

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

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## 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 inert 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-reactive 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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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 between 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

Let  $\Omega$  be a bounded domain in  $\mathbb{R}^3$  and  $\mathbf{x} := (x_1, x_2, z)$  the coordinates of a point in  $\Omega$  with  $\tilde{\mathbf{x}} = (x_1, x_2)$  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  $\mathcal{I}(k) := \{1, 2, \dots, k\}$  and  $\mathcal{I}_0(k) := \{0, 1, \dots, k\}$ . We consider  $n_c \in \mathbb{N}$  species of spherical solid particles dispersed in a viscous fluid whose vector of volume fractions is  $\phi := (\phi^{(1)}, \phi^{(2)}, \dots, \phi^{(n_c)})^\top$ , where the  $i$ -th phase volume fraction is denoted by  $\phi^{(i)} := \phi^{(i)}(\mathbf{x}, t)$  for

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

$$\rho := \rho(\Phi(\mathbf{x}, t)) = \rho_f \phi_f(\mathbf{x}, t) + \sum_{i=1}^{n_c} c^{(i)}(\mathbf{x}, t), \quad (1) \text{?def:rho?}$$

where  $\Phi := (\phi_f, \phi^{(1)}, \dots, \phi^{(n_c)})^\top$  is the vector of volume fractions including the fluid volume fraction. We also define the total solids volume fraction as  $\phi := \phi^{(1)} + \dots + \phi^{(n_c)}$ . Using the constitutive assumption that  $\phi_f + \phi = 1$ , we can express  $\phi_f$  in terms of  $\mathbf{c}$  as follows

$$\phi_f(\mathbf{c}) = 1 - \sum_{i=1}^{n_c} \frac{1}{\rho_i} c^{(i)},$$

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

$$\frac{\partial c^{(i)}}{\partial t} + \operatorname{div}(c^{(i)} \mathbf{v}_i) = \mathcal{R}_c^{(i)}(\mathbf{c}, \mathbf{s}) \quad \forall i \in \mathcal{I}(n_c), \quad (2) \text{eq:mass:c}$$

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

$$\rho_f \phi_f = s^{(1)} + \dots + s^{(n_s)} + \mathcal{W}.$$

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

$$\rho_f \frac{\partial \phi_f}{\partial t} + \operatorname{div}(\rho_f \phi_f \mathbf{v}_f) = \tilde{\mathcal{R}}_s(\mathbf{c}, \mathbf{s}) \quad \forall i \in \mathcal{I}(n_s) \quad (3) \text{eq:mass:phif}$$

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

$$\frac{\partial s^{(i)}}{\partial t} + \operatorname{div}(s^{(i)} \mathbf{v}_f) = \mathcal{R}_s^{(i)}(\mathbf{c}, \mathbf{s}) \quad \forall i \in \mathcal{I}(n_s), \quad (4a) \text{eq:mass:s}$$

$$\frac{\partial \mathcal{W}}{\partial t} + \operatorname{div}(\mathcal{W} \mathbf{v}_f) = 0, \quad (4b) \text{eq:mass:w}$$

$$s^{(1)} + \dots + s^{(n_s)} + \mathcal{W} = \rho_f \phi_f. \quad (4c) \text{?eq:sum:s?}$$

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  $\mathcal{W} = \rho_f \phi_f(\mathbf{c}) - (s^{(1)} + \dots + s^{(n_s)})$ . 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  $\mathbf{u}_i := \mathbf{v}_i - \mathbf{v}_f$  for  $i \in \mathcal{I}(n_c)$  and the so-called mass-average velocity, defined by

$$\mathbf{v} := \frac{1}{\rho(\Phi)} \left( \rho_f \phi_f \mathbf{v}_f + \sum_{j=1}^{n_s} c^{(j)} \mathbf{v}_j \right). \quad (5) \text{ ?def:mass-avera}$$

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

$$\mathbf{v}_i = \mathbf{v} + \mathbf{u}_i - \frac{1}{\rho} \sum_{j=1}^{n_c} c^{(j)} \mathbf{u}_j \quad \forall i \in \mathcal{I}(n_c), \quad (6) \text{ eq:relmassv}$$

$$\mathbf{v}_f = \mathbf{v} - \frac{1}{\rho_f \phi_f} \sum_{i=1}^{n_c} c^{(i)} \left( \mathbf{u}_i - \frac{1}{\rho} \sum_{j=1}^{n_c} c^{(j)} \mathbf{u}_j \right). \quad (7) \text{ eq:relslipv}$$

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

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

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

$$v_i^{\text{MLB}}(\mathbf{c}) := \mu v_{\text{hs}}(c_{\text{tot}}) \vartheta_i(\mathbf{c}), \quad (9) \text{ ?def:vLMB?}$$

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

where  $c_{\text{tot}} := c^{(1)} + \dots + c^{(n_c)}$  is the total solids concentration,  $v_{\text{hs}} := v_{\text{hs}}(c_{\text{tot}})$  is the hindered settling velocity,  $\sigma_e := \sigma_e(c_{\text{tot}}) \geq 0$  is the effective solid stress function with compact contained in  $[0, c_{\text{max}}]$ , and for each  $i \in \mathcal{I}(n_c)$ , the function  $\vartheta_i$  is given by

$$\vartheta_i(\mathbf{c}) := \delta_i (\rho_i + \phi_f(\mathbf{c}) \rho_f - c_{\text{tot}}) - \sum_{k=1}^{n_c} \frac{c^{(k)}}{\rho(\mathbf{c})} \delta_k (\rho_k + \phi_f(\mathbf{c}) \rho_f - c_{\text{tot}}).$$

