde{\mathcal{R}}_{\boldsymbol{s},\beta} + \widetilde{\mathcal{R}}_{\boldsymbol{c},\beta} \\ \mathbf{0}_2 \\ \boldsymbol{\mathcal{R}}_{\boldsymbol{c},\beta} \\ \boldsymbol{\mathcal{R}}_{\boldsymbol{s},\beta} \end{bmatrix},$$

each one in $\mathbb{R}^N$. Finally, system of equations can be written as

$$\partial_t\mathbf{W} + \mathbf{C}\left(\mathbf{div}_{\boldsymbol{x}}(\boldsymbol{F}(\tilde{\mathbf{W}})) + \boldsymbol{P}(\tilde{\mathbf{W}})\right) = \mathbf{C}\left(\boldsymbol{\mathcal{J}}_\mathrm{R}(\tilde{\mathbf{W}}) - \boldsymbol{\mathcal{J}}_\mathrm{L}(\tilde{\mathbf{W}})\right) + \mathbf{C}\boldsymbol{\mathcal{R}}(\tilde{\mathbf{W}}), \tag{35}$$ eq:systemfinalr

and for each α-layer

$$\partial_t\tilde{\mathbf{w}}_\alpha + \mathbf{div}_{\boldsymbol{x}}\big(\boldsymbol{F}_\alpha(\tilde{\mathbf{w}}_\alpha)\big) + \boldsymbol{P}_\alpha(\tilde{\mathbf{w}}_\alpha) = \boldsymbol{\mathcal{J}}_{\alpha+1/2}(\tilde{\mathbf{W}}) - \boldsymbol{\mathcal{J}}_{\alpha-1/2}(\tilde{\mathbf{W}}) + \boldsymbol{\mathcal{R}}_\alpha(\tilde{\mathbf{w}}_\alpha).$$

4.0.1 Marching formula

We now consider k control volumes $V_i \subset \mathbb{R}^2$ for $i = 1, \dots, k$, which in a uniform cartesian grid are diven by squares of size $\Delta x \times \Delta y$ with Δx and Δy positive, such that $\{V_i\}_{i=1}^k$ is a partition of the horizontal domain. In addition, we define $E_{i,j}$ as the edge between two adjacent control volume V_i and V_j, and $\boldsymbol{\eta}_{i,j}$ as the unitary normal vector at $E_{i,j}$ pointing from V_i to V_j. In turn, the set of control volumes neighboring V_i is defined by K_i. The center of mass of the i-th control volume is denoted by $\boldsymbol{x}_i$ while $|V_i|$ and $|E_{i,j}|$ stand for the area of V_i and length of $E_{i,j}$, respectively.

Ver que tanto cambia la CFL For the numerical simulation, we will use the following CFL condition to determine Δt in each iteration:

$$\max\left\{\frac{|\lambda_{i,j}|}{d_{i,j}},\ i=1,\dots,\mathcal{V},\ j\in K_i\right\}\Delta t\le \mathrm{CFL},$$

where $\lambda_{i,j}$ are bounds of the eigenvalues of the viscosity matrix, $d_{i,j}=||\boldsymbol{x}_j-\boldsymbol{x}_i||_2$, the distance between centers of the volume i and j and $\mathcal{V}$ the number of cells. We have fixed the Courant number by $\mathrm{CFL}=0.5$.

We approximate the solution at each time t_n by the averages

$$\boldsymbol{W}_i^n=\frac{1}{|V_i|}\int_{V_i}\boldsymbol{W}(\cdot,t_n)\,\mathrm{d}\boldsymbol{x},\qquad \forall i=1,\dots,k\,,$$

and propose the following first-order two-dimensional finite volume scheme to approximate (35):

$$\boldsymbol{W}_i^{n+1}=\boldsymbol{W}_i^n-\frac{\Delta t}{|V_i|}\sum_{j\in K_i}|E_{i,j}|\mathbf{C}\big(\boldsymbol{F}_{i,j}^n+\boldsymbol{P}_{i,j}^n-(\boldsymbol{\mathcal{J}}_{\mathrm{R},i,j}^n-\boldsymbol{\mathcal{J}}_{\mathrm{L},i,j}^n)\big)+\Delta t\boldsymbol{\mathcal{R}}_i^n,$$

where

$$\boldsymbol{F}_{i,j}^n=(\boldsymbol{F}_{i,j,\alpha}^n)_{1\le\alpha\le M}\,,\qquad \boldsymbol{P}_{i,j}^n=(\boldsymbol{P}_{i,j,\alpha}^n)_{1\le\alpha\le M}\,,\qquad \boldsymbol{\mathcal{R}}_i^n=(\boldsymbol{\mathcal{R}}_\alpha(\tilde{\mathbf{w}}_{i,\alpha}^n))_{1\le\alpha\le M}\,,$$
$$\boldsymbol{\mathcal{J}}_{\mathrm{L},i,j}^n=(\boldsymbol{\mathcal{J}}_{i,j,\alpha-1/2}^n)_{1\le\alpha\le M}\,,\qquad \boldsymbol{\mathcal{J}}_{\mathrm{R},i,j}^n=(\boldsymbol{\mathcal{J}}_{i,j,\alpha+1/2}^n)_{1\le\alpha\le M}.$$

