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a polydisperse model of flow and segregation in general domains

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AN INVARIANT-REGION-PRESERVING FINITE-VOLUME-ELEMENT SCHEME FOR A POLYDISPERSE MODEL OF FLOW AND SEGREGATION IN GENERAL DOMAINS*

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Abstract. A spatially two-dimensional model for the flow of a mixture of a continuous phase with a disperse phase that consists of particles (or droplets) of N species in general geometries consists of a system of N conservation laws for the concentrations of particles, coupled with a Stokes-type system of equations governing the velocity of the mixture. This model is studied for the special case of sedimentation of polydisperse solid-liquid suspensions. This coupled transport-flow problem is approximated by a numerical scheme in which the Stokes equations are discretized on a primal triangular mesh using a finite element approach, while the concentration equations are approximated on a dual diamond mesh by a finite volume scheme. The resulting finite volume element (FVE) scheme is second-order accurate in space and time. The concentration vector is required to take values in a set of physically relevant states (i.e., its components are non-negative and sum to at most a prescribed maximum value). It is proven that this invariant region is preserved by the numerical solutions produced by the FVE scheme. This property is ensured by applying a pair of linear scaling limiters to a second-order MUSCL reconstruction of the concentration field. The FVE scheme is applied to simulate the settling of polydisperse suspensions in various types of vessels.

Key words. Finite volume element scheme; MUSCL reconstruction; scaling limiters; transport-flow problem; invariant region; polydisperse sedimentation

MSC codes. 76T20, 65M08, 65M60

1. Introduction.

1.1. Scope. We are interested in second-order in space and time finite volume/finite element (in short, finite-volume-element, FVE) approximations of coupled transport-flow models of the form

$$(1.1a) \quad \partial_t \phi_l + \nabla \cdot (\phi_l \mathbf{u} + f_l(\Phi) \mathbf{k}) = 0, \quad f_l(\Phi) = \phi_l v_l(\Phi), \quad l = 1, \dots, N;$$

$$(1.1b) \quad -\nabla \cdot (\mu(\phi) \boldsymbol{\varepsilon}(\mathbf{u})) + \nabla p = \mathbf{g}(\phi), \quad \boldsymbol{\varepsilon}(\mathbf{u}) := \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T);$$

$$(1.1c) \quad \nabla \cdot \mathbf{u} = 0,$$

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where $\Phi := (\phi_1, \dots, \phi_N)^T$, $\phi := \phi_1 + \dots + \phi_N$, and (1.1) is posed on a bounded domain $\Omega \subset \mathbb{R}^2$ for $t > 0$, along with the initial and boundary conditions

$$(1.2) \quad \Phi(\mathbf{x}, 0) = \Phi_0(\mathbf{x}) \quad \text{for all } \mathbf{x} \in \Omega, \text{ where } \Phi_0 := (\phi_{1,0}, \dots, \phi_{N,0})^T,$$

$$(1.3) \quad \mathbf{u} = \mathbf{0} \quad \text{and} \quad (f_l(\Phi)\mathbf{k}) \cdot \mathbf{n} = 0, \quad l = 1, \dots, N, \quad \text{on } \partial\Omega,$$

$$(1.4) \quad \int_{\Omega} p(\mathbf{x}, t) d\mathbf{x} = 0 \quad \text{for all } t \geq 0.$$

The system (1.1) can be understood as a transport-flow model for a two-phase mixture consisting of a disperse phase with N species of particles or droplets moving in a viscous continuous phase. In particular it models a polydisperse suspension of solid particles of N species with diameters $d_1 \geq \dots \geq d_N$ and densities $\rho_1, \dots, \rho_N$ dispersed in a viscous fluid. The unknowns are the volume fractions $\phi_l = \phi_l(\mathbf{x}, t)$ of each particle species l (having diameter d_l and density ρ_l), which depend on spatial position $\mathbf{x}$ and time t , the volume-averaged mixture velocity $\mathbf{u} = \mathbf{u}(\mathbf{x}, t)$, and the pressure $p = p(\mathbf{x}, t)$. Here $\mathbf{k}$ denotes the downward-pointing unit vector while $v_1(\Phi), \dots, v_N(\Phi)$ are prescribed velocity functions that describe the relative motion of each particle species with respect to the mixture. The physically relevant set of states Φ is

$$\mathcal{D} := \{(\phi_1, \dots, \phi_N)^T \in \mathbb{R}^N : \phi_1 \geq 0, \dots, \phi_N \geq 0, \phi := \phi_1 + \dots + \phi_N \leq \phi_{\max}\},$$

where $\phi_{\max}$ denotes a given maximum total particle volume fraction.

It is the purpose of this work to introduce a FVE scheme for the solution of the initial-boundary value problem (IBVP) (1.1)–(1.4) that is second-order accurate in both space and time, and that provably satisfies the invariant region preservation (IRP) property, that is, if $\Phi_0(\mathbf{x}) \in \mathcal{D}$ for all $\mathbf{x} \in \Omega$, then the numerical solution assumes values in $\mathcal{D}$ for all times. The main novelties are as follows. While previously developed IRP methods for (1.1) were limited to the one-dimensional version of (1.1a) [2] or rectangular domains [3], we herein introduce a FVE approximation of (1.1) on general polygonal domains. Such domains include trapezoidal (roof-shaped) vessels and configurations of real solid-liquid separation equipment such as the reflux classifier [24]. To achieve this we define a primal triangular mesh for the nonconforming approximation of the Stokes problem (1.1b), (1.1c) by Crouzeix-Raviart finite elements along with a dual diamond mesh on which the concentration equations (1.1a) are discretized by a finite volume (FV) scheme with MUSCL reconstruction. Based on this dual-mesh construction the numerical flux may be approximated in a straightforward manner because the mixture velocity $\mathbf{u}$ is uniquely defined along the edges shared by adjacent control volumes of the dual mesh. On the other hand, the proof of the IRP property for the FVE scheme depends on a novel proof that the first-order LLF scheme on general meshes produces physically relevant solutions to the transport part of the model (1.1), as well as on an extension of the limiters introduced in [2, 3] to polygonal meshes. Finally, the version of the Masliyah-Lockett-Bassoon (MLB) model [21, 22] of polydisperse sedimentation utilized herein is more general than the one considered in [2, 3] since we admit a more general definition (see [4]) of hindered settling velocities (in a sense made precise in later parts of the paper).

1.2. Related work. Mathematical models for polydisperse sedimentation describe the coupled settling of particle species with different sizes and concentrations. Classical formulations of hindered settling include the models of Masliyah [22] and Lockett and Bassoon [21], while Richardson and Zaki [25] provided a widely used correlation for sedimentation and fluidization. Subsequent work has addressed the

mathematical structure of multispecies sedimentation models, including their hyperbolicity and instability regions [7, 9], as well as extensions involving particle-size-specific hindered-settling factors [4]. Specifically we refer to [9] for a derivation of the MLB model from principles of continuum mechanics, and to [7] for alternate models of polydisperse sedimentation. On the other hand, the governing model (1.1) also describes transport-flow processes for other a multispecies disperse phases, such as the settling and creaming of liquid-liquid dispersions [1, 26].

Numerical approximations of sedimentation and related transport-flow systems have been developed using FV, FE, and FVE techniques. In [8] Bürger et al. proposed a stabilized FVE formulation for sedimentation-consolidation processes. For transport problems on unstructured meshes, Castro et al. [11] developed a second-order FV method, providing a basis for the MUSCL reconstruction employed herein. The flow system (1.1b), (1.1c) is discretized using Crouzeix-Raviart nonconforming finite elements [14], together with stabilization techniques for piecewise H^1 fields [6, 15, 19].

A major challenge in high-order approximations of sedimentation models is maintaining the physically admissible concentration region $\mathcal{D}$. For the appropriate treatment of this issue in the general context of conservation laws we refer to [20]. Standard high-order reconstructions may violate the constraint $\Phi \in \mathcal{D}$, particularly near steep gradients. The authors' previous work addressed this issue through weighted essentially non-oscillatory (WENO) schemes equipped with the IRP property (IRP-WENO) schemes for one-dimensional multispecies kinematic flow models [2] and through a second-order finite-difference IRP method for a transport-flow model of polydisperse sedimentation on Cartesian meshes [3]. The present work extends these ideas to general polygonal domains and a FVE discretization. The scaling limiters used to enforce the IRP property are related to the positivity- and maximum-principle-preserving methodology developed by Zhang and collaborators. Zhang [28] introduced positivity-preserving high-order DG techniques for compressible Navier–Stokes equations. Zhang and Shu [29] developed maximum-principle-preserving high-order schemes for scalar conservation laws, establishing a general scaling strategy for constraining reconstructed polynomial solutions. Zhang et al. [30] subsequently extended maximum-principle and positivity-preserving ideas to high-order DG schemes on triangular meshes. These contributions provide the conceptual foundation for the scaling procedures adopted here, although the present application requires their modification to accommodate a vector-valued concentration field, the coupled transport-flow structure, and the invariant set defined by simultaneous lower and upper constraints.

The present second-order FVE approximation that preserves the admissible concentration region under an appropriate CFL restriction is particularly relevant to geometrically complex sedimentation and classification problems. Previous applications include enhanced sedimentation in inclined configurations [23, 27] and particle classification in reflux classifiers [24]. Thus, the principal contribution of the present work is the combination of second-order accuracy, the IRP property, and a FVE treatment capable of operating on polygonal meshes, thereby extending previous IRP sedimentation schemes to more general geometries.

1.3. Outline of the paper. The remainder of the paper is organized as follows. In Section 1.4 we state the assumptions of the analysis, in particular those related to the transport model (1.1a). These assumptions are met by the MLB model for equal-density spheres (see Section 1.5). Section 2 is dedicated to the formulation of the first-order versions of the FE and FV methods that form the basis of the FVE scheme. To obtain a discrete version of the problem (1.1), we first describe, in Sec-

tion 2.1, a FE approximation of the Stokes problem (1.1b), (1.1c) subject to boundary conditions (1.3), (1.4) on the primal triangular mesh, and then outline, in Section 2.2, the approximation of (1.1a) by a FV scheme defined on the dual mesh that is based on the local Lax-Friedrichs (LLF) numerical flux. In particular, since the discrete velocity field $\mathbf{u}_h$ coming from the FE solver satisfies a discrete divergence-free (DDF) property, we may prove that the FV scheme satisfies the IRP property under a suitable CFL condition (cf. Theorem 2.1). Next, in Section 3, we extend the FV scheme to second-order accuracy. To this end we outline in Section 3.1 the second-order MUSCL reconstruction that is mainly based on the work by Castro et al. [11]. The MUSCL reconstruction, applied to the piecewise constant approximations of Φ defined on the control volumes of the dual mesh $\mathcal{T}_h^*$, delivers a piecewise linear, second-order accurate approximation of Φ on the control volumes of the dual mesh and involves a slope limiter to avoid spurious oscillation. The MUSCL reconstruction does, however, not ensure the IRP property. The latter property is achieved by applying scaling limiters akin to those by Zhang [28] and Zhang and Shu [29], which are modified in Section 3.2 to handle the discretization of (1.1). The result is a second-order in space accurate FV scheme that has the IRP property, see Theorem 3.1. Then, in Section 3.3, we outline the strong-stability preserving (SSP) second-order TVD Runge-Kutta (SSPRK) time discretization [17, 18] applied to the FV scheme and describe the FVE scheme for the complete transport-flow problem (Algorithm 3.1). Numerical examples are presented in Section 4, including an accuracy test for a manufactured exact solution (Section 4.1), three cases of settling of a polydisperse suspension (Sections 4.2 to 4.4), and one case of the flow and settling through a tank with continuous in- and outflow (Section 4.5). Conclusions are collected in Section 5.