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  $\mathbf{v}$ ,  $\mathbf{c}$  and  $\nabla \mathbf{c}$ , as follows

$$c^{(i)} \mathbf{v}_i = c^{(i)} \mathbf{v} + f_i(\mathbf{c}) \mathbf{k} - \mathbf{a}_i(\mathbf{c}, \nabla \mathbf{c}) \quad \forall i \in \mathcal{I}(n_c),$$

$$s^{(i)} \mathbf{v}_f = s^{(i)} \mathbf{v} - \frac{s^{(i)}}{\rho_f \phi_f(\mathbf{c})} \sum_{j=1}^{n_c} \left( f_j(\mathbf{c}) \mathbf{k} - \mathbf{a}_j(\mathbf{c}, \nabla \mathbf{c}) \right) \quad \forall i \in \mathcal{I}(n_s),$$

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

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = \tilde{\mathcal{R}}_c(\mathbf{c}, \mathbf{s}) + \tilde{\mathcal{R}}_s(\mathbf{c}, \mathbf{s}). \quad (11) \text{?eq:mass:mixture}$$

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

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \operatorname{div}(\rho \mathbf{v} \otimes \mathbf{v} - \mu \mathbf{e}(\mathbf{v})) + \nabla p = -\rho g \mathbf{k}, \quad (12) \text{?eq:momentum:mixture}$$

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

:finalmodel)

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = \tilde{\mathcal{R}}_c(\mathbf{c}, \mathbf{s}) + \tilde{\mathcal{R}}_s(\mathbf{c}, \mathbf{s}), \quad (13a) \text{eq:fm:mass:mixture}$$

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

$$\frac{\partial c^{(i)}}{\partial t} + \operatorname{div}(c^{(i)} \mathbf{v} + f_i(\mathbf{c}) \mathbf{k} - \mathbf{a}_i(\mathbf{c}, \nabla \mathbf{c})) = \mathcal{R}_c^{(i)}(\mathbf{c}, \mathbf{s}) \quad \forall i \in \mathcal{I}(n_c). \quad (13c) \text{eq:fm:mass:c}$$

$$\frac{\partial s^{(i)}}{\partial t} + \operatorname{div}\left(s^{(i)} \mathbf{v} - s^{(i)} \sum_{j=1}^{n_c} \frac{f_j(\mathbf{c}) \mathbf{k} - \mathbf{a}_j(\mathbf{c}, \nabla \mathbf{c})}{\rho_f \phi_f(\mathbf{c})}\right) = \mathcal{R}_s^{(i)}(\mathbf{c}, \mathbf{s}) \quad \forall i \in \mathcal{I}(n_c). \quad (13d) \text{eq:fm:mass:s}$$

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).

### 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  $-\mathbf{k}$  into  $M \in \mathbb{N}$  different layers. More precisely, for each  $\alpha \in \mathcal{I}(M)$ , we consider surfaces  $z := z_{\alpha+1/2}(\tilde{\mathbf{x}}, t)$  with  $\tilde{\mathbf{x}} \in \mathbb{R}^2$ , such that layer  $\alpha$  at time  $t$  corresponds to the set comprehended between the curves  $z = z_{\alpha-1/2}(\tilde{\mathbf{x}}, t)$  and  $z = z_{\alpha+1/2}(\tilde{\mathbf{x}}, t)$ , i.e.  $z$  lies in the interval

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

Then, the layer and interfaces are defined by the sets

$$\Omega_\alpha(t) := \left\{ (\tilde{\mathbf{x}}, z) : z \in I_\alpha(\tilde{\mathbf{x}}, t), \quad \tilde{\mathbf{x}} \in \mathbf{\Pi}(t) \right\}, \quad \forall \alpha \in \mathcal{I}(M), \quad (14) \{?\}$$

$$\Gamma_{\alpha+1/2}(t) := \left\{ (\tilde{\mathbf{x}}, z) : z = z_{\alpha+1/2}(\tilde{\mathbf{x}}, t), \quad \tilde{\mathbf{x}} \in \mathbf{\Pi}(t) \right\}, \quad \forall \alpha \in \mathcal{I}_0(M), \quad (15) \{?\}$$

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

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

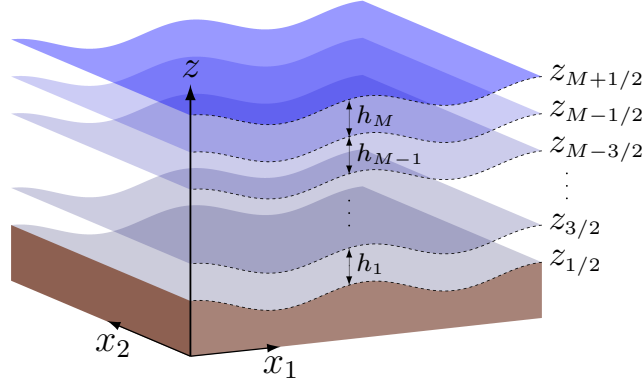


Figure 1: Illustration of the domain subdivision by layers.

where

$$\Theta_\alpha(t) := \left\{ (\tilde{\mathbf{x}}, z) : \tilde{\mathbf{x}} \in \partial\mathbf{\Pi}(t), \quad z \in I_\alpha(\tilde{\mathbf{x}}, t) \right\}.$$

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

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

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  $\varphi : \Omega \rightarrow \mathbb{R}$ , we define the one-sided limits