Given a discrete time $t=t^n$, each $\boldsymbol{F}_{i,j,\alpha}^n$ for $\alpha\in\mathcal{I}(M)$ corresponds to the approximation of the flux $\boldsymbol{F}_\alpha$ at the edge $E_{i,j}$ and time t^n. In turn, the first three components of $\boldsymbol{F}_{i,j,\alpha}^n$ are approximated by an HLL-PVM-1U method [24], which depends on left and right bounds of the eigenvalues of the transport matrix of the full system, denoted by σ_{L} and σ_{R}, respectively. (aqui creo que se puede hacer de la submatrix sin los substratos). In what follows, we will use the notation $[\,\cdot\,]_l$ to denote the l-th component of a vector, and for each function φ, we define $\{\!\{\varphi\}\!\}_{i,j}:=(\varphi_i+\varphi_j)/2$, the average of φ at the edge $E_{i,j}$, which is defined analogously for vector and tensor variables. For the rest of components of $\boldsymbol{F}_{i,j\alpha}^n$, we use the fact that they are linear and depend on $[\boldsymbol{F}_\alpha]_1(\tilde{\mathbf{w}}_\alpha^n)$, so that an upwind approach is employed. Then, the components $[\boldsymbol{F}_{i,j,\alpha}^n]_l$ for $l=1,2,3$ are given by the HLL-PVM-1U scheme

$$[F_{i,j,\alpha}^n]_l=\Big[\big\{\!\!\big\{\boldsymbol{F}_\alpha(\tilde{\mathbf{w}}_\alpha^n)\big\}\!\!\big\}_{i,j}\cdot\boldsymbol{\eta}_{i,j}-\frac{1}{2}\Big(\theta_{0,i,j}^n\big(\tilde{\mathbf{w}}_{j,\alpha}^n-\tilde{\mathbf{w}}_{i,\alpha}^n+\boldsymbol{b}_{i,j,\alpha}^n\big)$$
$$+\theta_{1,i,j}^n\big((\boldsymbol{F}_\alpha(\tilde{\mathbf{w}}_{j,\alpha}^n)-\boldsymbol{F}_\alpha(\tilde{\mathbf{w}}_{i,\alpha}^n))\cdot\boldsymbol{\eta}_{i,j}+\boldsymbol{P}_{i,j,\alpha}^n\big)\Big)\Big]_l.$$

and for $l=4,\dots,N$, by the upwind scheme

$$[F_{i,j,\alpha}^n]_l=[F_{i,j,\alpha}^n]_1\left(\frac{[\tilde{\mathbf{w}}_{i,\alpha}^n]_l}{[\tilde{\mathbf{w}}_{i,\alpha}^n]_1}\frac{1+\mathrm{sgn}([F_{i,j,\alpha}^n]_1)}{2}+\frac{[\tilde{\mathbf{w}}_{j,\alpha}^n]_l}{[\tilde{\mathbf{w}}_{j,\alpha}^n]_1}\frac{1-\mathrm{sgn}([F_{i,j,\alpha}^n]_1)}{2}\right).$$

The coefficients $\theta_{0,i,j}^n$ and $\theta_{1,i,j}^n$ are respectively defined by

$$\theta_{0,i,j}^n=\frac{\sigma_{\mathrm{R},i,j}^n|\sigma_{\mathrm{L},i,j}^n|-\sigma_{\mathrm{L},i,j}^n|\sigma_{\mathrm{R},i,j}^n|}{\sigma_{\mathrm{R},i,j}^n-\sigma_{\mathrm{L},i,j}^n},\qquad \theta_{1,i,j}^n=\frac{|\sigma_{\mathrm{R},i,j}^n|-|\sigma_{\mathrm{L},i,j}^n|}{\sigma_{\mathrm{R},i,j}^n-\sigma_{\mathrm{L},i,j}^n},$$

where the characteristic velocities $\sigma_{\mathrm{L},i,j}^n$ and $\sigma_{\mathrm{R},i,j}^n$ are global approximations of the minimum and maximum wave speed of the system (poner systema). poner blabla sobre por que tomamos las velocidades del 1D. We make use of eigenvalues obtained in the one-dimensional case in [17], for which we define $\sigma_{\mathrm{L},i,j}$ and $\sigma_{\mathrm{R},i,j}$ as follows:

?⟨ssd⟩?

$$\sigma_{\mathrm{L},i,j}^n:=\bar{v}_{i,j}^n-\Psi_{i,j}^n,\qquad \sigma_{\mathrm{R},i,j}^n:=\bar{v}_{i,j}^n+\Psi_{i,j}^n,\tag{36}$$?wave1?

where

$$\bar{v}_{i,j}^n := \frac{1}{M}\sum_{\beta=1}^{M} \left\{\!\!\left\{ \widetilde{\boldsymbol{v}}_\beta^{\,n} \right\}\!\!\right\}_{i,j}^{\mathtt{t}} \boldsymbol{\eta}_{i,j}, \tag{37}$$?wave2?

$$\begin{aligned}\Psi_{i,j}^n := \left(4 - \frac{2}{M}\right)^{1/2} \Bigg(&\sum_{\beta=1}^{M} (\bar{v}_{i,j}^n - v_{\beta,i,j}^n)^2 \\ &+ \frac{g}{2}\left\{\!\!\left\{ h^n \right\}\!\!\right\}_{i,j} \left(1 + \sum_{\beta=1}^{M} \frac{(2\beta-1)}{M\rho_{\mathrm{f}}} \left\{\!\!\left\{ \rho_\beta^n \right\}\!\!\right\}_{i,j}\right)\Bigg)^{1/2}.\end{aligned} \tag{38}$$?wave3?