1.4. Assumptions. We assume that there exist continuous, piecewise differentiable functions $w_l = w_l(\phi)$, $l = 1, \dots, N$, which are differentiable on $[0, \phi_{\max}]$, and parameters $\kappa_1 \geq \kappa_2 \geq \dots \geq \kappa_N > 0$ such that the vectors $\mathbf{v}(\Phi) := (v_1(\Phi), \dots, v_N(\Phi))^T$, $\boldsymbol{\kappa} := (\kappa_1, \dots, \kappa_N)^T$, and $\mathbf{w}(\phi) := (w_1(\phi), \dots, w_N(\phi))^T$ satisfy

$$(1.5) \quad \mathbf{v}(\Phi)^T \Phi = \boldsymbol{\kappa}^T (\Phi * \mathbf{w}) \quad \text{for all } \Phi \in \mathcal{D},$$

where for $\mathbf{a} = (a_1, \dots, a_N)^T$, $\mathbf{b} = (b_1, \dots, b_N)^T$ we define $(\mathbf{a} * \mathbf{b}) := (a_1 b_1, \dots, a_N b_N)^T$. The functions w_l must satisfy $w_l(\phi) \geq 0$ for all $\phi \in [0, \phi_{\max}]$, $w_l(\phi_{\max}) = 0$, and $w'_l(\phi) \leq w'_l(\tilde{\phi})$ if $0 \leq \phi \leq \tilde{\phi} \leq \phi_{\max}$. Note that this implies that $w'_l(\phi) \leq 0$ for all $\phi \in (0, \phi_{\max})$, for $l = 1, \dots, N$. Furthermore, the one-dimensional system

$$(1.6) \quad \partial_t \Phi + \partial_z \mathbf{f}(\Phi) = \mathbf{0}$$

where $\mathbf{f}(\Phi) = (f_1(\Phi), \dots, f_N(\Phi))^T$, is assumed to be hyperbolic on $\mathcal{D}$. Let $\lambda_1(\Phi) \geq \dots \geq \lambda_N(\Phi)$ denote the eigenvalues of the Jacobian matrix $\mathcal{J}(\Phi)$ of $\mathbf{f}(\Phi)$ at $\Phi \in \mathcal{D}$. It is assumed that there exist piecewise continuous functions $\psi_l = \psi_l(\phi)$ such that $\boldsymbol{\kappa}^T (\Phi * \boldsymbol{\psi}) \leq \min\{v_N(\Phi), \lambda_N(\Phi)\}$ and $w'_l(\phi) \geq \psi_l(\phi)$ for all $\Phi \in \mathcal{D}$, $l = 1, \dots, N$; that $v_1(\Phi) \geq 0$ for all $\Phi \in \mathcal{D}$; and that there exists a known upper bound $M_2 = M_2(\Phi)$ such that $M_2(\Phi) \geq \max\{v_1(\Phi), \lambda_1(\Phi)\}$ for all $\Phi \in \mathcal{D}$. Summarizing, we assume that

$$(1.7) \quad \begin{aligned} M_1(\Phi) &:= \boldsymbol{\kappa}^T (\Phi * \boldsymbol{\psi}) \leq \min\{v_i(\Phi), \lambda_i(\Phi) : 1 \leq i \leq N\} \\ &\leq \max\{v_i(\Phi), \lambda_i(\Phi) : 1 \leq i \leq N\} \leq M_2(\Phi) \quad \text{for all } \Phi \in \mathcal{D}. \end{aligned}$$

1.5. The MLB model with particle-size-specific hindered-settling factors. For particle of diameters $d_1 \geq \dots \geq d_N$ and equal density ρ_s , parameters

$\delta_l := d_l^2/d_1^2$, $\boldsymbol{\delta} := (\delta_1 = 1, \delta_2, \dots, \delta_N)^T$, and $\tilde{\mu}_{\text{sed}} := g d_1^2/(18\mu_f)$, where g is the acceleration of gravity, ρ_f is the density of the fluid, and μ_f is the viscosity of the fluid, the MLB model states that

(1.8)

$$v_l(\Phi) = \mu_{\text{sed}}(1 - \phi)(\delta_l V_l(\phi) - \boldsymbol{\delta}^T(\Phi * \mathbf{V}(\phi))), \quad l = 1, \dots, N; \quad \mu_{\text{sed}} := (\rho_s - \rho_f)\tilde{\mu}_{\text{sed}},$$

where $\mathbf{V}(\phi) = (V_1(\phi), \dots, V_N(\phi))^T$ and $V_l(\phi)$ are hindrance factors assumed to satisfy

$$(1.9) \quad V_l(0) = 1, \quad V_l'(\phi) \leq 0 \quad \text{for } 0 \leq \phi \leq \phi_{\max}, \quad V_l(\phi_{\max}) = 0 \quad \text{for } l = 1, \dots, N.$$

One can prove (cf., e.g., [7, Lemma 4.1]) that if $v_l(\Phi)$, $l = 1, \dots, N$ are given by (1.8) and the functions $V_l(\phi)$, besides (1.9), satisfy

$$V_l(\phi) \geq V_j(\phi) \quad \text{for all } \phi \in [0, \phi_{\max}] \text{ if } l < j,$$

then (1.1a) is strictly hyperbolic on the interior of $\mathcal{D}$, and the eigenvalues $\lambda_1, \dots, \lambda_N$ and velocities $v_1, \dots, v_N$ (all depending on Φ) satisfy the interlacing property

$$\begin{aligned} M_1(\Phi) &:= \mu_{\text{sed}} \sum_{l=1}^N \delta_l \phi_l ((1 - \phi)V_l'(\phi) - 2V_l(\phi)) \\ &< \lambda_N < v_N < \lambda_{N-1} < \dots < \lambda_1 < v_1 =: M_2(\Phi) \quad \text{for all } \Phi \in \mathcal{D}. \end{aligned}$$

Notice that for $\rho_s > \rho_f$, there holds $v_1(\Phi) \geq 0$ for all $\Phi \in \mathcal{D}$. It is straightforward to prove that the present MLB model with equal-density particles satisfies the assumptions of Section 1.4 for $w_l(\phi) := \mu_{\text{sed}}(1 - \phi)^2 V_l(\phi)$, $\boldsymbol{\kappa} := \boldsymbol{\delta}$, and $\psi_l(\phi) := \mu_{\text{sed}}((1 - \phi)V_l'(\phi) - 2V_l(\phi))$. Note that $w_l'(\phi) = (1 - \phi)\psi_l(\phi)$.

2. Numerical scheme. Let $\Omega \subset \mathbb{R}^2$ be a bounded polygonal Lipschitz domain and let $L_0^2(\Omega)$ denote the space of L^2 functions with zero average. We assume that $\phi \in L^\infty(\Omega)$ with $0 \leq \phi \leq \phi_{\max}$ a.e. is given and assume that μ satisfies $0 < \mu_{\min} \leq \mu(s) \leq \mu_{\max} < \infty$ for all $s \in [0, \phi_{\max}]$, and that $\mathbf{g}(\phi) \in [L^2(\Omega)]^2$.

2.1. Approximation of the Stokes system. We define the bilinear forms

$$a(\phi; \mathbf{u}, \mathbf{v}) := \int_{\Omega} \mu(\phi) \boldsymbol{\varepsilon}(\mathbf{u}) : \boldsymbol{\varepsilon}(\mathbf{v}) \, d\mathbf{x}, \quad b(\mathbf{v}, q) := - \int_{\Omega} (\nabla \cdot \mathbf{v}) q \, d\mathbf{x}.$$

Then, the variational formulation of the Stokes problem (1.1b), (1.1c) reads: find $(\mathbf{u}, p) \in [H_0^1(\Omega)]^2 \times L_0^2(\Omega)$ such that

$$(2.1) \quad \begin{aligned} a(\phi; \mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) &= \int_{\Omega} \mathbf{g}(\phi) \cdot \mathbf{v} \, d\mathbf{x} \quad \forall \mathbf{v} \in [H_0^1(\Omega)]^2, \\ b(\mathbf{u}, q) &= 0 \quad \forall q \in L_0^2(\Omega). \end{aligned}$$

By Korn's first inequality the bilinear form $a(\phi; \cdot, \cdot)$ is $[H_0^1(\Omega)]^2$ -elliptic, and the pair $([H_0^1(\Omega)]^2, L_0^2(\Omega))$ satisfies the inf-sup condition

$$\inf_{q \in L_0^2(\Omega)} \sup_{\mathbf{v} \in [H_0^1(\Omega)]^2} \frac{(\nabla \cdot \mathbf{v}, q)}{\|\mathbf{v}\|_{1,\Omega} \|q\|_{0,\Omega}} > 0,$$

hence (2.1) has a unique solution [16].