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

If  $\varphi$  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  $\alpha$ -layer, we need to take into account the flux transmissions at the interfaces  $\Gamma_{\alpha+1/2}$ . Before delving deeper, we introduce the divergence and gradient operators in the horizontal coordinates as  $\text{div}_{\mathbf{x}}$  and  $\nabla_{\mathbf{x}}$ , this is

$$\text{div}_{\mathbf{x}} := \frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2}, \quad \nabla_{\mathbf{x}} := (\partial_{x_1}, \partial_{x_2})^{\mathbf{t}},$$

and define  $\mathbf{div}_{\mathbf{x}}$  as the row-wise tensorial version of the divergence  $\text{div}_{\mathbf{x}}$ . For all  $\alpha \in \mathcal{I}(M)$ , we employ the subscript  $\alpha$  to denote the restriction of each function to the layer  $\alpha$ , i.e.  $\mathbf{c}_\alpha = \mathbf{c}|_{\Omega_\alpha(t)}$ ,  $\mathbf{s}_\alpha = \mathbf{s}|_{\Omega_\alpha(t)}$  and  $\mathbf{v}_\alpha = \mathbf{v}|_{\Omega_\alpha(t)}$ , and similarly with the rest of scalar, vector and tensor variables. In addition, we split the volume-average velocity at the  $\alpha$ -layer into its horizontal component  $\tilde{\mathbf{v}}_\alpha$  and

vertical velocity  $w_\alpha$ , this is  $\mathbf{v}_\alpha := (\tilde{\mathbf{v}}_\alpha, w_\alpha)$ . 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

$$\partial_z \tilde{\mathbf{v}}_\alpha = \mathbf{0} \quad \text{and} \quad \partial_z \mathbf{c}_\alpha = \partial_z \mathbf{s}_\alpha = \mathbf{0} \quad \forall \alpha \in \mathcal{I}(M). \quad (16) \text{ ?u\_constant?}$$

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

$$\partial_z w_\alpha = (\partial_z w_\alpha)(\mathbf{x}, t) \quad \text{and} \quad \partial_z p_\alpha = (\partial_z p_\alpha)(\mathbf{x}, t) \quad \forall \alpha \in \mathcal{I}(M). \quad (17) \text{ ?strucvp?}$$

More precisely, the assumption of a hydrostatic pressure means that

$$p_\alpha(\mathbf{x}, z, t) = p_{\alpha+1/2}(\mathbf{x}, t) + \rho_\alpha g(z_{\alpha+1/2} - z), \quad p_{\alpha+1/2}(\mathbf{x}, t) := p_S(\mathbf{x}, t) + g \sum_{\beta=\alpha+1}^M \rho_\beta h_\beta(\mathbf{x}, t),$$

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  $I_\alpha$ , this is

$$\partial_t(\rho_\alpha h_\alpha) + \text{div}_{\mathbf{x}}(\rho_\alpha h_\alpha \tilde{\mathbf{v}}_\alpha) = \mathcal{G}_{\alpha+1/2}^- - \mathcal{G}_{\alpha-1/2}^+ + h_\alpha(\tilde{\mathcal{R}}_{\mathbf{c}}(\mathbf{c}_\alpha, \mathbf{s}_\alpha) + \tilde{\mathcal{R}}_{\mathbf{s}}(\mathbf{c}_\alpha, \mathbf{s}_\alpha)), \quad (18) \text{ eq:PDErho}$$

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

$$\mathcal{G}_{\alpha+1/2} := \rho_\alpha(\partial_t z_{\alpha+1/2} + \tilde{\mathbf{v}}_\alpha \cdot \nabla_{\mathbf{x}} z_{\alpha+1/2} - w_\alpha) \quad \forall \alpha \in \mathcal{I}(M). \quad (19) \text{ def:flux:G}$$

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

$$\partial_t(c_\alpha^{(i)} h_\alpha) + \text{div}_{\mathbf{x}}(c_\alpha^{(i)} h_\alpha \tilde{\mathbf{v}}_\alpha) = \mathcal{G}_{\alpha+1/2}^{(i)} - \mathcal{G}_{\alpha-1/2}^{(i)} + h_\alpha \mathcal{R}_{\mathbf{c}}^{(i)}(\mathbf{c}_\alpha, \mathbf{s}_\alpha), \quad (20) \text{ eq:PDEc}$$

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  $\Gamma_{\alpha+1/2}$ , so that adding up  $\mathcal{G}_{\alpha+1/2}^{(i)}$  from  $i = 1$  to  $i = n_c$ , 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

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

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

$$\tilde{\mathbf{c}}_{\alpha+1/2} := (\tilde{c}_{\alpha+1/2}^{(i)})_{i \in \mathcal{I}(n_c)}, \quad \tilde{\mathbf{f}}_{\alpha+1/2} := (\tilde{f}_{\alpha+1/2}^{(i)})_{i \in \mathcal{I}(n_c)}, \quad \tilde{\mathbf{a}}_{3,\alpha+1/2} := (\tilde{a}_{3,\alpha+1/2}^{(i)})_{i \in \mathcal{I}(n_c)}.$$



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  $\tilde{\mathbf{v}}_\alpha$ )

$$\partial_t(s_\alpha^{(i)}h_\alpha) + \operatorname{div}_{\mathbf{x}}(s_\alpha^{(i)}h_\alpha\tilde{\mathbf{v}}_\alpha) = \mathcal{S}_{\alpha+1/2}^{(i)} - \mathcal{S}_{\alpha-1/2}^{(i)} + h_\alpha\mathcal{R}_s^{(i)}(\mathbf{c}_\alpha, \mathbf{s}_\alpha) \quad \forall i \in \mathcal{I}(n_s), \quad (21) \quad \boxed{\text{eq:PDEs}}$$

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

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

and as for the solid phase, we also the vector  $\mathcal{S}_{\alpha+1/2} := (\mathcal{S}_{\alpha+1/2}^{(i)})_{i \in \mathcal{I}(n_s)}$ . 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

$$\begin{aligned} & \partial_t(h_\alpha\rho_\alpha\tilde{\mathbf{v}}_\alpha) + \nabla_{\mathbf{x}} \cdot (h_\alpha\rho_\alpha\tilde{\mathbf{v}}_\alpha \otimes \tilde{\mathbf{v}}_\alpha) + h_\alpha(\nabla_{\mathbf{x}}\bar{p}_\alpha + g\rho_\alpha\nabla_{\mathbf{x}}\bar{z}_\alpha) \\ &= \frac{1}{2}G_{\alpha+1/2}(\tilde{\mathbf{v}}_{\alpha+1} - \tilde{\mathbf{v}}_\alpha) - \frac{1}{2}G_{\alpha-1/2}(\tilde{\mathbf{v}}_\alpha - \tilde{\mathbf{v}}_{\alpha-1}) + \mathbf{K}_{\alpha+1/2} - \mathbf{K}_{\alpha-1/2}, \end{aligned} \quad (22) \quad \boxed{\text{eq:PDEv}}$$

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

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

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

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

then

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

with  $h_{\alpha+1/2}$  the distance between the midpoints of layers  $\alpha$  and  $\alpha+1/2$ . On the other hand  $\bar{p}_\alpha$  and  $\bar{z}_\alpha$  are defined by (24) and (25), respectively.