For the pressure-related term $\boldsymbol{P}_{i,j,\alpha}^n = \left[0, (\boldsymbol{\psi}_{i,j,\alpha}^n)^{\mathtt{t}}, \mathbf{0}_{n_{\boldsymbol{c}}}^{\mathtt{t}}, \mathbf{0}_{n_{\boldsymbol{s}}}^{\mathtt{t}}\right]^{\mathtt{t}} \in \mathbb{R}^N$, in the same way as in [18], we approximate the products and gradients appearing in (34) by averages and differences so that

$$\begin{aligned}\boldsymbol{\psi}_{i,j,\alpha}^n = g\Bigg(&\left\{\!\!\left\{ m_\alpha^n \right\}\!\!\right\}_{i,j} \left(z_{\mathrm{B},j} - z_{\mathrm{B},i} + h_j^n - h_i^n\right) + \left\{\!\!\left\{ (h^n)^2 \right\}\!\!\right\}_{i,j} \left(\frac{l_\alpha}{2} + \sum_{\beta=\alpha+1}^{M} l_\beta\right)\left(\rho_{j,\alpha}^n - \rho_{i,\alpha}^n\right) \\ &+ \left\{\!\!\left\{ h^n \right\}\!\!\right\}_{i,j} \sum_{\beta=\alpha+1}^{M} l_\beta \left(m_{j,\beta}^n - m_{i,\beta}^n - (m_{j,\alpha}^n - m_{i,\beta}^n)\right)\Bigg)\boldsymbol{\eta}_{i,j}\,.\end{aligned} \tag{39}$$ {?}

Next, for the normal mass flux, for all $\alpha \in \mathcal{I}_0(M)$, we compute each of the approximated terms involved in $\boldsymbol{\mathcal{J}}_{i,j,\alpha+1/2}^n$ as follows

$$\mathcal{G}_{i,j,\alpha+1/2}^n = \frac{\tilde{\rho}_{i,j,\alpha+1/2}^n}{\rho_{\mathrm{f}}} \sum_{\beta=1}^{\alpha} l_\beta \left((\boldsymbol{R}_{j,\beta}^n - \bar{\boldsymbol{R}}_j^n)^{\mathtt{t}} - (\boldsymbol{R}_{i,\beta}^n - \bar{\boldsymbol{R}}_i^n)^{\mathtt{t}}\right)\boldsymbol{\eta}_{i,j} + \tilde{\mathcal{G}}_{i,\alpha+1/2}^n \ell_{i,j}\,, \tag{40}$$ {?}

$$\tilde{\boldsymbol{q}}_{i,j,\alpha+1/2}^n = \frac{1}{2}\left\{\!\!\left\{ \boldsymbol{q}_\alpha^n + \boldsymbol{q}_{\alpha+1}^n \right\}\!\!\right\}_{i,j}, \tag{41}$$ {?}

$$\boldsymbol{\mathcal{G}}_{i,j,\alpha+1/2}^n = \tilde{\boldsymbol{c}}_{i,j,\alpha+1/2}^n \mathcal{G}_{i,j,\alpha+1/2}^n - \left(\tilde{\boldsymbol{f}}_{i,\alpha+1/2}^n - \tilde{\boldsymbol{a}}_{i,3,\alpha+1/2}^n\right)\ell_{i,j}\,, \tag{42}$$ {?}

$$\boldsymbol{\mathcal{S}}_{i,j,\alpha+1/2}^n = \tilde{\boldsymbol{s}}_{i,j,\alpha+1/2}^n \mathcal{G}_{i,j,\alpha+1/2}^n + \tilde{\boldsymbol{s}}_{i,j,\alpha+1/2}^{\mathrm{f},n} \sum_{l=1}^{n_{\boldsymbol{c}}} \left(\tilde{f}_{i,\alpha+1/2}^{(l),n} - \tilde{a}_{i,3,\alpha+1/2}^{(l),n}\right)\ell_{i,j}\,, \tag{43}$$ {?}

where $\ell_{i,j} := \frac{1}{2}(\boldsymbol{x}_{i,j} - \boldsymbol{x}_i)^{\mathtt{t}}\boldsymbol{\eta}_{i,j}$ and the averages

$$\tilde{\rho}_{i,j,\alpha+1/2}^n = \left\{\!\!\left\{ \frac{2\rho_\alpha^n \rho_{\alpha+1}^n}{\rho_\alpha^n + \rho_{\alpha+1}^n} \right\}\!\!\right\}_{i,j}, \qquad \tilde{\boldsymbol{c}}_{i,j,\alpha+1/2}^n = \frac{1}{2}\left\{\!\!\left\{ \frac{\boldsymbol{c}_{\alpha+1}^n}{\rho_{\alpha+1}^n} + \frac{\boldsymbol{c}_\alpha^n}{\rho_\alpha^n} \right\}\!\!\right\}_{i,j},$$