To discretize (2.1) we assume that $\{\mathcal{T}_h\}_{h>0}$ is a regular family of triangulations of Ω made up of triangles T of diameter h_T , where h stands for both a sub-index of each triangulation $\mathcal{T}_h$, as well as for the largest diameter, that is $h = \max\{h_T : T \in \mathcal{T}_h\}$. Next, given $k \in \mathbb{N}_0$ and a subset $\Lambda \subset \mathbb{R}^2$, we denote by $\mathbb{P}_k(\Lambda)$ the space of polynomials of degree less than or equal to k . We employ the Crouzeix–Raviart finite elements [14] where the degrees of freedom (DOFs) consist of the values of the shape functions at the centers of the edges/faces. We denote by $\mathcal{E}_h$ the set of the edges of all $T \in \mathcal{T}_h$, by $\mathcal{E}_h^{\text{int}} \subset \mathcal{E}_h$ the set of edges interior to Ω , and by $\mathcal{E}_h^{\text{ext}} := \mathcal{E}_h \setminus \mathcal{E}_h^{\text{int}}$ the set of boundary edges. We now define the (nonconforming) Crouzeix–Raviart space

$$\mathbf{P}_1^{\text{CR}}(\mathcal{T}_h) := \left\{ \mathbf{v}_h \in [L^2(\Omega)]^2 : \mathbf{v}_h|_T \in [\mathbb{P}_1(T)]^2 \ \forall T \in \mathcal{T}_h, \int_e \llbracket \mathbf{v}_h \rrbracket_e \, ds = 0 \ \forall e \in \mathcal{E}_h^{\text{int}}, \right. \\ \left. \int_e \mathbf{v}_h \, ds = 0 \ \forall e \in \mathcal{E}_h^{\text{ext}} \right\},$$

where we define the jump across an interior $e \in \mathcal{E}_h^{\text{int}}$ shared by T_- and T_+ as $\llbracket \mathbf{v}_h \rrbracket_e := \mathbf{v}_h|_{T_-} - \mathbf{v}_h|_{T_+}$, and $\llbracket \mathbf{v}_h \rrbracket_e := \mathbf{v}_h|_e$, for $e \in \mathcal{E}_h^{\text{ext}}$. We set $\mathbf{V}_h := \mathbf{P}_1^{\text{CR}}(\mathcal{T}_h)$ and endow this space with the broken norm $\|\mathbf{v}_h\|_{1,h}^2 := \sum_{T \in \mathcal{T}_h} \|\mathbf{v}_h\|_{1,T}^2$. We approximate pressure by piecewise constant functions from

$$Q_h := \{q_h \in L_0^2(\Omega) : q_h|_T \in \mathbb{P}_0(T) \ \forall T \in \mathcal{T}_h\}.$$

Since $\mathbf{V}_h \not\subset [H_0^1(\Omega)]^2$, the forms in (2.1) must be replaced by their broken counterparts. Moreover, the Crouzeix–Raviart space does not satisfy a discrete Korn inequality for the symmetric-gradient form [6, 15, 19]. Following [8, 19] we therefore add a weakly consistent jump stabilization and define for $\gamma > 0$

$$a_h(\phi; \mathbf{u}_h, \mathbf{v}_h) := \sum_{T \in \mathcal{T}_h} \int_T \mu(\phi) \boldsymbol{\varepsilon}(\mathbf{u}_h) : \boldsymbol{\varepsilon}(\mathbf{v}_h) \, d\mathbf{x} + \gamma \sum_{e \in \mathcal{E}_h} \frac{\bar{\mu}_e}{h_e} \int_e \llbracket \mathbf{u}_h \rrbracket \cdot \llbracket \mathbf{v}_h \rrbracket \, ds, \\ b_h(\mathbf{v}_h, q_h) := - \sum_{T \in \mathcal{T}_h} \int_T (\nabla \cdot \mathbf{v}_h) q_h \, d\mathbf{x},$$

where $\bar{\mu}_e$ denotes the average of $\mu(\phi)$ over the elements sharing e . The discrete problem now reads: given $\phi \in L^\infty(\Omega; [0, \phi_{\max}])$, find $(\mathbf{u}_h, p_h) \in \mathbf{V}_h \times Q_h$ such that

$$(2.2a) \quad a_h(\phi; \mathbf{u}_h, \mathbf{v}_h) + b_h(\mathbf{v}_h, p_h) = \int_\Omega \mathbf{g}(\phi) \cdot \mathbf{v}_h \, d\mathbf{x} \quad \forall \mathbf{v}_h \in \mathbf{V}_h,$$

$$(2.2b) \quad b_h(\mathbf{u}_h, q_h) = 0 \quad \forall q_h \in Q_h.$$

The Korn inequality for piecewise H^1 vector fields [6] implies that there exists a constant $C_K > 0$ such that

$$\|\mathbf{v}_h\|_{1,h}^2 \leq C_K \left(\sum_{T \in \mathcal{T}_h} \|\boldsymbol{\varepsilon}(\mathbf{v}_h)\|_{0,T}^2 + \sum_{e \in \mathcal{E}_h} h_e^{-1} \|\llbracket \mathbf{v}_h \rrbracket\|_{0,e}^2 \right).$$

Then using $\mu \geq \mu_{\min}$ and $\bar{\mu}_e \geq \mu_{\min}$ and taking $\alpha_* := \min\{1, \gamma\}/C_K$, we obtain

$$a_h(\phi; \mathbf{v}_h, \mathbf{v}_h) \geq \alpha_* \mu_{\min} \|\mathbf{v}_h\|_{1,h}^2 \quad \forall \mathbf{v}_h \in \mathbf{V}_h,$$

so the bilinear form a_h is coercive. In addition, it is well known that the pair $(\mathbf{V}_h, Q_h)$ satisfies the inf-sup condition [14, 16]

$$\inf_{q_h \in Q_h} \sup_{\mathbf{v}_h \in \mathbf{V}_h} \frac{b_h(\mathbf{v}_h, q_h)}{\|\mathbf{v}_h\|_{1,h} \|q_h\|_{0,\Omega}} \geq \beta_*,$$

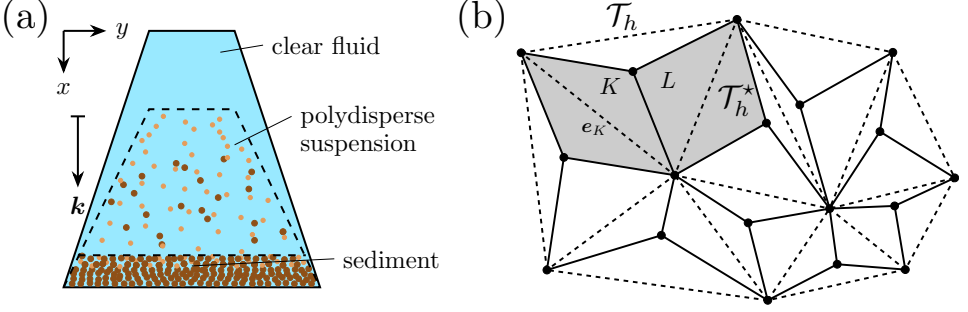


FIG. 1. (a) Settling of a polydisperse suspension in a polygonal (here, roof-shaped) domain; (b) schematic of the primal mesh $\mathcal{T}_h$ (dashed) and the corresponding dual mesh $\mathcal{T}_h^*$ (solid lines).

where $\beta_* > 0$ is a constant independent of h and ϕ . Consequently, from the Babuška-Brezzi theory we conclude that (2.2) has a unique solution.

By testing (2.2b) with $q_h = \chi_T - m(T)/m(\Omega)$, it follows that $\int_T \nabla \cdot \mathbf{u}_h \, dx = 0$. Since $\nabla \cdot \mathbf{u}_h$ is constant on T , we obtain the local DDF property

$$(2.3) \quad (\nabla \cdot \mathbf{u}_h)|_T = 0 \quad \forall T \in \mathcal{T}_h.$$

2.2. Approximation of the concentration equations. Given the primal triangulation $\mathcal{T}_h$, we construct a dual FV mesh $\mathcal{T}_h^*$ by using the edges of the primal triangulation. For a given edge $e_K \in \mathcal{E}_h^{\text{int}}$ of the triangulation, the vertices of the corresponding finite volume K are given by the endpoints of e_K and the barycenters of the two triangles containing e_K . If $e_K \in \mathcal{E}_h^{\text{ext}}$, then the vertices of K are given by the endpoints of e_K and the barycenter of the triangle containing the edge e_K (see Fig. 1). We denoted the midpoint of e_K by $\mathbf{x}_K$. Let us denote by $\mathcal{E}_h^*$ the set of edges of the dual mesh $\mathcal{T}_h^*$ and by $\sigma_{K,L}$ the edge of K shared with its neighbor control volume $L \in \mathcal{T}_h^*$ (see Figure 1). In addition, we define m_σ as the measure of the edge $\sigma \in \mathcal{E}_h^*$, and $\mathbf{n}_{K,\sigma}$ as the unit normal vector at σ pointing outward to K . We also consider the set $\mathcal{N}(K)$ of neighboring control volumes to K and the measure $m(K)$ of K , and define $S_h \subset L^2(\Omega)$ as the space of piecewise constant functions on each control volume of $\mathcal{T}_h^*$, i.e.

$$S_h := \{w \in L^2(\Omega) : w|_K \in \mathbb{P}_0(K) \quad \forall K \in \mathcal{T}_h^*\}.$$

We also define $\mathbf{S}_h := (S_h)^N$. Then, the sought unknown is approximated by $\Phi_h(t) = (\phi_{1,h}(t), \dots, \phi_{N,h}(t)) \in \mathbf{S}_h$, i.e., for each $t > 0$, Φ_h is a piecewise constant function on $\mathcal{T}_h^*$. Here we also assume that the piecewise linear discrete velocity $\mathbf{u}_h$ is known (it has been computed in a previous step). The system (1.1a) is now written as

$$(2.4) \quad \partial_t \Phi + \partial_x \mathbf{F}_1(\Phi, u^x) + \partial_y \mathbf{F}_2(\Phi, u^y) = \mathbf{0},$$

where $\mathbf{F}_1(\Phi, u^x) = u^x \Phi + k^x \mathbf{f}(\Phi)$, $\mathbf{F}_2(\Phi, u^y) = u^y \Phi + k^y \mathbf{f}(\Phi)$, and $\mathbf{k} = (k^x, k^y)^\top$. Integrating (2.4) over K and using the divergence theorem yields

$$\frac{d}{dt} \int_K \Phi_h(\mathbf{x}, t) \, d\mathbf{x} + \int_{\partial K} \mathbf{F}(\Phi_h(\mathbf{x}, t), \mathbf{u}_h(\mathbf{x})) \cdot \mathbf{n}_K \, ds = 0,$$

where $\mathbf{F}(\Phi, \mathbf{u}) := (\mathbf{F}_1(\Phi, u^x), \mathbf{F}_2(\Phi, u^y))^T$. Let us define

$$\Phi_K(t) := \frac{1}{m(K)} \int_K \Phi_h(\mathbf{x}, t) d\mathbf{x}, \quad \Phi_K^n := \Phi_K(t_n), \quad \text{and} \quad \mathbf{u}_h^n := \mathbf{u}_h(t_n).$$

Discretizing the time derivative by a forward Euler step, we arrive at

$$(2.5) \quad \Phi_K^{n+1} = \Phi_K^n - \frac{\Delta t}{m(K)} \sum_{L \in \mathcal{N}(K)} \int_{\sigma_{K,L}} \mathbf{F}(\Phi_h(\mathbf{x}, t_n), \mathbf{u}_h(\mathbf{x}, t_n)) \cdot \mathbf{n}_{K,L} ds.$$