Next, to close the system, we further assume that the thickness of each layer  $h_\alpha$  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  $m_\alpha := \rho_\alpha h$ ,  $\mathbf{q}_\alpha := \rho_\alpha h \tilde{\mathbf{v}}_\alpha$ ,  $\mathbf{r}_\alpha := \mathbf{c}_\alpha h$  and  $\zeta_\alpha := \mathbf{s}_\alpha h$  for  $\alpha \in \mathcal{I}(M)$  and replacing them into (18), (22), (20) and (21), we can write the multilayer formulation of (13) as

$$\partial_t m_\alpha + \operatorname{div}_{\mathbf{x}}(\mathbf{q}_\alpha) = \frac{1}{l_\alpha} (\mathcal{G}_{\alpha+1/2} - \mathcal{G}_{\alpha-1/2}) + h (\tilde{\mathcal{R}}_{s,\alpha} + \tilde{\mathcal{R}}_{c,\alpha}), \quad (23a) \quad \boxed{\text{eq:ml:m}}$$

$$\begin{aligned} & \partial_t \mathbf{q}_\alpha + \operatorname{div}_{\mathbf{x}} \left( \frac{\mathbf{q}_\alpha \otimes \mathbf{q}_\alpha}{m_\alpha} \right) + h (\nabla_{\mathbf{x}} \bar{p}_\alpha + g \rho_\alpha \nabla_{\mathbf{x}} \bar{z}_\alpha) \\ &= \frac{1}{l_\alpha} (\tilde{\mathbf{q}}_{\alpha+1/2} G_{\alpha+1/2} - \tilde{\mathbf{q}}_{\alpha-1/2} G_{\alpha-1/2}) + \frac{1}{l_\alpha} (\mathbf{K}_{\alpha+1/2} - \mathbf{K}_{\alpha-1/2}), \end{aligned} \quad (23b) \quad \boxed{\text{eq:ml:v}}$$

$$\partial_t r_\alpha^{(i)} + \operatorname{div}_{\mathbf{x}} \left( \frac{r_\alpha^{(i)} \mathbf{q}_\alpha}{m_\alpha} \right) = \frac{1}{l_\alpha} (\mathcal{G}_{\alpha+1/2}^{(i)} - \mathcal{G}_{\alpha-1/2}^{(i)}) + h \mathcal{R}_{c,\alpha}^{(i)} \quad \forall i \in \mathcal{I}(n_c), \quad (23c) \quad \boxed{\text{eq:ml:c}}$$

$$\partial_t \zeta_\alpha^{(i)} + \operatorname{div}_{\mathbf{x}} \left( \frac{\zeta_\alpha^{(i)} \mathbf{q}_\alpha}{m_\alpha} \right) = \frac{1}{l_\alpha} (\mathcal{S}_{\alpha+1/2}^{(i)} - \mathcal{S}_{\alpha-1/2}^{(i)}) + h \mathcal{R}_{s,\alpha}^{(i)} \quad \forall i \in \mathcal{I}(n_s), \quad (23d) \quad \boxed{\text{eq:ml:s}}$$



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

$$\bar{p}_\alpha := p_S + \frac{1}{2}gl_\alpha m_\alpha + \sum_{\beta=\alpha+1}^M gl_\beta m_\beta, \quad (24) \text{def:pbar}$$

$$\bar{z}_\alpha := z_B + \frac{1}{2}l_\alpha h + \sum_{\beta=1}^{\alpha-1} l_\beta h, \quad (25) \text{def:zbar}$$

$$\tilde{\mathbf{q}}_{\alpha+1/2} := \frac{1}{2} \left( \frac{\mathbf{q}_{\alpha+1}}{m_{\alpha+1}} + \frac{\mathbf{q}_\alpha}{m_\alpha} \right). \quad (26) \text{?def:vbar?}$$

Using the definitions (24) and (25), together with  $l_1 + \dots + l_M = 1$  and  $m_\alpha = \rho_\alpha h$ , the third term on the left-hand side of (23b), accounting for the gradient of pressure, can be written as

$$\begin{aligned} h(\nabla_{\mathbf{x}} \bar{p}_\alpha + g\rho_\alpha \nabla_{\mathbf{x}} \bar{z}_\alpha) &= gm_\alpha \nabla_{\mathbf{x}}(z_B + h) + gh^2 \left( \frac{1}{2}l_\alpha + \sum_{\beta=\alpha+1}^M l_\beta \right) \nabla_{\mathbf{x}} \rho_\alpha \\ &\quad + gh \sum_{\beta=\alpha+1}^M l_\beta \nabla_{\mathbf{x}}(m_\beta - m_\alpha). \end{aligned} \quad (27) \text{eq:expressionP}$$

The conservation equation for the total mass of the solid phase is obtained by adding up equation (23a) (after multiplying by  $l_\alpha$  in both sides of the equation) from  $\alpha = 0$  to  $\alpha = M$ , this is

$$\partial_t \bar{m} + \nabla_{\mathbf{x}} \cdot \left( \sum_{\beta=1}^M l_\beta \mathbf{q}_\beta \right) = \mathcal{G}_{M+1/2} - \mathcal{G}_{1/2}, \quad (28) \text{?eq:ml:mtot?}$$

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 (19), depends explicitly on the vertical velocities  $w_\alpha$ , 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