$$\tilde{\boldsymbol{s}}_{i,j,\alpha+1/2}^n = \frac{1}{2}\left\{\!\!\left\{ \frac{\boldsymbol{s}_{\alpha+1}^n}{\rho_{\alpha+1}^n} + \frac{\boldsymbol{s}_\alpha^n}{\rho_\alpha^n} \right\}\!\!\right\}_{i,j}, \qquad \tilde{\boldsymbol{s}}_{i,j,\alpha+1/2}^{\mathrm{f},n} = \frac{1}{2\rho_{\mathrm{f}}}\left\{\!\!\left\{ \frac{\boldsymbol{s}_{\alpha+1}^n}{\phi_{\mathrm{f},\alpha+1}^n} + \frac{\boldsymbol{s}_\alpha^n}{\phi_{\mathrm{f},\alpha}^n} \right\}\!\!\right\}_{i,j},$$

where $\tilde{\boldsymbol{f}}_{i,\alpha+1/2}^n = \left(\tilde{f}_{\alpha+1/2}^{(i),n}\right)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}$ is the numerical approximation of the vertical flux given by

$$\begin{aligned}\tilde{f}_{\alpha+1/2}^{(j),n} = &\frac{1}{2}\left(\phi_{j,\alpha} v_j^{\mathrm{MLB}}(\Phi_\alpha) + \phi_{j,\alpha+1} v_j^{\mathrm{MLB}}(\Phi_{\alpha+1})\right) - \frac{E_{\alpha+1}}{2}(\phi_{j,\alpha+1} - \phi_{j,\alpha}) \\ &- \frac{\phi_{j,\alpha}}{2}\left|v_j^{\mathrm{MLB}}(\Phi_{\alpha+1}) - v_j^{\mathrm{MLB}}(\Phi_\alpha)\right| \operatorname{sgn}(\phi_{j,\alpha+1} - \phi_{j,\alpha}), \quad \text{for } j \in \mathcal{I}(n_{\boldsymbol{c}}),\end{aligned}$$

and where $\Phi_\alpha := (\phi_{1,\alpha}, \ldots, \phi_{N,\alpha})^{\mathrm{T}}$ and $E_\alpha := \max_{j=1,\ldots,N} |v_j^{\mathrm{MLB}}(\Phi_\alpha)|$, where v_j^{MLB} is the hindered settling velocity. For $\tilde{\boldsymbol{a}}_{3,\alpha+1/2} := \left(\tilde{a}_{3,\alpha+1/2}^{(i)}\right)_{i\in\mathcal{I}(n_{\boldsymbol{c}})}$ first note that from (10) the third component of

vector $\boldsymbol{a}_i(\boldsymbol{c}, \nabla \boldsymbol{c})$ can be write as

$$\tilde{a}_3^{(i)} = \sum_{j=1}^{N} \eta_{ij} \frac{\partial \phi_j}{\partial z} \tag{44}$$ def:a3

with

$$\eta_{ij} = -\frac{\mu}{g\phi} \rho_j V(\phi) \left\{ (1-\phi)\phi_j(\delta_j - \boldsymbol{\delta}^t \boldsymbol{\lambda})\sigma_e' + \left[\delta_j \delta_{ji} - \frac{\phi_j \rho_i \delta_i}{\rho} - \frac{\phi_j}{\phi}(\delta_j - \boldsymbol{\delta}^t \boldsymbol{\lambda}) \right] \sigma_e \right\}, \tag{45}$$ {?}

then $\tilde{a}_{3,\alpha+1/2}^{(i)}$ is an approximation of (44) at the interface $\Gamma_{\alpha+1/2}$. Finally, the term $\boldsymbol{b}_{i,j,\alpha}$ is included to preserve the well-balance and the stationary solution deduced in [18, Proposition 1], this is

$$\boldsymbol{b}_{i,j,\alpha} = \{\!\{\bar{\rho}_\alpha^n\}\!\}_{i,j}(z_{\mathrm{B},j} - z_{\mathrm{B},i})\mathbf{e}_1 \,.$$

Hacer distinción que se resuelve con un método semi-implicito con splitting

Viscous term approximation

For each cell $i \in \{1, \ldots, \mathcal{V}\}$, from the end of Section **??** we have that

$$\boldsymbol{Q}_{i,\alpha+1/2} - \partial_z \boldsymbol{v}_{i,\alpha+1/2} = 0.$$

Thus, we may approximate the viscous terms as

$$\boldsymbol{K}_{i,\alpha+1/2} = \frac{\eta_{i,\alpha+1/2}}{2}(\widetilde{\boldsymbol{v}}_{i,\alpha+1} - \widetilde{\boldsymbol{v}}_{i,\alpha}),$$

which allows us to update the horizontal velocities by solving the tri-diagonal linear system

$$\begin{bmatrix} a_{i,1}^n & b_{i,1}^n & 0 & \cdots & 0 \\ b_{i,1}^n & a_{i,2}^n & b_{i,2}^n & \ddots & \vdots \\ 0 & b_{i,2}^n & a_{i,3}^n & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & b_{i,M-1}^n \\ 0 & \cdots & 0 & b_{i,M-1}^n & a_{i,M}^n \end{bmatrix} \begin{pmatrix} \widetilde{\boldsymbol{v}}_{i,1}^{n+1} \\ \vdots \\ \widetilde{\boldsymbol{v}}_{i,\alpha}^{n+1} \\ \vdots \\ \widetilde{\boldsymbol{v}}_{i,M}^{n+1} \end{pmatrix} = \begin{pmatrix} m_{i,1}^n \widetilde{\boldsymbol{v}}_{i,1}^n \\ \vdots \\ m_{i,\alpha}^n \widetilde{\boldsymbol{v}}_{i,\alpha}^n \\ \vdots \\ m_{i,M}^n \widetilde{\boldsymbol{v}}_{i,M}^n \end{pmatrix},$$

where $a_{i,\alpha}^n$ and $b_{i,\alpha}^n$ are given by

$$a_{i,\alpha}^n = m_{i,\alpha}^n + \frac{\Delta t}{2l_\alpha^2}\left(\eta(\phi_{i,\alpha+1/2}^n) + \eta(\phi_{i,\alpha-1/2}^n)\right), \quad b_{i,\alpha}^n = -\frac{\Delta t}{2l_\alpha^2}\eta(\phi_{i,\alpha+1/2}^n).$$