The integrand $\mathbf{F}(\Phi_h(\mathbf{x}, t_n), \mathbf{u}_h(\mathbf{x}, t_n))$ has to be specified appropriately, since Φ_h is not necessarily continuous across the element boundary. If $\mathbf{H}$ denotes a numerical flux function associated with the projection of system (1.1a) in the direction of the normal vector $\mathbf{n}_{K,L}$ (see [3] for details), then the integrals in (2.5) can be approximated by a Gauss quadrature rule. This yields the discrete approximation of (1.1a)

$$(2.6) \quad \Phi_K^{n+1} = \Phi_K^n - \frac{\Delta t}{m(K)} \sum_{L \in \mathcal{N}(K)} \mathbf{H}(\Phi_K^n, \Phi_L^n, \mathbf{u}_{K,L}^n, \mathbf{n}_{K,L}) m_{K,L},$$

where $\mathbf{u}_{K,L}^n := \mathbf{u}_h^n(\mathbf{x}_{K,L})$ and $\mathbf{x}_{K,L}$ denotes the midpoint of $\sigma_{K,L}$. This suggests defining $\mathbf{H}$ as some approximation of the flux at $z = 0$ of the solution of the one-dimensional Riemann problem

$$(2.7) \quad \partial_t U + \partial_z(\mathbf{F}(U, \mathbf{u}_{K,L}) \cdot \mathbf{n}_{K,L}) = \mathbf{0} \quad \text{in } \mathbb{R} \times (0, \infty), \quad U(z, 0) = \begin{cases} \Phi_K & \text{if } z < 0, \\ \Phi_L & \text{if } z > 0, \end{cases}$$

defined for $\Phi_K, \Phi_L \in \mathcal{D}$. To this end, we propose an LLF numerical flux given by

$$(2.8) \quad \begin{aligned} \mathbf{H}(\Phi_K^n, \Phi_L^n, \mathbf{u}_{K,L}^n, \mathbf{n}_{K,L}) &= \frac{1}{2} \left(\mathbf{F}(\Phi_L^n, \mathbf{u}_{K,L}^n) + \mathbf{F}(\Phi_K^n, \mathbf{u}_{K,L}^n) \right) \cdot \mathbf{n}_{K,L} \\ &\quad - \frac{1}{2} \alpha_{K,L}^n (\Phi_L^n - \Phi_K^n), \end{aligned}$$

where $\alpha_{K,L}^n := \alpha(\Phi_K^n, \Phi_L^n)$ is a local upper bound for the eigenvalues $\tilde{\lambda}_i(U)$ of the Jacobian matrix associated to the system (2.7). As in [3] this bound can be derived from those arising in (1.7) if we choose a direction $\boldsymbol{\eta} \in \mathbb{R}^2$, $\|\boldsymbol{\eta}\|_2 = 1$, and assume that U varies only in that direction in a neighborhood of a point $\mathbf{x}_0$; if we set $\boldsymbol{\xi}(z, t) := U(z\boldsymbol{\eta} + \mathbf{x}_0)$, then $\boldsymbol{\xi}$ satisfies $\partial_t \boldsymbol{\xi} + \partial_z(\mathbf{F}(\boldsymbol{\xi}, \mathbf{u}) \cdot \boldsymbol{\eta}) = \mathbf{0}$. Thus, taking into account the definition of $\mathbf{F}(\boldsymbol{\xi}, \mathbf{u})$, we obtain the bounds $\tilde{M}_1(U) \leq \tilde{\lambda}_i(U) \leq \tilde{M}_2(U)$ for all $i = 1, \dots, N$, where in light of (1.7),

$$(2.9) \quad \tilde{M}_p(U) := \begin{cases} \mathbf{u} \cdot \boldsymbol{\eta} + (\mathbf{k} \cdot \boldsymbol{\eta}) M_p(U) & \text{if } \mathbf{k} \cdot \boldsymbol{\eta} > 0, \\ \mathbf{u} \cdot \boldsymbol{\eta} + (\mathbf{k} \cdot \boldsymbol{\eta}) M_{3-p}(U) & \text{if } \mathbf{k} \cdot \boldsymbol{\eta} \leq 0, \end{cases} \quad p = 1, 2,$$

for any unit vector $\boldsymbol{\eta}$. Consequently, a suitable definition of $\alpha(\Phi_K^n, \Phi_L^n)$ is given by

$$\alpha(\Phi_K, \Phi_L) := \max\{|\min_{\Phi \in [\Phi_K, \Phi_L]} \tilde{M}_1(\Phi)|, |\max_{\Phi \in [\Phi_K, \Phi_L]} \tilde{M}_2(\Phi)|\},$$

where we define $[\Phi_K, \Phi_L] := \{s\Phi_K + (1-s)\Phi_L : s \in [0, 1]\}$.

The time step $\Delta t = \Delta t_n$ is computed for each iteration by enforcing the CFL condition

$$(2.10) \quad \alpha_n \frac{\Delta t_n}{m(K)} \sum_{L \in \mathcal{N}(K)} m_{K,L} \leq 1 \quad \forall K \in \mathcal{T}_h^*, \quad \alpha_n := \max_{K \in \mathcal{T}_h^*} \left\{ \max_{L \in \mathcal{N}(K)} \alpha_{K,L}^n \right\}.$$

Remark 2.1. Since $\mathbf{u}_h$ is piecewise linear on every triangle in $\mathcal{T}_h$, using the divergence theorem and the local DDF condition (2.3) we obtain

$$\begin{aligned} \sum_{L \in \mathcal{N}(K)} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} &= \int_{\partial K} \mathbf{u}_h \cdot \mathbf{n}_K \, ds = \int_K \nabla \cdot \mathbf{u}_h \, d\mathbf{x} \\ &= \sum_{\substack{T \in \mathcal{T}_h \\ T \cap K \neq \emptyset}} \int_{T \cap K} \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0. \end{aligned}$$

Let $K \in \mathcal{T}_h^*$ and $L \in \mathcal{N}(K)$ be given. For $\lambda \in \mathbb{R}^+$, we analyze the function

$$\mathbf{G}(\Phi_K, \Phi_L, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}) := \Phi_K - \lambda \mathbf{H}(\Phi_K, \Phi_L, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}).$$

We set $\mathbf{G}_{K,L} = (G_{K,L}^1, \dots, G_{K,L}^N)^\top := \mathbf{G}(\Phi_K, \Phi_L, \mathbf{u}_{K,L}, \mathbf{n}_{K,L})$ to simplify notation.

LEMMA 2.2. *If the velocity functions $v_l(\Phi)$ satisfy the assumptions of Section 1.4, $\Phi_K, \Phi_L \in \mathcal{D}$, and $\lambda > 0$ satisfies*

$$(2.11) \quad \alpha(\Phi_K, \Phi_L) \lambda \leq 1,$$

then the function $\mathbf{G}$ satisfies

$$(2.12) \quad G_{K,L}^l \geq 0 \quad \text{for all } l = 1, \dots, N,$$

$$(2.13) \quad G_{K,L}^1 + \dots + G_{K,L}^N \leq \phi_{\max} - \lambda \phi_{\max}(\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}).$$

Proof. In this proof it is always understood that $\mathbf{u} = \mathbf{u}_{K,L}$ and $\mathbf{n} = \mathbf{n}_{K,L}$. First, by using the definition of the flux $\mathbf{H}$ we notice that

$$(2.14) \quad G_{K,L}^l = \left(1 - \frac{\lambda \alpha_{K,L}}{2} - \frac{\lambda}{2} (\mathbf{u} \cdot \mathbf{n} + (\mathbf{k} \cdot \mathbf{n}) v_l(\Phi_K)) \right) \phi_{l,K} + \frac{\lambda \alpha_{K,L}}{2} \tilde{G}_{K,L}^l$$

for $l = 1, \dots, N$, where $\tilde{G}_{K,L}^l := \phi_{l,L} - (1/\alpha_{K,L})((\mathbf{u} \cdot \mathbf{n})\phi_{l,L} + (\mathbf{k} \cdot \mathbf{n})\phi_{l,L}v_l(\Phi_L))$. Let us check (2.12) first. We notice from (1.7) and (2.9) that

$$|\mathbf{u} \cdot \mathbf{n} + (\mathbf{k} \cdot \mathbf{n}) v_l(\Phi_U)| \leq \alpha_{K,L}, \quad U \in \{L, K\}.$$

Therefore, $\tilde{G}_{K,L}^l \geq 0$, and thanks to (2.11),

$$1 - \frac{\lambda \alpha_{K,L}}{2} - \frac{\lambda}{2} (\mathbf{u} \cdot \mathbf{n} + (\mathbf{k} \cdot \mathbf{n}) v_l(\Phi_K)) \geq 1 - \lambda \alpha_{K,L} \geq 0,$$

so we deduce (2.12) from (2.14). To prove (2.13), we first rewrite (2.14) as

$$\begin{aligned} G_{K,L}^l &= \left(1 - \frac{\lambda \alpha_{K,L}}{2} - \frac{\lambda}{2} (\mathbf{u} \cdot \mathbf{n} + (\mathbf{k} \cdot \mathbf{n}) v_l(\Phi_K)) \right) \phi_{l,K} + \frac{\lambda \alpha_{K,L}}{2} \phi_{l,L} \\ &\quad - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n})\phi_{l,L} + (\mathbf{k} \cdot \mathbf{n})\phi_{l,L}v_l(\Phi_L)). \end{aligned}$$

Summing over $l = 1, \dots, N$ yields

$$\sum_{l=1}^N G_{K,L}^l = \left(1 - \frac{\lambda \alpha_{K,L}}{2} \right) \phi_K - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n})\phi_K + (\mathbf{k} \cdot \mathbf{n})\Phi_K^\top \mathbf{v}(\Phi_K))$$

$$\begin{aligned}
& + \frac{\lambda \alpha_{K,L}}{2} \phi_L - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n}) \phi_L + (\mathbf{k} \cdot \mathbf{n}) \Phi_L^T \mathbf{v}(\Phi_L)) \\
& = (1 - \lambda \alpha_{K,L}) \phi_K + \frac{\lambda \alpha_{K,L}}{2} \phi_K - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n}) \phi_K + (\mathbf{k} \cdot \mathbf{n}) \Phi_K^T \mathbf{v}(\Phi_K)) \\
& + \frac{\lambda \alpha_{K,L}}{2} \phi_L - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n}) \phi_L + (\mathbf{k} \cdot \mathbf{n}) \Phi_L^T \mathbf{v}(\Phi_L)).
\end{aligned}$$

Using (1.5) and adding and subtracting the term $(\mathbf{u} \cdot \mathbf{n}) \phi_{\max}$, we obtain

$$(2.15) \quad \sum_{l=1}^N G_{K,L}^l = (1 - \lambda \alpha_{K,L}) \phi_K + \lambda \alpha_{K,L} \phi_{\max} + \mathcal{Y}_1 + \mathcal{Y}_2 - \lambda (\mathbf{u} \cdot \mathbf{n}) \phi_{\max},$$

where the terms $\mathcal{Y}_1$ and $\mathcal{Y}_2$ are defined by

$$\begin{aligned}
\mathcal{Y}_1 &:= \frac{\lambda \alpha_{K,L}}{2} (\phi_L - \phi_{\max}) - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n}) (\phi_L - \phi_{\max}) + (\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}(\phi_L))), \\
\mathcal{Y}_2 &:= \frac{\lambda \alpha_{K,L}}{2} (\phi_K - \phi_{\max}) - \frac{\lambda}{2} ((\mathbf{u} \cdot \mathbf{n}) (\phi_K - \phi_{\max}) + (\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_K * \mathbf{w}(\phi_K))).
\end{aligned}$$