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

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

$$\mathcal{G}_{\alpha+1/2} = \frac{\tilde{\rho}_{\alpha+1/2}}{\rho_f} \sum_{\beta=1}^\alpha l_\beta \operatorname{div}_{\mathbf{x}}(\mathbf{R}_\beta - \bar{\mathbf{R}}) + \tilde{\mathcal{G}}_{\alpha+1/2} \quad \forall \alpha \in \mathcal{I}_0(M), \quad (29) \text{?eq:fluxGnew?}$$

where

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

and for  $l = 1/2$  and  $l = M + 1/2$

$$C_l := \frac{\rho_f}{\tilde{\rho}_l} \mathcal{G}_l + \sum_{j=1}^N \frac{(\rho_j - \rho_f)}{\rho_j} \left( \tilde{f}_l^{(j)} - \tilde{a}_{3,l}^{(j)} \right).$$

### 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

$$w_{1/2}^+ = \partial_t z_B + \tilde{\mathbf{v}}_1 \cdot \nabla_{\mathbf{x}} z_B - \frac{G_{1/2}}{\rho_1}. \quad (30) \text{ ?v:1?}$$

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

$$\begin{aligned} w_\alpha(\mathbf{x}, z, t) &= w_{\alpha-1/2}^+ - \frac{1}{\rho_\alpha} (\partial_t \rho_\alpha + \nabla_{\mathbf{x}} \cdot (\rho_\alpha \tilde{\mathbf{v}}_\alpha)) (z - z_{\alpha-1/2}), \\ w_{\alpha+1/2}^- &= w_{\alpha-1/2}^+ - \frac{h_\alpha}{\rho_\alpha} (\partial_t \rho_\alpha + \nabla_{\mathbf{x}} \cdot (\rho_\alpha \tilde{\mathbf{v}}_\alpha)), \\ w_{\alpha+1/2}^+ &= \frac{1}{\rho_\alpha} \left( (\rho_\alpha - \rho_{\alpha-1}) \partial_t z_{\alpha-1/2} + (\rho_\alpha \tilde{\mathbf{v}}_\alpha - \rho_{\alpha-1} \tilde{\mathbf{v}}_{\alpha-1}) \cdot \nabla_{\mathbf{x}} z_{\alpha-1/2} + \rho_{\alpha-1} w_{\alpha-1/2}^- \right). \end{aligned} \quad (31) \text{ ?v:2?}$$

**Ver hiperbolicidad, y alguna otra propiedad.**

## 4 Numerical scheme

ec:numschem)

In this section, we describe the numerical method designed to approximate system (23) 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 (23b) separately, we start by writing system (23) in compact form, without including the term  $\mathbf{K}_{\alpha+1/2} - \mathbf{K}_{\alpha-1/2}$ . Considering that for each  $\alpha \in \mathcal{I}(M)$ ,  $\mathbf{q}_\alpha \in \mathbb{R}^2$ ,  $\mathbf{r}_\alpha \in \mathbb{R}^{n_c}$  and  $\boldsymbol{\zeta}_\alpha \in \mathbb{R}^{n_s}$ , we define the vector of unknowns of (23) on each  $\alpha$ -layer as  $\tilde{\mathbf{w}}_\alpha := (m_\alpha, \mathbf{q}_\alpha, \mathbf{r}_\alpha, \boldsymbol{\zeta}_\alpha)^t \in \mathbb{R}^N$ , where  $N := 3 + n_c + n_s$  and  $\mathbf{w}_\alpha := (\mathbf{q}_\alpha, \mathbf{r}_\alpha, \boldsymbol{\zeta}_\alpha) \in \mathbb{R}^{N-1}$ . The vector solution gathering the  $M$  layers is defined by  $\tilde{\mathbf{W}} := (\tilde{\mathbf{w}}_1, \dots, \tilde{\mathbf{w}}_M) \in \mathbb{R}^{NM}$ , and the transformed vector taking into account the total mass  $\tilde{m}$  is

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

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

$$\mathbf{W} = \mathbf{C} \tilde{\mathbf{W}}, \quad (32) \text{ ?eq:relWhatW?}$$

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

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

The convective fluxes corresponding to each equation (23a), (23c), (23d) and (23b), for  $\alpha \in \mathcal{I}(M)$  are denoted by the single matrix  $\mathbf{F} := (\mathbf{F}_1^\mathbf{t}, \dots, \mathbf{F}_M^\mathbf{t})^\mathbf{t} \in \mathbb{R}^{NM \times 2}$  where

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

For the third term on the left-hand side of Equation (23b), we define the vector  $\mathbf{P} := (\mathbf{P}_1^\mathbf{t}, \dots, \mathbf{P}_M^\mathbf{t})^\mathbf{t} \in \mathbb{R}^{NM}$ , where  $\mathbf{P}_\alpha := [0, \boldsymbol{\psi}_\alpha^\mathbf{t}, \mathbf{0}_{n_c}, \mathbf{0}_{n_s}]^\mathbf{t} \in \mathbb{R}^N$  for all  $\alpha \in \mathcal{I}(M)$ , with  $\boldsymbol{\psi}_\alpha \in \mathbb{R}^2$  given by (27), this is

$$\boldsymbol{\psi}_\alpha := g m_\alpha \nabla_{\mathbf{x}}(z_B + h) + g h^2 \left( \frac{1}{2} l_\alpha + \sum_{\beta=\alpha+1}^M l_\beta \right) \nabla_{\mathbf{x}} \rho_\alpha + g h \sum_{\beta=\alpha+1}^M l_\beta \nabla_{\mathbf{x}}(m_\beta - m_\alpha). \quad (33) \quad \boxed{\text{def:psi}}$$