5 Simulations

numexamples⟩

For the first example, we consider the reduced denitrification process [9], which consists of converting nitrate into nitrogen gas. The solid phase is composed by two species, the ordinary heterotrophic organisms $c^{(1)}$ and undegradable organics $c^{(2)}$, and the substrates are three, nitrate $s^{(1)}$, readily biodegradable substrate $s^{(2)}$, and nitrogen $s^{(3)}$. The vectors of concentration are $\boldsymbol{c} = \left(c^{(1)}, c^{(2)}\right)$ and $\boldsymbol{s} = \left(s^{(1)}, s^{(2)}, s^{(3)}\right)$, which in [9] are denoted by $\boldsymbol{c} = \left(X_{\mathrm{OHO}}, X_{\mathrm{U}}\right)$ and $\boldsymbol{s} = \left(S_{\mathrm{NO_3}}, S_{\mathrm{S}}, S_{\mathrm{N_2}}\right)$. The vector of reaction rates and stoichiometric matrices are respectively given by

$$\boldsymbol{\kappa}(\boldsymbol{c}, \boldsymbol{s}) = c^{(1)} \begin{bmatrix} \mu(s^{(1)}, s^{(2)}) \\ b \end{bmatrix}, \quad \boldsymbol{\sigma}_{\boldsymbol{c}} = \begin{bmatrix} 1 & -1 \\ 0 & f_{\mathrm{p}} \end{bmatrix}, \qquad \boldsymbol{\sigma}_{\boldsymbol{s}} = \begin{bmatrix} -\bar{Y} & -1/Y & \bar{Y} \\ 0 & 0.8 & 0 \end{bmatrix},$$

where $b = 6.94 \times 10^{-6}\mathrm{s}^{-1}$ is the decay rate of heterotrophic organisms, $f_\mathrm{p} = 0.2$ is the portion of these that decays to undegradable organics, $Y = 0.67$ and $\bar{Y} = 0.172216$ are (dimensionless) yield factors. The specific growth rate function is defined by

$$\mu(\boldsymbol{s}) = \mu_{\max} \frac{s^{(1)}}{\kappa_1 + s^{(1)}} \frac{s^{(2)}}{\kappa_2 + s^{(2)}} ,$$

with $\mu_{\max} = 5.56 \times 10^{-5}\,\mathrm{s}^{-1}$ being the maximum growth rate, and $\kappa_1 = 5 \times 10^{-4}\,\mathrm{kg/m^3}$ and $\kappa_2 = 0.02\,\mathrm{kg/m^3}$ are saturation constants. Then, the reaction terms read as follows

$$\boldsymbol{\mathcal{R}}_{\boldsymbol{c}}(\boldsymbol{c}, \boldsymbol{s}) = c^{(1)} \begin{bmatrix} \mu(\boldsymbol{s}) - b \\ f_\mathrm{p} b \end{bmatrix} , \qquad \boldsymbol{\mathcal{R}}_{\boldsymbol{s}}(\boldsymbol{c}, \boldsymbol{s}) = c^{(1)} \begin{bmatrix} -\bar{Y}\mu(\boldsymbol{s}) \\ -\mu(\boldsymbol{s})/Y + 0.8b \\ \bar{Y}\mu(\boldsymbol{s}) \end{bmatrix} ,$$

The maximal total solids concentration is set to $u_{\max} = 30\,\mathrm{kg/m^3}$. The constitutive functions used in all simulations are

$$v_{\mathrm{hs}}(\phi(\boldsymbol{c})) = v_0 \left(1 - \sum_{j=1}^{n_{\boldsymbol{c}}} \frac{c^{(j)}}{\rho_j} \right)^n , \qquad n > 2$$

$$\sigma_\mathrm{e}(u) := \beta \chi_{\{u \geq u_\mathrm{c}\}}(u - u_\mathrm{c})$$

with constants $v_0 = 1.76 \times 10^{-3}\,\mathrm{m/s}$, $\breve{u} = 3.87\,\mathrm{kg/m^3}$, $\eta = 3.58$, $u_\mathrm{c} = 5\,\mathrm{kg/m^3}$ and $\beta = 0.2\,\mathrm{m^2/s^2}$. Other parameters are $\rho = 1050\,\mathrm{kg/m^3}$, $\rho_\mathrm{L} = 998\,\mathrm{kg/m^3}$, $g = 9.81\,\mathrm{m/s^2}$, $A = 400\,\mathrm{m^2}$, $H = 1\mathrm{m}$ and $B = 3\,\mathrm{m}$.

$$\boldsymbol{c}_0(t) = u_0(t) \begin{bmatrix} 5/7 \\ 2/7 \end{bmatrix} , \quad \text{where} \quad u_0(z) = \begin{cases} 0\,\mathrm{kg/m^3} & \text{if } z < 0.5\,\mathrm{m}, \\ 3.8z + 1.6\,\mathrm{kg/m^3} & \text{if } z \geq 0.5\,\mathrm{m}, \end{cases}$$

$$\boldsymbol{s}_0(z) = \begin{cases} (0.006, 0, 0)^\mathtt{t}\,\mathrm{kg/m^3} & \text{if } z < 0.5\,\mathrm{m}, \\ (0, 0.12(z - 0.5), 0.006)^\mathtt{t}\,\mathrm{kg/m^3} & \text{if } z \geq 0.5\,\mathrm{m}, \end{cases}$$

6 Conclusions

(conclusions?)