Let us now show that $\mathcal{Y}_1 \leq 0$. If $\phi_L = \phi_{\max}$, then $w_l(\phi_{\max}) = 0$ for all $l = 1, \dots, N$ implies that $\mathcal{Y}_1 = 0$. If $\phi_L \neq \phi_{\max}$, it follows that $\mathcal{Y}_1 = \frac{\lambda}{2} (\phi_L - \phi_{\max}) \mathcal{Y}_{K,L}$, where

$$\mathcal{Y}_{K,L} := \alpha_{K,L} - \mathbf{u} \cdot \mathbf{n} - (\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}(\phi_L)) / (\phi_L - \phi_{\max}).$$

Now, we notice that there exists a number $\xi_L^{(l)} \in [\phi_L, \phi_{\max}]$ such that

$$\frac{w_l(\phi_L)}{\phi_L - \phi_{\max}} = \frac{w_l(\phi_L) - w_l(\phi_{\max})}{\phi_L - \phi_{\max}} = w'_l(\xi_L^{(l)}).$$

For $\xi_L := (\xi_L^{(1)}, \dots, \xi_L^{(N)})^T$ and $\mathbf{w}'(\xi_L) := (w'_1(\xi_L^{(1)}), \dots, w'_N(\xi_L^{(N)}))^T$ we obtain

$$\mathcal{Y}_{K,L} = \alpha_{K,L} - (\mathbf{u} \cdot \mathbf{n} + (\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}'(\xi_L))).$$

If $\mathbf{k} \cdot \mathbf{n} > 0$, then $(\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}'(\xi_L)) \leq 0$, thus $\mathcal{Y}_{K,L} \geq \alpha_{K,L} - \mathbf{u} \cdot \mathbf{n}$. In addition, $M_2(\Phi_L) \geq v_1(\Phi_L) \geq 0$, hence

$$\mathcal{Y}_{K,L} \geq \alpha_{K,L} - \mathbf{u} \cdot \mathbf{n} - (\mathbf{k} \cdot \mathbf{n}) M_2(\Phi_L) = \alpha_{K,L} - \tilde{M}_2(\Phi_L) \geq 0.$$

On the other hand, if $\mathbf{k} \cdot \mathbf{n} \leq 0$, then we may use that w'_l is nondecreasing to obtain that $w'_l(\xi_L^{(l)}) \geq w'_l(\phi_L)$. Moreover, the assumptions of Section 1.4 imply that $w'_l(\phi) \geq \psi_l(\phi)$. Let $\psi(\phi) := (\psi_1(\phi), \dots, \psi_N(\phi))^T$. Then

$$\begin{aligned}
(-\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}'(\xi_L)) &\geq (-\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \mathbf{w}'(\phi_L)) \\
&\geq (-\mathbf{k} \cdot \mathbf{n}) \kappa^T (\Phi_L * \psi(\phi_L)) = (-\mathbf{k} \cdot \mathbf{n}) M_1(\Phi_L)
\end{aligned}$$

implies that

$$\mathcal{Y}_{K,L} \geq \alpha_{K,L} - \mathbf{u} \cdot \mathbf{n} - (\mathbf{k} \cdot \mathbf{n}) M_1(\Phi_L) = \alpha_{K,L} - \tilde{M}_2(\Phi_L) \geq 0.$$

In both cases, we get $\mathcal{Y}_{K,L} \geq 0$, hence $\mathcal{Y}_1 \leq 0$. Repeating the same argument with Φ_K instead of Φ_L yields $\mathcal{Y}_2 \leq 0$. Then, since $\phi_K \in [0, \phi_{\max}]$, (2.15) implies (2.13). $\square$

Using Lemma 2.2 we may now prove that the first-order numerical scheme used to approximate the polydisperse system (1.1a) preserves the region $\mathcal{D}$.

THEOREM 2.1. *If the CFL condition (2.10) is in effect and the velocity functions $v_l(\Phi)$ satisfy the assumptions of Section 1.4, then the LLF scheme defined by (2.6) with the numerical flux (2.8) satisfies the IRP property*

$$\Phi_K^n \in \mathcal{D} \text{ for all } K \in \mathcal{T}_h^* \Rightarrow \Phi_K^{n+1} \in \mathcal{D} \text{ for all } K \in \mathcal{T}_h^* \text{ and all } n \in \mathbb{N}_0.$$

Proof. Let $K \in \mathcal{T}_h^*$ be given. For practical reasons, during the proof we omit the superscript n on the right-hand side of the marching formula, i.e., we set $\Phi_K := \Phi_K^n$, $\alpha_{K,L} := \alpha_{K,L}^n$, and $\Delta t := \Delta t_n$. Let us define $\lambda_{K,L} := \frac{\Delta t}{m(K)} m_{K,L}$, $\lambda := \sum_{L \in \mathcal{N}(K)} \lambda_{K,L}$, and $\tilde{\lambda}_{K,L} := \lambda_{K,L}/\lambda$, so that $\sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} = 1$. Then we can write

$$\begin{aligned} \Phi_K^{n+1} &= \Phi_K - \frac{\Delta t}{m(K)} \sum_{L \in \mathcal{N}(K)} \mathbf{H}(\Phi_K, \Phi_L, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}) m_{K,L} \\ &= \sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} (\Phi_K - \lambda \mathbf{H}(\Phi_K, \Phi_L, \mathbf{u}_{K,L}, \mathbf{n}_{K,L})) = \sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} \mathbf{G}_{K,L}. \end{aligned}$$

Thus,

$$\phi_{l,K}^{n+1} = \sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} G_{K,L}^l \quad \text{for } l = 1, \dots, N.$$

Then, (2.12) implies that $G_{K,L}^l \geq 0$, so $\phi_{l,K}^{n+1} \geq 0$ for all $l = 1, \dots, N$. In addition, employing (2.13) and Remark 2.1 yields

$$\begin{aligned} \phi_K^{n+1} &= \sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} (G_{K,L}^1 + \dots + G_{K,L}^N) \leq \sum_{L \in \mathcal{N}(K)} \tilde{\lambda}_{K,L} \phi_{\max} (1 - \lambda(\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L})) \\ &= \phi_{\max} - \frac{\Delta t \phi_{\max}}{m(K)} \sum_{L \in \mathcal{N}(K)} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} = \phi_{\max}. \end{aligned}$$

This completes the proof. $\square$

3. Second-order finite volume scheme.

3.1. Second-order MUSCL reconstruction. We will look for a linear approximation function on K of the form $\mathbf{P}_K(\mathbf{x}) = \Phi_K + \nabla \Phi_K \cdot (\mathbf{x} - \mathbf{c}_K)^T$ for $\mathbf{x} \in K$, where $\mathbf{c}_K$ is the barycenter of K and $\nabla \Phi_K$ represents a constant approximation of the gradient of Φ over the control cell K . To describe this approximation, let us consider $K \in \mathcal{T}_h^*$ such that $\partial K \cap \partial \Omega = \emptyset$, so K has four neighboring elements $K^{(1)}, \dots, K^{(4)}$. Then we define four triangles $T_K^{(1)}, \dots, T_K^{(4)}$, where $T_K^{(j)}$ is the triangle formed by joining the barycenter $\mathbf{c}_K$ of K with the two barycenters $\mathbf{c}_K^{(j)}$ and $\mathbf{c}_K^{(\ell(j))}$ of two neighboring elements (see Figure 2), where $\ell(j) = j + 1$ for $j = 1, \dots, 3$ and $\ell(4) = 1$. On each triangle $T_K^{(j)}$ we use the values Φ_K and $\Phi_{K^{(1)}}, \dots, \Phi_{K^{(4)}}$ to obtain the following linear approximation of the gradient $\nabla \Phi$:

$$\nabla \Phi|_{T_K^{(j)}} := \Phi_K \nabla \lambda_K^{(0)} + \Phi_{K^{(j)}} \nabla \lambda_K^{(j)} + \Phi_{K^{(\ell(j))}} \nabla \lambda_K^{(\ell(j))},$$

where $\lambda_K^{(0)}$, $\lambda_K^{(j)}$, and $\lambda_K^{(\ell(j))}$ are the barycentric coordinates of the vertices of $T_K^{(j)}$. Finally, we consider the first-order approximation of the gradient $\nabla \Phi(\mathbf{x})$ in K

$$(3.1) \quad \nabla \Phi(\mathbf{x})|_K \approx \nabla \Phi_K = \frac{\sum_{j=1}^4 m(T_K^{(j)}) \nabla \Phi|_{T_K^{(j)}}}{\sum_{j=1}^4 m(T_K^{(j)})}.$$

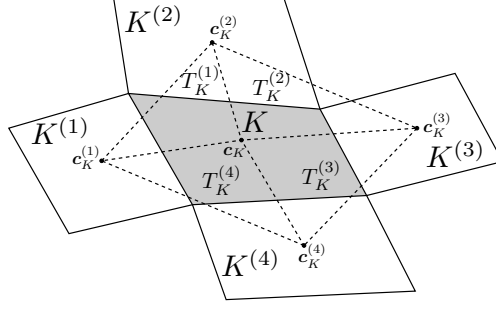


FIG. 2. Triangles $T_K^{(1)}, \dots, T_K^{(4)}$ associated with MUSCL reconstruction on $K \in \mathcal{T}_h^*$.

To handle discontinuities in the solution, we modify the gradient approximation by introducing slope limiters that control spurious oscillations near discontinuities. Let us employ the notation $\nabla \Phi_K := (\nabla \phi_{1,K}, \dots, \nabla \phi_{N,K})^T$ and define the operator

$$(3.2) \quad P_K(\mathbf{x}) = \Phi_K + \widehat{\nabla \Phi}_K(\mathbf{x} - \mathbf{c}_K)^T, \quad \text{where } \widehat{\nabla \Phi}_K := \boldsymbol{\varphi}_K * \nabla \Phi_K,$$

and $\boldsymbol{\varphi}_K = (\varphi_{1,K}, \dots, \varphi_{N,K})^T$ is the vector of componentwise slope-limiter coefficients related to the control volume K . These coefficients are given by

$$(3.3) \quad \varphi_{l,K} = \min_{L \in \mathcal{N}(K)} \{\varphi_{l,K,L}^l\}, \quad \varphi_{l,K,L}^l = \max\{0, \min\{r_{l,K,L}^l, 1\}\}, \quad l = 1, \dots, N.$$