For the right-hand sides of (23) we introduce the following vectors  $\mathcal{J}_L := (\mathcal{J}_{1-1/2}^\mathbf{t}, \dots, \mathcal{J}_{M-1/2}^\mathbf{t})^\mathbf{t}$ ,  $\mathcal{J}_R := (\mathcal{J}_{1+1/2}^\mathbf{t}, \dots, \mathcal{J}_{M+1/2}^\mathbf{t})^\mathbf{t}$  and  $\mathcal{R} := (\mathcal{R}_1^\mathbf{t}, \dots, \mathcal{R}_M^\mathbf{t})^\mathbf{t}$  in  $\mathbb{R}^{NM}$  where for  $\alpha \in \mathcal{I}_0(M)$  and  $\beta \in \mathcal{I}(M)$ :

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

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

$$\partial_t \mathbf{W} + \mathbf{C} \left( \text{div}_{\mathbf{x}}(\mathbf{F}(\tilde{\mathbf{W}})) + \mathbf{P}(\tilde{\mathbf{W}}) \right) = \mathbf{C} \left( \mathcal{J}_R(\tilde{\mathbf{W}}) - \mathcal{J}_L(\tilde{\mathbf{W}}) \right) + \mathbf{C} \mathcal{R}(\tilde{\mathbf{W}}), \quad (34) \quad \boxed{\text{eq:systemfinal}}$$

and for each  $\alpha$ -layer

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

#### 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 given by squares of size  $\Delta x \times \Delta y$  with  $\Delta x$  and  $\Delta y$  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  $\mathbf{x}_i$  while  $|V_i|$  and  $|E_{i,j}|$  stand for the area of  $V_i$  and length of  $E_{i,j}$ , respectively.

For the numerical simulation, we will use the following CFL condition to determine  $\Delta t$  in each iteration:

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

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

We approximate the solution at each time  $t_n$  by the averages

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

and propose the following first-order two-dimensional finite volume scheme to approximate (34):

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

where

$$\begin{aligned} \mathbf{F}_{i,j} &= (\mathbf{F}_{i,j,\alpha})_{1 \leq \alpha \leq M}, & \mathbf{P}_{i,j} &= (\mathbf{P}_{i,j,\alpha})_{1 \leq \alpha \leq M}, & \mathbf{R}_i &= (\mathbf{R}_\alpha(\tilde{\mathbf{w}}_{i,\alpha}))_{1 \leq \alpha \leq M}, \\ \mathcal{J}_{L,i,j} &= (\mathcal{J}_{i,j,\alpha-1/2})_{1 \leq \alpha \leq M}, & \mathcal{J}_{R,i,j} &= (\mathcal{J}_{i,j,\alpha+1/2})_{1 \leq \alpha \leq M}. \end{aligned}$$

Each  $\mathbf{F}_{i,j,\alpha}$  for  $\alpha \in \mathcal{I}(M)$  corresponds to the approximation of the flux  $\mathbf{F}_\alpha$  at the edge  $E_{i,j}$ . The first three components of  $\mathbf{F}_{i,j,\alpha}$  are approximated by an HLL-PVM-1U method [24], which depends on left and right bounds of the eigenvalues, denoted by  $\sigma_L$  and  $\sigma_R$ , respectively, of the transport matrix of the **full system (aquí 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  $\varphi$ , we define  $\{\{\varphi\}\}_{i,j} := (\varphi_i + \varphi_j)/2$ , the average of  $\varphi$  at the edge  $E_{i,j}$ , which is defined analogously for vector and tensor variables. For the rest of components of  $\mathbf{F}_{i,j,\alpha}$ , we use the fact that they are linear and depend on  $[\mathbf{F}_\alpha]_1(\tilde{\mathbf{w}}_\alpha)$ , so that an upwind approach is employed. Then, the components  $[\mathbf{F}_{i,j,\alpha}]_l$  for  $l = 1, 2, 3$  are given by the HLL-PVM-1U scheme

$$\begin{aligned} [F_{i,j,\alpha}]_l &= \left[ \left\{ \mathbf{F}_\alpha(\tilde{\mathbf{w}}_\alpha) \right\}_{i,j} \cdot \boldsymbol{\eta}_{i,j} - \frac{1}{2} \left( \theta_{0,i,j} (\tilde{\mathbf{w}}_{j,\alpha} - \tilde{\mathbf{w}}_{i,\alpha} + \mathbf{b}_{i,j,\alpha}) \right. \right. \\ &\quad \left. \left. + \theta_{1,i,j} ((\mathbf{F}_\alpha(\tilde{\mathbf{w}}_{j,\alpha}) - \mathbf{F}_\alpha(\tilde{\mathbf{w}}_{i,\alpha})) \cdot \boldsymbol{\eta}_{i,j} + \mathbf{P}_{i,j,\alpha}) \right) \right]_l. \end{aligned}$$

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

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

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

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

where the characteristic velocities  $\sigma_{L,i,j}^n$  and  $\sigma_{R,i,j}^n$  are global approximations of the minimum and maximum wave speed of the system (**poner sistema**). **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  $\sigma_{L,i,j}$  and  $\sigma_{R,i,j}$  as follows:

$$\sigma_{L,i,j} := \bar{v}_{i,j}^n - \Psi_{i,j}^n, \quad \sigma_{R,i,j} := \bar{v}_{i,j}^n + \Psi_{i,j}^n, \quad (35) \text{ ?wave1?}$$

where

$$\bar{v}_{i,j}^n := \frac{1}{M} \sum_{\beta=1}^M \{\{\tilde{\mathbf{v}}_\beta^n\}\}_{i,j}^\mathbf{t} \boldsymbol{\eta}_{i,j}, \quad (36) \text{ ?wave2?}$$

$$\begin{aligned} \Psi_{i,j}^n &:= \left( 4 - \frac{2}{M} \right)^{1/2} \left( \sum_{\beta=1}^M (\bar{v}_{i,j}^n - \mathbf{v}_{\beta,i,j}^n)^2 \right. \\ &\quad \left. + \frac{g}{2} \{\{h^n\}\}_{i,j} \left( 1 + \sum_{\beta=1}^M \frac{(2\beta-1)}{M\rho_f} \{\{\rho_\beta^n\}\}_{i,j} \right) \right)^{1/2}. \end{aligned} \quad (37) \text{ ?wave3?}$$