Some conclusions here.

A Appendix

For a scalar quantity θ driven by a vector (velocity) field $\boldsymbol{\nu} = (\widetilde{\boldsymbol{\nu}}, \nu)$, such that θ and $\widetilde{\boldsymbol{\nu}}$ are independent of z, we consider the conservation law $\partial_t \theta + \mathrm{div}(\theta \boldsymbol{\nu}) = 0$. Integrating this equation on the vertical coordinate over the interval I_α, we can obtain its αth-multilayer approach

$$\begin{aligned} 0 = \int_{I_\alpha} \big(\partial_t \theta + \mathrm{div}(\theta \boldsymbol{\nu})\big) \mathrm{d}z &= h_\alpha(\partial_t \theta) + \int_{I_\alpha} \mathrm{div}_{\boldsymbol{x}}(\theta \boldsymbol{\nu}) \mathrm{d}z + \theta \int_{I_\alpha} \partial_z \nu \mathrm{d}z \\ & h_\alpha(\partial_t \theta) - \theta \left(\widetilde{\boldsymbol{\nu}}|^-_{z_{\alpha+1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha+1/2} - \widetilde{\boldsymbol{\nu}}|^+_{z_{\alpha-1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha-1/2} \right) + \theta \nu|^-_{z_{\alpha+1/2}} - \theta \nu|^+_{z_{\alpha-1/2}} \\ & \quad + \mathrm{div}_{\boldsymbol{x}} \Big(\int_{I_\alpha} \theta \widetilde{\boldsymbol{\nu}} \, \mathrm{d}z \Big) \end{aligned}$$

where we have used that $\mathrm{div} = \mathrm{div}_{\boldsymbol{x}} + \partial_z$ and Leibnitz's rule. Using once again that θ and $\widetilde{\boldsymbol{\nu}}$ are independent of z and that $(\partial_t\theta)h_\alpha = (\partial_t\theta)h_\alpha + \theta\partial_t h_\alpha - \theta\partial_t h_\alpha = \partial_t(\theta h_\alpha) - \theta(\partial_t z_{\alpha+1/2} - \partial_t z_{\alpha-1/2})$, we obtain

$$\begin{aligned} 0 = \partial_t(\theta h_\alpha) - \theta\big(\partial_t z_{\alpha+1/2} - \partial_t z_{\alpha-1/2}\big) - \theta\left(\widetilde{\boldsymbol{\nu}}|^-_{z_{\alpha+1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha+1/2} - \widetilde{\boldsymbol{\nu}}|^+_{z_{\alpha-1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha-1/2}\right) \\ + \theta\nu|^-_{z_{\alpha+1/2}} - \theta\nu|^+_{z_{\alpha-1/2}} + \mathrm{div}_{\boldsymbol{x}}\big(\theta h_\alpha \widetilde{\boldsymbol{\nu}}\big)\,, \end{aligned}$$

The above equation implies

$$\begin{aligned} \partial_t(\theta h_\alpha) + \mathrm{div}_{\boldsymbol{x}}\big(\theta h_\alpha \widetilde{\boldsymbol{\nu}}\big) = \theta\big(\partial_t z_{\alpha+1/2} + \widetilde{\boldsymbol{\nu}}|^-_{z_{\alpha+1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha+1/2} - \nu|^-_{z_{\alpha+1/2}}\big) \\ - \theta\big(\partial_t z_{\alpha-1/2} + \widetilde{\boldsymbol{\nu}}|^+_{z_{\alpha-1/2}} \cdot \nabla_{\boldsymbol{x}} z_{\alpha-1/2} - \nu|^+_{z_{\alpha-1/2}}\big)\,. \end{aligned}$$

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$$\mathcal{D}_{(i-1)M+l,(j-1)M+l} = h_{i,j}\delta_{i,j} + \frac{\rho_j \Delta t}{\Delta z^2 h_{i,j}}(\eta_{i,j}(\phi_{\mathrm{int},i,j,l+1}, \rho_{t,i,j,l+1}) + \eta_{i,j}(\phi_{\mathrm{int},i,j,l}, \rho_{t,i,j,l}))$$

$$\mathcal{D}_{(i-1)M+l,(j-1)M+l-1} = \frac{\rho_j \Delta t}{\Delta z^2 h_{i,j}}\eta_{i,j}(\phi_{\mathrm{int},i,j,l-1}, \rho_{t,i,j,l-1})$$

$$\mathcal{D}_{(i-1)M+l,(j-1)M+l+1} = \frac{\rho_j \Delta t}{\Delta z^2 h_{i,j}}\eta_{i,j}(\phi_{\mathrm{int},i,j,l+1}, \rho_{t,i,j,l-1})$$

$$\eta_{i,j} = \mu\rho_i \frac{v_{\mathrm{hs}}(\phi)}{g\phi}\left((1-\phi)\phi_i\left(\delta_i - \sum \delta_k\lambda_k\right)\sigma'(\phi) + \left(\delta_i\delta_{i,j} - \delta_j\frac{\rho_j\phi_i}{\rho} - \frac{\phi_i}{\phi}\left(\delta_i - \sum \delta_k\lambda_k\right)\right)\sigma(\phi)\right)$$

References

Anestis1981 [1] G. Anestis. *Eine eindimensionale Theorie der Sedimentation in Absetzbehältern veränderlichen Querschnitts und in Zentrifugen.* PhD thesis, TU Vienna, Austria, 1981.