The quantities $r_{l,K,L}^l$ are defined as

$$r_{l,K,L}^l := \begin{cases} (\phi_{l,K}^{\max} - \phi_{l,K}) / (\phi_{l,K,L}^* - \phi_{l,K}) & \text{if } \phi_{l,K,L}^* - \phi_{l,K} > 0, \\ (\phi_{l,K}^{\min} - \phi_{l,K}) / (\phi_{l,K,L}^* - \phi_{l,K}) & \text{if } \phi_{l,K,L}^* - \phi_{l,K} < 0, \\ 1 & \text{if } \phi_{l,K,L}^* = \phi_{l,K}, \end{cases} \quad l = 1, \dots, N,$$

where $\phi_{l,K}^{\min} := \min\{\phi_{l,K}, \min_{L \in \mathcal{N}(K)} \phi_{l,L}\}$, $\phi_{l,K}^{\max} := \max\{\phi_{l,K}, \max_{L \in \mathcal{N}(K)} \phi_{l,L}\}$, and

$$\Phi_{K,L}^* := (\phi_{1,K,L}^*, \dots, \phi_{N,K,L}^*)^T = \Phi_K + \nabla \Phi_K(\mathbf{x}_{K,L} - \mathbf{c}_K)^T,$$

where $\mathbf{c}_K$ is the center of mass of K . To obtain a second-order approximation we replace (2.6) by

$$(3.4) \quad \Phi_K^{n+1} = \Phi_K^n - \frac{\Delta t}{m(K)} \sum_{L \in \mathcal{N}(K)} \mathbf{H}(\Phi_{K,L}^{\text{int}(K)}, \Phi_{K,L}^{\text{ext}(K)}, \mathbf{u}_{K,L}^n, \mathbf{n}_{K,L}) m_{K,L},$$

where $\Phi_{K,L}^{\text{int}(K)}$ and $\Phi_{K,L}^{\text{ext}(K)}$ denote the MUSCL reconstructions of the cell-average concentration vector on the interior and exterior sides of K , respectively, evaluated at the midpoint $\mathbf{x}_{K,L}$ of the edge shared by K and L , i.e.

$$(3.5) \quad \Phi_{K,L}^{\text{int}(K)} := P_K(\mathbf{x}_{K,L}), \quad \Phi_{K,L}^{\text{ext}(K)} := P_L(\mathbf{x}_{K,L}),$$

where the reconstruction polynomials are given by (3.2).

Although MUSCL reconstructions generally reduce numerical oscillations, they do not eliminate them entirely. In some numerical tests, the remaining oscillations prevent the scheme from guaranteeing the IRP property. In particular, the positivity of each component and the bound-preserving property of the total concentration may be violated; see Examples 2 and 3 in Section 4. This issue is addressed by introducing two scaling limiters that ensure the IRP property.

3.2. Scaling limiters. To adapt the Zhang and Shu [28, 29] scaling limiters to handle (1.1), we first limit each concentration ϕ_l . Let us assume that $\Phi_K^n \in \mathcal{D}$ and let $\tilde{S}$ be a prescribed subset of K . The polynomials $P_K^{(l)}(\mathbf{x})$ are then replaced by $\tilde{P}_K^{(l)}(\mathbf{x}) := \theta_l(P_K^{(l)}(\mathbf{x}) - \phi_{l,K}^n) + \phi_{l,K}^n$, where

$$\theta_l := \min\{|\phi_{l,K}^n/(\phi_{l,K}^n - m_K^{(l)})|, 1\}, \quad m_K^{(l)} := \min_{\mathbf{x} \in \tilde{S}} P_K^{(l)}(\mathbf{x}), \quad l = 1, \dots, N.$$

Then the cell average of $\tilde{P}_K^{(l)}(\mathbf{x})$ over K is still $\phi_{l,K}^n$ and

$$(3.6) \quad \tilde{P}_K^{(l)}(\mathbf{x}) \geq 0 \quad \text{for all } \mathbf{x} \in \tilde{S} \text{ and } l = 1, \dots, N.$$

Next, we define the polynomial $\hat{P}_K(\mathbf{x}) := \hat{\theta}(\tilde{P}_K^{(1)}(\mathbf{x}) + \dots + \tilde{P}_K^{(N)}(\mathbf{x}) - \phi_K^n) + \phi_K^n$, where

$$\hat{\theta} := \min\{|(\phi_{\max} - \phi_K^n)/(M_K - \phi_K^n)|, 1\}, \quad M_K := \max_{\mathbf{x} \in \tilde{S}} (\tilde{P}_K^{(1)}(\mathbf{x}) + \dots + \tilde{P}_K^{(N)}(\mathbf{x})).$$

Thus, $\hat{P}_K(\mathbf{x}) \leq \phi_{\max}$ for all $\mathbf{x} \in \tilde{S}$. We now define the modified polynomials

$$(3.7) \quad \bar{P}_K^{(l)}(\mathbf{x}) := \hat{\theta}(\tilde{P}_K^{(l)}(\mathbf{x}) - \phi_{l,K}^n) + \phi_{l,K}^n, \quad l = 1, \dots, N,$$

and setting $\bar{\mathbf{P}}_K := (\bar{P}_K^{(1)}, \dots, \bar{P}_K^{(N)})^T$, replace (3.5) by

$$\Phi_{K,L}^{\text{int}(K)} := \bar{\mathbf{P}}_K(\mathbf{x}_{K,L}), \quad \Phi_{K,L}^{\text{ext}(K)} := \bar{\mathbf{P}}_L(\mathbf{x}_{K,L}).$$

Remark 3.1. The accuracy analysis of [2, section 4.4] shows that the limiters $\theta_1, \dots, \theta_N$ and $\hat{\theta}$ do not destroy the order of accuracy of the reconstruction.

We first prove the following lemma.

LEMMA 3.2. *If $\Phi_K^n \in \mathcal{D}$, then $\bar{\mathbf{P}}_K(\mathbf{x}) \in \mathcal{D}$ for all $\mathbf{x} \in \tilde{S}$.*

Proof. Let $\mathbf{x} \in \tilde{S}$. By definition (3.7), (3.6), and since $\hat{\theta} \in [0, 1]$,

$$(3.8) \quad \bar{P}_K^{(l)}(\mathbf{x}) = \hat{\theta}\tilde{P}_K^{(l)}(\mathbf{x}) + (1 - \hat{\theta})\phi_{l,K}^n \geq 0, \quad l = 1, \dots, N,$$

$$(3.9) \quad \begin{aligned} \bar{P}_K^{(1)}(\mathbf{x}) + \dots + \bar{P}_K^{(N)}(\mathbf{x}) &= \hat{\theta}(\tilde{P}_K^{(1)}(\mathbf{x}) + \dots + \tilde{P}_K^{(N)}(\mathbf{x}) - \phi_K^n) + \phi_K^n \\ &= \hat{P}_K(\mathbf{x}) \leq \phi_{\max}. \end{aligned}$$

Combining (3.8) and (3.9) we deduce that $\bar{\mathbf{P}}_K(\mathbf{x}) \in \mathcal{D}$ for all $\mathbf{x} \in \tilde{S}$. $\square$

To show that the marching formula (3.4) produces solutions belonging to $\mathcal{D}$, we notice that if $K \in \mathcal{T}_h^*$ is an interior volume, i.e. $\partial K \cap \partial\Omega = \emptyset$, then the diamond can be decomposed as $K = T_{K,1} \cup T_{K,2}$, where $T_{K,j}$ are triangles having the diagonal of K as a common side. Following the approach of [30], on each triangle $T_{K,j}$ with vertices $\mathbf{V}_{1,j}$, $\mathbf{V}_{2,j}$, and $\mathbf{V}_{3,j}$, we introduce the mappings

$$\begin{aligned} \mathbf{G}_{1,j}(u, v) &= \left(\frac{1}{2} + v\right) \mathbf{V}_{1,j} + \left(\frac{1}{2} + u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{2,j} + \left(\frac{1}{2} - u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{3,j}, \\ \mathbf{G}_{2,j}(u, v) &= \left(\frac{1}{2} + v\right) \mathbf{V}_{2,j} + \left(\frac{1}{2} + u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{3,j} + \left(\frac{1}{2} - u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{1,j}, \\ \mathbf{G}_{3,j}(u, v) &= \left(\frac{1}{2} + v\right) \mathbf{V}_{3,j} + \left(\frac{1}{2} + u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{1,j} + \left(\frac{1}{2} - u\right) \left(\frac{1}{2} - v\right) \mathbf{V}_{2,j}, \end{aligned}$$

which map the top edge of the rectangle $[-\frac{1}{2}, \frac{1}{2}] \times [-\frac{1}{2}, \frac{1}{2}]$ into one vertex and the other three edges to the edges of $T_{K,j}$. We define the quadrature points by

$$(3.10) \quad \begin{aligned} S_K &:= S_{K,1} \cup S_{K,2}, \\ S_{K,j} &= \left\{ \mathbf{G}_{1,j}(0, -\frac{1}{2}), \mathbf{G}_{2,j}(0, -\frac{1}{2}), \mathbf{G}_{3,j}(0, -\frac{1}{2}) \right\} \\ &= \left\{ \frac{1}{2}(\mathbf{V}_{1,j} + \mathbf{V}_{2,j}), \frac{1}{2}(\mathbf{V}_{2,j} + \mathbf{V}_{3,j}), \frac{1}{2}(\mathbf{V}_{3,j} + \mathbf{V}_{1,j}) \right\}, \quad j = 1, 2, \end{aligned}$$

that is, $S_{K,j}$ consists only of the midpoints of the three edges of $T_{K,j}$. Let us define the averages of the reconstruction polynomials over each sub-triangle $T_{K,j}$ of K

$$\Phi_{T_{K,j}}^n := \frac{1}{m(T_{K,j})} \int_{T_{K,j}} \bar{\mathbf{P}}_K(\mathbf{x}) d\mathbf{x}, \quad j = 1, 2.$$

and the set $\mathcal{N}_{K,j}$ of neighbors of the triangle $T_{K,j}$. Thus

$$\mathcal{N}(K) := (\mathcal{N}_{K,1} \cup \mathcal{N}_{K,2}) \setminus \{T_{K,1}, T_{K,2}\}.$$

Using the quadrature (3.10) and following [30], we can write

$$\Phi_{T_{K,j}}^n = \frac{1}{3} \sum_{L \in \mathcal{N}_{K,j}} \Phi_{K,L}^{\text{int}(K)}, \quad j = 1, 2.$$

Now, if K is a boundary element, i.e. $\partial K \cap \partial\Omega \neq \emptyset$, then there exists a segment $\sigma \in \mathcal{E}_h^*$ such that $\sigma \subset \partial K \cap \partial\Omega$. We denote by $\mathbf{x}_K^{\text{ext}}$ the midpoint of this segment and set $N(K)^\circ := \{L \in \mathcal{N}(K) : \sigma_{K,L} \subset \partial K \setminus \partial\Omega\}$. We also denote by $\mathbf{x}_{K,L_j}$, the midpoint of the edge shared by K and the interior neighbor L_j , $j = 1, 2$. In this case we define the stencil as $S_K = \{\mathbf{x}_{K,L_1}, \mathbf{x}_{K,L_2}, \mathbf{x}_K^{\text{ext}}\}$ and adopt the convention $T_{K,1} = T_{K,2} = K$.