For the pressure-related term  $\mathbf{P}_{i,j,\alpha}^n = [0, (\boldsymbol{\psi}_{i,j,\alpha}^n)^\mathbf{t}, \mathbf{0}_{n_c}^\mathbf{t}, \mathbf{0}_{n_s}^\mathbf{t}]^\mathbf{t} \in \mathbb{R}^N$ , in the same way as in [18], we approximate the products and gradients appearing in (33) by averages and differences so that

$$\begin{aligned} \boldsymbol{\psi}_{i,j,\alpha}^n = g \left( \left\{ \left\{ m_\alpha^n \right\} \right\}_{i,j} \left( z_{B,j} - z_{B,i} + h_j^n - h_i^n \right) + \left\{ (h^n)^2 \right\}_{i,j} \left( \frac{l_\alpha}{2} + \sum_{\beta=\alpha+1}^M l_\beta \right) \left( \rho_{j,\alpha}^n - \rho_{i,\alpha}^n \right) \right. \\ \left. + \left\{ h^n \right\}_{i,j} \sum_{\beta=\alpha+1}^M l_\beta \left( m_{j,\beta}^n - m_{i,\beta}^n - (m_{j,\alpha}^n - m_{i,\beta}^n) \right) \right) \boldsymbol{\eta}_{i,j}. \end{aligned} \quad (38) \{?\}$$

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

$$\mathcal{G}_{i,j,\alpha+1/2}^n = \frac{\tilde{\rho}_{i,j,\alpha+1/2}^n}{\rho_f} \sum_{\beta=1}^{\alpha} l_\beta \left( (\mathbf{R}_{j,\beta}^n - \bar{\mathbf{R}}_j^n)^\mathbf{t} - (\mathbf{R}_{i,\beta}^n - \bar{\mathbf{R}}_i^n)^\mathbf{t} \right) \boldsymbol{\eta}_{i,j} + \tilde{\mathcal{G}}_{i,\alpha+1/2}^n \ell_{i,j}, \quad (39) \{?\}$$

$$\tilde{\mathbf{q}}_{i,j,\alpha+1/2}^n = \frac{1}{2} \left\{ \mathbf{q}_\alpha^n + \mathbf{q}_{\alpha+1}^n \right\}_{i,j}, \quad (40) \{?\}$$

$$\mathcal{G}_{i,j,\alpha+1/2}^n = \tilde{\mathbf{c}}_{i,j,\alpha+1/2}^n \mathcal{G}_{i,j,\alpha+1/2}^n - \left( \tilde{\mathbf{f}}_{i,\alpha+1/2}^n - \tilde{\mathbf{a}}_{i,3,\alpha+1/2}^n \right) \ell_{i,j}, \quad (41) \{?\}$$

$$\mathcal{S}_{i,j,\alpha+1/2}^n = \tilde{\mathbf{s}}_{i,j,\alpha+1/2}^n \mathcal{G}_{i,j,\alpha+1/2}^n + \tilde{\mathbf{s}}_{i,j,\alpha+1/2}^{\mathbf{f},n} \sum_{l=1}^{n_c} \left( \tilde{f}_{i,\alpha+1/2}^{(l),n} - \tilde{a}_{i,3,\alpha+1/2}^{(l),n} \right) \ell_{i,j}, \quad (42) \{?\}$$

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

$$\begin{aligned} \tilde{\rho}_{i,j,\alpha+1/2}^n &= \left\{ \left\{ \frac{2\rho_\alpha^n \rho_{\alpha+1}^n}{\rho_\alpha^n + \rho_{\alpha+1}^n} \right\} \right\}_{i,j}, & \tilde{\mathbf{c}}_{i,j,\alpha+1/2}^n &= \frac{1}{2} \left\{ \left\{ \frac{\mathbf{c}_{\alpha+1}^n}{\rho_{\alpha+1}^n} + \frac{\mathbf{c}_\alpha^n}{\rho_\alpha^n} \right\} \right\}_{i,j}, \\ \tilde{\mathbf{s}}_{i,j,\alpha+1/2}^n &= \frac{1}{2} \left\{ \left\{ \frac{\mathbf{s}_{\alpha+1}^n}{\rho_{\alpha+1}^n} + \frac{\mathbf{s}_\alpha^n}{\rho_\alpha^n} \right\} \right\}_{i,j}, & \tilde{\mathbf{s}}_{i,j,\alpha+1/2}^{\mathbf{f},n} &= \frac{1}{2\rho_f} \left\{ \left\{ \frac{\mathbf{s}_{\alpha+1}^n}{\phi_{f,\alpha+1}^n} + \frac{\mathbf{s}_\alpha^n}{\phi_{f,\alpha}^n} \right\} \right\}_{i,j}, \end{aligned}$$

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

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

and where  $\Phi_\alpha := (\phi_{1,\alpha}, \dots, \phi_{N,\alpha})^\mathbf{T}$  and  $E_\alpha := \max_{j=1,\dots,N} |v_j^{\text{MLB}}(\Phi_\alpha)|$ , where  $v_j^{\text{MLB}}$  is the hindered settling velocity. For  $\tilde{\mathbf{a}}_{3,\alpha+1/2}^{(i)} := (\tilde{a}_{3,\alpha+1/2}^{(i)})_{i \in \mathcal{I}(n_c)}$  first note that from (10) the third component of vector  $\mathbf{a}_i(\mathbf{c}, \nabla \mathbf{c})$  can be write as

$$\tilde{a}_3^{(i)} = \sum_{j=1}^N \eta_{ij} \frac{\partial \phi_j}{\partial z} \quad (43) \text{def:a3}$$

with

$$\eta_{ij} = -\frac{\mu}{g\rho} \rho_j V(\phi) \left\{ (1-\phi) \phi_j (\delta_j - \boldsymbol{\delta}^t \boldsymbol{\phi}) \sigma'_e \left[ \delta_j \delta_{ji} - \frac{\phi_j \rho_i \delta_i}{\rho} - \frac{\phi_j}{\phi} (\delta_j - \boldsymbol{\delta}^t \boldsymbol{\lambda}) \right] \sigma_e \right\}, \quad (44) \{?\}$$

then  $\tilde{a}_{3,\alpha+1/2}^{(i)}$  is an approximation of (43) at the interface  $\Gamma_{\alpha+1/2}$ . Finally, the term  $\mathbf{b}_{i,j,\alpha}$  is included to preserve the well-balance and the stationary solution deduced in [18, Proposition 1], this is