Audusse2005 [2] E. Audusse. A multilayer saint-venant model: Derivation and numerical validation. *Discrete Continuous Dyn. Syst. Ser. B*, 5(2):189–214, 2005.

Audusse2011 [3] E. Audusse, M.-O. Bristeau, M. Pelanti, and J. Sainte-Marie. Approximation of the hydrostatic navier–stokes system for density stratified flows by a multilayer model: Kinetic interpretation and numerical solution. *J. Comput. Phys.*, 230(9):3453–3478, 2011.

Audusse2010 [4] E. Audusse, M.-O. Bristeau, B. Perthame, and J. Sainte-Marie. A multilayer saint-venant system with mass exchanges for shallow water flows. derivation and numerical validation. *ESAIM: Math. Model. Numer. Anal.*, 45(1):169–200, 2010.

Basson2009 [5] D.K. Basson, S. Berres, and R. Bürger. On models of polydisperse sedimentation with particle-size-specific hindered-settling factors. *Appl. Math. Model.*, 33(4):1815–1835, 2009.

siap_varyingA [6] R. Bürger, J. Careaga, and S. Diehl. Entropy solutions of a scalar conservation law modeling sedimentation in vessels with varying cross-sectional area. *SIAM J. Appl. Math.*, 77(2):789–811, 2017.

Dcec_varyingA [7] R. Bürger, J. Careaga, and S. Diehl. A simulation model for settling tanks with varying cross-sectional area. *Chem. Eng. Commun.*, 204(11):1270–1281, 2017.

SDIMA_MOL [8] R. Bürger, J. Careaga, and S. Diehl. A method-of-lines formulation for a model of reactive settling in tanks with varying cross-sectional area. *IMA J. Appl. Math.*, 86(3):514–546, 2021.

cace_reactive [9] R. Bürger, J. Careaga, S. Diehl, C. Mejías, I. Nopens, E. Torfs, and P. A. Vanrolleghem. Simulations of reactive settling of activated sludge with a reduced biokinetic model. *Computers Chem. Eng.*, 92:216–229, 2016.

SDAMM_SBR1 [10] R. Bürger, J. Careaga, S. Diehl, and R. Pineda. A moving-boundary model of reactive settling in wastewater treatment. Part 1: Governing equations. *Appl. Math. Modelling*, 106:390–401, 2022.

SDAMM_SBR2 [11] R. Bürger, J. Careaga, S. Diehl, and R. Pineda. A moving-boundary model of reactive settling in wastewater treatment. Part 2: Numerical scheme. *Appl. Math. Modelling*, 111:247–269, 2022.

Burger2023a [12] R. Bürger, J. Careaga, S. Diehl, and R. Pineda. A model of reactive settling of activated sludge: Comparison with experimental data. *Chem. Eng. Sci.*, 267:118244, March 2023.

Burger2023b [13] R. Bürger, J. Careaga, S. Diehl, and R. Pineda. Numerical schemes for a moving-boundary convection-diffusion-reaction model of sequencing batch reactors. *ESAIM: Math. Model. Numer. Anal.*, 57(5):2931–2976, 2023.

rger&D&K2004 [14] R. Bürger, J. J. R. Damasceno, and K. H. Karlsen. A mathematical model for batch and continuous thickening of flocculated suspensions in vessels with varying cross-section. *Int. J. Miner. Process.*, 73:183–208, 2004.

SDcace1 [15] R. Bürger, S. Diehl, S. Farås, and I. Nopens. On reliable and unreliable numerical methods for the simulation of secondary settling tanks in wastewater treatment. *Computers Chem. Eng.*, 41:93–105, 2012.

er&E&K&L2000 [16] R. Bürger, S. Evje, K. H. Karlsen, and K.-A. Lie. Numerical methods for the simulation of the settling of flocculated suspensions. *Chem. Eng. J.*, 80:91–104, 2000.

Osores2019 [17] R. Bürger, E.D. Fernández-Nieto, and V. Osores. A dynamic multilayer shallow water model for polydisperse sedimentation. *ESAIM: Math. Model. Numer. Anal.*, 53(4):1391–1432, 2019.

Osores2020 [18] R. Bürger, E.D. Fernández-Nieto, and V. Osores. A multilayer shallow water approach for polydisperse sedimentation with sediment compressibility and mixture viscosity. *J. Sci. Comput.*, 85(2), 2020.

ger&K&T2005a [19] R. Bürger, K. H. Karlsen, and J. D. Towers. A model of continuous sedimentation of flocculated suspensions in clarifier-thickener units. *SIAM J. Appl. Math.*, 65:882–940, 2005.