Hence, in general the stencil is

$$(3.11) \quad S_K = \begin{cases} S_{K,1} \cup S_{K,2} & \text{if } \partial K \cap \partial\Omega = \emptyset, \\ \{\mathbf{x}_{K,L_1}, \mathbf{x}_{K,L_2}, \mathbf{x}_K^{\text{ext}}\} & \text{if } \partial K \cap \partial\Omega \neq \emptyset. \end{cases}$$

THEOREM 3.1. *Consider the FV scheme (3.4) associated with the reconstruction polynomials $\bar{\mathbf{P}}_K(\mathbf{x})$ defined by (3.7) and $\hat{S} = S_K$ (cf. (3.11)). If the CFL condition*

$$(3.12) \quad \frac{\alpha \Delta t}{\min\{m(T_{K,1}), m(T_{K,2})\}} \sum_{L \in \mathcal{N}(K)} m_{K,L} \leq \frac{1}{3} \quad \forall K \in \mathcal{T}_h^*, \quad \alpha := \max_{K \in \mathcal{T}_h^*} \left\{ \max_{L \in \mathcal{N}(K)} \alpha_{K,L} \right\}$$

is in effect and $\Phi_K^n \in \mathcal{D}$ for all $K \in \mathcal{T}_h^$, then $\Phi_K^{n+1} \in \mathcal{D}$ for all $K \in \mathcal{T}_h^*$.*

Proof. Let us focus first on the case when $K \in \mathcal{T}_h^*$ is an interior volume. Since we can write the average of Φ over K as

$$(3.13) \quad \Phi_K^n = \sum_{j=1}^2 \frac{m(T_{K,j})}{m(K)} \Phi_{T_{K,j}}^n,$$

the marching formula (3.4) can be expressed as

$$(3.14) \quad \Phi_K^{n+1} = \sum_{j=1}^2 \frac{m(T_{K,j})}{m(K)} \mathbf{H}_{T_{K,j}}, \quad \mathbf{H}_{T_{K,j}} := \frac{1}{3} \sum_{L \in \mathcal{N}_{K,j}} \mathbf{H}_{K,L,j},$$

where

$$\begin{aligned}\mathbf{H}_{K,L,j} &:= \Phi_{K,L}^{\text{int}(K)} - \frac{3\Delta t}{m(T_{K,j})} \mathbf{H}(\Phi_{K,L}^{\text{int}(K)}, \Phi_{K,L}^{\text{ext}(K)}, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}) m_{K,L} \\ &\quad \forall L \in \mathcal{N}_{K,j} \setminus \{T_{K,3-j}\}, \\ \mathbf{H}_{K,T_{K,3-j},j} &:= \Phi_{K,T_{K,j}}^{\text{int}(K)}.\end{aligned}$$

Applying Lemma 2.2 yields for $j = 1, 2$

$$(3.15) \quad \mathbf{H}_{K,L,j}^l \geq 0, \quad \forall l = 1, \dots, N, \quad \forall L \in \mathcal{N}_{K,j},$$

$$(3.16) \quad \sum_{l=1}^N \mathbf{H}_{K,L,j}^l \leq \phi_{\max} - \frac{3\Delta t \phi_{\max}}{m(T_{K,j})} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} \quad \forall L \in \mathcal{N}_{K,j} \setminus \{T_{K,3-j}\},$$

$$(3.17) \quad \sum_{l=1}^N \mathbf{H}_{K,T_{K,3-j},j}^l \leq \phi_{\max}.$$

Therefore, (3.13), (3.14) and (3.15) imply that $\phi_{l,K}^{n+1} \geq 0$. Moreover, from (3.13), (3.14), (3.16), (3.17), and the DDF property (2.3) it follows that

$$\begin{aligned}\phi_K^{n+1} &\leq \sum_{j=1}^2 \frac{m(T_{K,j})}{m(K)} \frac{1}{3} \sum_{L \in \mathcal{N}_{K,j}} \sum_{l=1}^N \mathbf{H}_{K,L,j}^l \\ &\leq \sum_{j=1}^2 \frac{m(T_{K,j})}{m(K)} \left(\phi_{\max} - \frac{\Delta t \phi_{\max}}{m(T_{K,j})} \sum_{L \in \mathcal{N}_{K,j} \setminus \{T_{K,3-j}\}} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} \right) \\ &= \phi_{\max} - \frac{\Delta t \phi_{\max}}{m(K)} \sum_{L \in \mathcal{N}(K)} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} = \phi_{\max}.\end{aligned}$$

Hence it follows that $\Phi_K^{n+1} \in \mathcal{D}$. For the case when K is a boundary element, the zero-flux boundary condition implies that

$$\Phi_K^{n+1} = \frac{1}{3} \left(\sum_{L \in \mathcal{N}(K)^\circ} \mathbf{G}_{K,L} + \bar{\mathbf{P}}_K(\mathbf{x}_K^{\text{ext}}) \right),$$

where

$$\mathbf{G}_{K,L} := \Phi_{K,L}^{\text{int}(K)} - \frac{3\Delta t}{m(K)} \mathbf{H}(\Phi_{K,L}^{\text{int}(K)}, \Phi_{K,L}^{\text{ext}(K)}, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}) m_{K,L} \quad \forall L \in \mathcal{N}(K)^\circ.$$

Then proceeding as before and using Lemmas 2.2 and 3.2 yields $\phi_{l,K}^{n+1} \geq 0$ and

$$\begin{aligned}\phi_K^{n+1} &\leq \frac{1}{3} \left(\sum_{L \in \mathcal{N}(K)^\circ} \left(\phi_{\max} - \frac{3\Delta t \phi_{\max}}{m(K)} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} \right) + \phi_{\max} \right) \\ &= \phi_{\max} - \frac{\Delta t \phi_{\max}}{m(K)} \sum_{L \in \mathcal{N}(K)^\circ} (\mathbf{u}_{K,L} \cdot \mathbf{n}_{K,L}) m_{K,L} \\ &= \phi_{\max} - \frac{\Delta t \phi_{\max}}{m(K)} \int_{\partial K \setminus \partial \Omega} \mathbf{u}_h \cdot \mathbf{n}_K \, ds.\end{aligned}$$

By construction of the dual mesh, K is the triangle whose vertices are the endpoints of $\mathbf{e}_K$ and the barycenter of the unique $T \in \mathcal{T}_h$ containing $\mathbf{e}_K$; in particular $K \subset T$, so $\mathbf{u}_h|_K$ is affine, and $\partial K \cap \partial\Omega = \mathbf{e}_K$. Thus, the divergence theorem and (2.3) give

$$(3.18) \quad \int_{\partial K} \mathbf{u}_h \cdot \mathbf{n}_K \, ds = \int_K \nabla \cdot \mathbf{u}_h \, d\mathbf{x} = 0,$$

whereas, since $\mathbf{e}_K$ is a straight segment, $\mathbf{n}_K$ is constant on $\mathbf{e}_K$ and the definition of the space $\mathbf{P}_1^{\text{CR}}(\mathcal{T}_h)$ yields

$$(3.19) \quad \int_{\partial K \cap \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_K \, ds = \mathbf{n}_K \cdot \left(\int_{\mathbf{e}_K} \mathbf{u}_h \, ds \right) = 0.$$

Subtracting (3.19) from (3.18), we get $\int_{\partial K \setminus \partial\Omega} \mathbf{u}_h \cdot \mathbf{n}_K \, ds = 0$. Thus, it also follows in this case that $\Phi_K^{n+1} \in \mathcal{D}$. $\square$

3.3. Time discretization and FVE scheme. To describe the SSPRK time discretization we assume that Φ^n is the vector of approximate solution values of $\Phi' = \mathcal{L}(\Phi)$ at $t = t_n$. Then the vector Φ^{n+1} for $t_{n+1} = t_n + \Delta t$ is computed by

$$\begin{aligned} \Phi^{(1)} &= \Phi^n + \Delta t \mathcal{L}(\Phi^n), \\ \Phi^{n+1} &= \frac{1}{2} \Phi^n + \frac{1}{2} (\Phi^{(1)} + \Delta t \mathcal{L}(\Phi^{(1)})). \end{aligned}$$

Due to convexity in the intermediate stages, this time discretization preserves the IRP property. The two subproblems are solved sequentially within each Runge-Kutta stage: given a concentration vector, the flow problem (1.1b), (1.1c) is solved first, and the resulting velocity is then held fixed while the conservation law (1.1a) is advanced. We denote by $\text{STOKES}(\Phi_h)$ the solution operator of (1.1b), (1.1c) and set

$$\Delta t_{\max}(\Phi_h, \mathbf{u}_h) := \frac{1}{3} \min_{K \in \mathcal{T}_h} \frac{\min_{j \in \{1,2\}} m(T_{K,j})}{\alpha \sum_{L \in \mathcal{N}(K)} m_{K,L}}, \quad \alpha := \max_{K \in \mathcal{T}_h} \left\{ \max_{L \in \mathcal{N}(K)} \alpha_{K,L} \right\},$$

so that $\Delta t \leq \Delta t_{\max}$ is precisely the CFL condition (3.12) and the time step Δt is computed adaptively at every time step so this condition is satisfied. The procedure is summarized in Algorithm 3.1.

4. Numerical examples. In part following [23], we define dimensionless (starred) variables via $\mathbf{x} = X_{\text{ref}} \mathbf{x}^*$, $t = T_{\text{ref}} t^*$, and $\mathbf{u} = (X_{\text{ref}}/T_{\text{ref}}) \mathbf{u}^*$, where X_{ref} is a reference length and $T_{\text{ref}} := X_{\text{ref}}/v_{\text{St}}$ is a reference time, where $v_{\text{St}} := (\rho_s - \rho_f) g d_1^2 / (18 \mu_f)$ is the Stokes velocity, i.e., the settling velocity of a single particle of the largest species, where μ_f is the viscosity of the fluid. We now omit the asterisk to simplify notation.