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

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

## Viscous term approximation

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

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

Thus, we may approximate the viscous terms as

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

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

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

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)

We consider a reduced biokinetic model, the denitrification process of converting nitrate ( $NO_3$ ) into nitrogen gas ( $N_2$ ) presented in [9], where  $\mathbf{c} = (c^{(1)}, c^{(2)})$ , with  $c^{(1)}$  and  $c^{(2)}$  correspond to the concentration of ordinary heterotrophic organisms (often denoted by  $X_{\text{OHO}}$ ) and undegradable organics (often denoted by  $X_{\text{U}}$ ), respectively, and  $\mathbf{s} = (s^{(1)}, s^{(2)}, s^{(3)})$  with  $s^{(1)}$ ,  $s^{(2)}$  and  $s^{(3)}$  correspond to the concentration of nitrate  $S_{\text{NO}_3}$ , readily biodegradable substrate  $S_{\text{S}}$  and nitrogen  $S_{\text{N}_2}$ , respectively. The vector of nonlinear reactions and stoichiometric matrices are given by

$$\mathbf{r} = c^{(1)} \begin{bmatrix} \mu(s^{(1)}, s^{(2)}) \\ b \end{bmatrix}, \quad \boldsymbol{\sigma}_{\mathbf{c}} = \begin{bmatrix} 1 & -1 \\ 0 & f_p \end{bmatrix}, \quad \boldsymbol{\sigma}_{\mathbf{s}} = \begin{bmatrix} -\bar{Y} & -1/Y & \bar{Y} \\ 0 & -0.8 & 0 \end{bmatrix},$$

where  $b = 6.94 \times 10^{-6}$  is the decay rate of heterotrophic organisms,  $f_p = 0.2$  is the portion of these that decays to undegradable organics,  $Y = 0.67$  and  $\bar{Y} = 0.172216$  are a yield factors, and

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

with  $\mu_{\max} = 5.56 \times 10^{-5}$ ,  $\kappa_1 = 5 \times 10^{-4}$ ,  $\kappa_2 = 0.02$ . The reaction terms are

$$\boldsymbol{\sigma}_{\mathbf{c}} \mathbf{r} = c^{(1)} \begin{bmatrix} \mu(s^{(1)}, s^{(2)}) - b \\ f_p b \end{bmatrix}, \quad \boldsymbol{\sigma}_{\mathbf{s}} \mathbf{r} = c^{(1)} \begin{bmatrix} -\bar{Y} \mu(s^{(1)}, s^{(2)}) \\ -\tilde{\mu}(s^{(1)}, s^{(2)})/Y - 0.8b \\ \bar{Y} \mu(s^{(1)}, s^{(2)}) \end{bmatrix},$$

$$v_{\text{hs}}(\phi(\mathbf{c})) = \left( 1 - \sum_{j=1}^{n_{\mathbf{c}}} \frac{c^{(j)}}{\rho_j} \right)^n, \quad n > 2$$

## 6 Conclusions

Some conclusions here.

## A Appendix

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

$$\begin{aligned} 0 &= \int_{I_\alpha} (\partial_t \theta + \text{div}(\theta \boldsymbol{\nu})) dz = h_\alpha (\partial_t \theta) + \int_{I_\alpha} \text{div}_{\mathbf{x}}(\theta \boldsymbol{\nu}) dz + \theta \int_{I_\alpha} \partial_z \nu dz \\ &= h_\alpha (\partial_t \theta) - \theta \left( \tilde{\boldsymbol{\nu}}|_{z_{\alpha+1/2}}^- \cdot \nabla_{\mathbf{x}} z_{\alpha+1/2} - \tilde{\boldsymbol{\nu}}|_{z_{\alpha-1/2}}^+ \cdot \nabla_{\mathbf{x}} z_{\alpha-1/2} \right) + \theta \nu|_{z_{\alpha+1/2}}^- - \theta \nu|_{z_{\alpha-1/2}}^+ \\ &\quad + \text{div}_{\mathbf{x}} \left( \int_{I_\alpha} \theta \tilde{\boldsymbol{\nu}} dz \right) \end{aligned}$$

where we have used that  $\text{div} = \text{div}_{\mathbf{x}} + \partial_z$  and Leibnitz's rule. Using once again that  $\theta$  and  $\tilde{\boldsymbol{\nu}}$  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

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

The above equation implies

$$\begin{aligned} \partial_t(\theta h_\alpha) + \text{div}_{\mathbf{x}}(\theta h_\alpha \tilde{\boldsymbol{\nu}}) &= \theta(\partial_t z_{\alpha+1/2} + \tilde{\boldsymbol{\nu}}|_{z_{\alpha+1/2}}^- \cdot \nabla_{\mathbf{x}} z_{\alpha+1/2} - \nu|_{z_{\alpha+1/2}}^-) \\ &\quad - \theta(\partial_t z_{\alpha-1/2} + \tilde{\boldsymbol{\nu}}|_{z_{\alpha-1/2}}^+ \cdot \nabla_{\mathbf{x}} z_{\alpha-1/2} - \nu|_{z_{\alpha-1/2}}^+). \end{aligned}$$

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