Burger2012b [20] R. Bürger, R. Ruiz-Baier, K. Schneider, and H. Torres. A multiresolution method for the simulation of sedimentation in inclined channels. *Int. J. Numer. Anal. Model.*, 9(3):479–504, 2012.

ger&RB&T2012 [21] R. Bürger, R. Ruiz-Baier, and H. Torres. A stabilized finite volume element formulation for sedimentation-consolidation processes. *SIAM J. Sci. Comput.*, 34:B265–B289, 2012.

Careaga2023 [22] J. Careaga and G.N. Gatica. Coupled mixed finite element and finite volume methods for a solid velocity-based model of multidimensional sedimentation. *ESAIM: Math. Model. Numer. Anal.*, 57:2529–2556, 2023.

ancelier1994 [23] J.-Ph. Chancelier, M. Cohen de Lara, and F. Pacard. Analysis of a conservation PDE with discontinuous flux: a model of settler. *SIAM J. Appl. Math.*, 54(4):954–995, 1994.

Castro2012 [24] M. J. Castro Díaz and E. Fernández-Nieto. A class of computationally fast first order finite volume solvers: PVM methods. *SIAM Journal on Scientific Computing*, 34(4):A2173–A2196, 2012.

astroDaz2012 [25] M.J. Castro Díaz, E.D. Fernández-Nieto, T. Morales de Luna, G. Narbona-Reina, and C. Parés. A HLLC scheme for nonconservative hyperbolic problems. application to turbidity currents with sediment transport. *ESAIM: Math. Model. Numer. Anal.*, 47(1):1–32, 2012.

astroDaz2009 [26] M.J. Castro Díaz, E.D. Fernández-Nieto, A.M. Ferreiro, and C. Parés. Two-dimensional sediment transport models in shallow water equations. a second order finite volume approach on unstructured meshes. *Comput. Methods Appl. Mech. Eng.*, 198(33-36):2520–2538, 2009.

SDsiam3 [27] S. Diehl. Dynamic and steady-state behavior of continuous sedimentation. *SIAM J. Appl. Math.*, 57(4):991–1018, 1997.

SDwatres2 [28] S. Diehl. The solids-flux theory – confirmation and extension by using partial differential equations. *Water Res.*, 42(20):4976–4988, 2008.

Dupont1992 [29] R. Dupont and M. Henze. Modelling of the secondary clarifier combined with the activated sludge model no. 1. *Water Sci. Tech.*, 25(6):285–300, 1992.

Ekama1997 [30] G. A. Ekama, J. L. Barnard, F. W. Günthert, P. Krebs, J. A. McCorquodale, D. S. Parker, and E. J. Wahlberg. *Secondary Settling Tanks: Theory, Modelling, Design and Operation.* IAWQ scientific and technical report no. 6. International Association on Water Quality, England, 1997.

Flores2008 [31] X. Flores-Alsina, I. Rodriguez-Roda, G. Sin, and K.V. Gernaey. Multi-criteria evaluation of wastewater treatment plant control strategies under uncertainty. *Water Res.*, 42(17):4485–4497, 2008.

Gernaey2004 [32] K. V. Gernaey, M. C. M. van Loosdrecht, M. Henze, M. Lind, and S. B Jørgensen. Activated sludge wastewater treatment plant modelling and simulation: state of the art. *Environ. Model. Software*, 19(9):763–783, 2004.

stavsson2000 [33] K. Gustavsson and J. Oppelstrup. Consolidation of concentrated suspensions – numerical simulations using a two-phase fluid model. *Comput. Visual. Sci.*, 3(1–2):39–45, 2000.

Henze1987WR [34] M. Henze, C. P. L. Grady, W. Gujer, G. V. R. Marais, and T. Matsuo. A general model for single-sludge wastewater treatment systems. *Water Res.*, 21(5):505–515, 1987.

e2000ASMbook [35] M. Henze, W. Gujer, T. Mino, and M. C. M. van Loosdrecht. *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3.* IWA Publishing, London, UK, 2000. IWA Scientific and Technical Report No. 9.

Hu2003 [36] Z. R. Hu, M. C. Wentzel, and G. A. Ekama. Modelling biological nutrient removal activated sludge systems – a review. *Water Res.*, 37(14):3430–3444, 2003.

Lockett1979 [37] M.J. Lockett and K.S. Bassoon. Sedimentation of binary particle mixtures. *Powder Technology*, 24(1):1–7, 1979.

Masliyah1979 [38] J.H. Masliyah. Hindered settling in a multi-species particle system. *Chemical Engineering Science*, 34(9):1166–1168, 1979.

DalMaso1995 [39] G. Dal Maso, P. Le Floch, and F. Murat. Definition and weak stability of nonconservative products. *J. Math. Pures Appl.*, 74:483–548, 1995.

Rao2002 [40] R. Rao, L. Mondy, A. Sun, and S. Altobelli. A numerical and experimental study of batch sedimentation and viscous resuspension. *International Journal for Numerical Methods in Fluids*, 39(6):465–483, 2002.

Tory2003 [41] E.M. Tory, K.H. Karlsen, R. Bürger, and S. Berres. Strongly degenerate parabolic-hyperbolic systems modeling polydisperse sedimentation with compression. *SIAM J. Appl. Math.*, 64(1):41–80, 2003.

Watts1996a [42] R. W. Watts, S. A. Svoronos, and B. Koopman. One-dimensional modeling of secondary clarifiers using a concentration and feed velocity-dependent dispersion coefficient. *Water Res.*, 30(9):2112–2124, 1996.