We assume that the functions $V_l(\phi)$, $l = 1, \dots, N$, are given by the modified Richardson-Zaki function [25]

$$V_l(\phi) := \begin{cases} \tilde{V}_l(\phi) & \text{for } 0 \leq \phi < \phi_{l,*}, \\ \tilde{V}_l(\phi_{l,*}) + \tilde{V}_l'(\phi_{l,*})(\phi - \phi_{l,*}) & \text{for } \phi_{l,*} \leq \phi \leq \phi_{\max}, \\ 0 & \text{otherwise,} \end{cases}$$

Following [4] we employ hindered settling functions with different exponents:

$$\tilde{V}_l(\phi) = \begin{cases} (1 - \phi)^{n_l - 2} & \text{if } \Phi \in \mathcal{D}, \\ 0 & \text{otherwise,} \end{cases} \quad n_l > 3, \quad n_i \leq n_j \text{ for } i < j, \quad i, j, l = 1, \dots, N.$$

Algorithm 3.1 Coupled FVE algorithm with IRP MUSCL reconstruction

Require: meshes $\mathcal{T}_h$, $\mathcal{T}_h^*$; datum Φ_0 with $\Phi_0(\mathbf{x}) \in \mathcal{D}$; t_{end} ; $\text{CFL} \in (0, 1]$; model parameters

- 1: $\Phi_K^0 \leftarrow m(K)^{-1} \int_K \Phi_0 \, d\mathbf{x}$, $K \in \mathcal{T}_h^*$; $t \leftarrow 0$; $n \leftarrow 0$
- 2: **while** $t < t_{\text{end}}$ **do**
- 3: $\mathbf{u}_h^n \leftarrow \text{STOKES}(\Phi^n)$
- 4: $\Delta t \leftarrow \min\{\text{CFL} \cdot \Delta t_{\text{max}}(\Phi^n, \mathbf{u}_h^n), t_{\text{end}} - t\}$
- 5: $\Phi^{(1)} \leftarrow \Phi^n + \Delta t \text{RESIDUAL}(\Phi^n, \mathbf{u}_h^n)$
- 6: $\mathbf{u}_h^{(1)} \leftarrow \text{STOKES}(\Phi^{(1)})$
- 7: $\Phi^{n+1} \leftarrow \frac{1}{2}\Phi^n + \frac{1}{2}(\Phi^{(1)} + \Delta t \text{RESIDUAL}(\Phi^{(1)}, \mathbf{u}_h^{(1)}))$
- 8: $t \leftarrow t + \Delta t$; $n \leftarrow n + 1$
- 9: **end while**

Ensure: $\{(\Phi^n, \mathbf{u}_h^n)\}_{n \geq 0}$, $\Phi_K^n \in \mathcal{D} \, \forall K \in \mathcal{T}_h^*, \forall n$

- 10: **procedure** $\text{RESIDUAL}(\Phi_h, \mathbf{u}_h)$
- 11: **for** $K \in \mathcal{T}_h^*$ **do**
- 12: Compute $\nabla \Phi_K$, from (3.1) and φ_K from (3.3).
- 13: $\widehat{\nabla \Phi_K} \leftarrow \varphi_K * \nabla \Phi_K$
- 14: $\mathbf{P}_K(\mathbf{x}) \leftarrow \Phi_K + \widehat{\nabla \Phi_K}(\mathbf{x} - \mathbf{c}_K)$
- 15: $m_K^{(l)} \leftarrow \min_{\mathbf{x} \in S_K} \mathbf{P}_K^{(l)}(\mathbf{x})$, $\theta_l \leftarrow \min\{|\phi_{l,K}^n / (\phi_{l,K}^n - m_K^{(l)})|, 1\}$, $l = 1, \dots, N$
- 16: $\tilde{\mathbf{P}}_K^{(l)} \leftarrow \theta_l(\mathbf{P}_K^{(l)} - \phi_{l,K}^n) + \phi_{l,K}^n$
- 17: $M_K \leftarrow \max_{\mathbf{x} \in S_K} \sum_{l=1}^N \tilde{\mathbf{P}}_K^{(l)}(\mathbf{x})$, $\hat{\theta} \leftarrow \min\{|\phi_{\text{max}} - \phi_K^n| / (M_K - \phi_K^n), 1\}$
- 18: $\bar{\mathbf{P}}_K^{(l)} \leftarrow \hat{\theta}(\tilde{\mathbf{P}}_K^{(l)} - \phi_{l,K}^n) + \phi_{l,K}^n$, $l = 1, \dots, N$
- 19: **end for**
- 20: **for** $K \in \mathcal{T}_h^*$ and $L \in \mathcal{N}(K)$ **do**
- 21: $\Phi_{K,L}^{\text{int}(K)} \leftarrow \bar{\mathbf{P}}_K(\mathbf{x}_{K,L})$, $\Phi_{K,L}^{\text{ext}(K)} \leftarrow \bar{\mathbf{P}}_L(\mathbf{x}_{K,L})$, $\mathbf{u}_{K,L} \leftarrow \mathbf{u}_h(\mathbf{x}_{K,L})$
- 22: **end for**
- 23: **return** $-m(K)^{-1} \sum_{L \in \mathcal{N}(K)} \mathbf{H}(\Phi_{K,L}^{\text{int}(K)}, \Phi_{K,L}^{\text{ext}(K)}, \mathbf{u}_{K,L}, \mathbf{n}_{K,L}) m_{K,L}$, $K \in \mathcal{T}_h^*$
- 24: **end procedure**

If $\tau_l(\phi) := \tilde{V}_l(\phi_{l,*}) + \tilde{V}_l'(\phi_{l,*})(\phi - \phi_{l,*})$ is the tangent to $\tilde{V}_l(\phi)$ at $(\phi_{l,*}, \tilde{V}_l(\phi_{l,*}))$, then $\phi_{l,*}$ is chosen such that $\tau_l(\phi_{\text{max}}) = 0$, i.e., $\phi_{l,*} = ((n_l - 2)\phi_{\text{max}} - 1)/(n_l - 3)$.

We define the function $\mu(\phi) = (1/\mu_0)(1 - \max(\eta, \min(\phi/\phi_{\text{max}}, 1 - \eta)))^{-v}$, where the parameter $\eta = 1 \times 10^{-8}$ is introduced to ensure that $\mu(\phi)$ remains bounded as $\phi \rightarrow \phi_{\text{max}}$. In addition we set $\mathbf{g}(\phi) := (\rho_s - \rho_f)\phi \mathbf{k} / \rho_f$, with $\mathbf{k} = (1, 0)^T$. In all examples we employ $X_{\text{ref}} = 1 \text{ m}$, $v = 2$, $\rho_s = 2790 \text{ kg/m}^3$, $\rho_f = 1208 \text{ kg/m}^3$, and $\mu_f = 0.02416 \text{ Pa.s}$. The stabilization parameter for the Stokes problem is set to $\gamma = 1$. We use the constant $\text{CFL} = 0.45$ (see Algorithm 3.1). We denote by “FVE” and “IRP-FVE” the numerical scheme without and with the limiters, respectively. The numerical scheme and all simulations presented in this work have been implemented in MATLAB, and the current solver can be found in the following Github repository:

<https://github.com/juanbarajasalonge/fve-polydisperse-sed>.

4.1. Example 1: $N = 3$, numerical order of accuracy. To verify numerically the convergence rate of the IRP-FVE scheme, we choose the ingredients in (1.1) in such a way that an exact solution is known. We set $\Omega := (0, 1) \times (0, 1)$ and $N = 3$

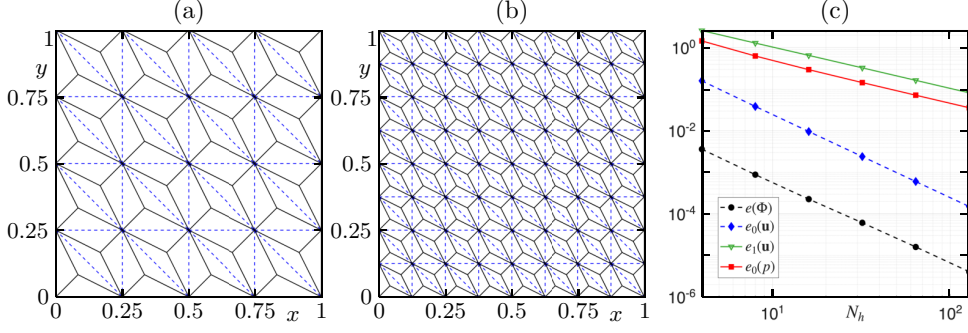


FIG. 3. Example 1: (a), (b) quasi-uniform triangulations of the unit square with (a) $h = 2^{-2}$, (b) $h = 2^{-3}$; (c) errors of the numerical solution against the number of control volumes N_h at simulated time $t = 0.01$.

TABLE 1

Example 1: convergence test using a manufactured exact solution, based on approximations of Φ , $\mathbf{u}$, and p on a sequence of uniformly refined triangulations of the unit square.

h	$e(\Phi)$	$r(\Phi)$	$e_0(\mathbf{u})$	$r_0(\mathbf{u})$	$e_1(\mathbf{u})$	$r_1(\mathbf{u})$	$e_0(p)$	$r_0(p)$
2.50e-01	3.62e-03	—	1.59e-01	—	2.59e+0	—	1.46e+0	—
1.25e-01	8.82e-04	2.038	3.86e-02	2.045	1.29e+0	1.000	6.32e-01	1.208
6.25e-02	2.27e-04	1.957	9.61e-03	2.008	6.53e-01	0.986	2.97e-01	1.092
3.12e-02	6.14e-05	1.888	2.41e-03	1.998	3.28e-01	0.995	1.45e-01	1.033
1.56e-02	1.61e-05	1.933	6.02e-04	1.999	1.64e-01	0.999	7.20e-02	1.010
7.81e-03	4.06e-06	1.986	1.51e-04	1.999	8.21e-02	1.000	3.59e-02	1.002

with $\boldsymbol{\delta} = (1, 0.8, 0.6)^T$. We choose $\phi_{\max} = 1.0$, $\mu_0 = 1$ and $n_l = 4.6$, $l = 1, 2, 3$. We modify the system by adding forcing terms that impose a known solution. In this case, the solution is

$$\begin{aligned} \Phi_{\text{ex}}(x, y, t) &= (\phi_{1,\text{ex}}(x, y, t), \phi_{2,\text{ex}}(x, y, t), \phi_{3,\text{ex}}(x, y, t))^T = \phi_0(x, y, t)(1/2, 1/3, 1/6)^T, \\ \phi_0(x, y, t) &= 0.2 \sin(\pi x)^2 \sin(\pi y)^2 \cos(t), \\ \mathbf{u}_{\text{ex}}(x, y, t) &= \begin{pmatrix} -\cos(2\pi x) \sin(2\pi y) + \sin(2\pi y) \\ \sin(2\pi x) \cos(2\pi y) - \sin(2\pi x) \end{pmatrix}, \quad p_{\text{ex}}(x, y, t) = \cos(\pi x) + \cos(\pi y), \end{aligned}$$

which satisfies (1.3) and (1.4). Therefore, the equations that are solved are

$$\begin{aligned} \partial_t \phi_l + \nabla \cdot (\phi_l \mathbf{u} + f_l(\Phi) \mathbf{k}) &= \partial_t \phi_{l,\text{ex}} + \nabla \cdot (\phi_{l,\text{ex}} \mathbf{u}_{\text{ex}} + f_l(\Phi_{\text{ex}}) \mathbf{k}), \quad l = 1, 2, 3; \\ -\nabla \cdot (\mu(\phi) \boldsymbol{\varepsilon}(\mathbf{u})) + \nabla p &= \mathbf{g}(\phi) - \nabla \cdot (\mu(\phi_{\text{ex}}) \boldsymbol{\varepsilon}(\mathbf{u}_{\text{ex}})) + \nabla p_{\text{ex}} - \mathbf{g}(\phi_{\text{ex}}), \\ \nabla \cdot \mathbf{u} &= 0, \end{aligned}$$

where $\phi_{\text{ex}} = \phi_{1,\text{ex}} + \phi_{2,\text{ex}} + \phi_{3,\text{ex}}$. We first apply the proposed IRP-FVE method on meshes obtained by successive subdivision of Ω into quasi-uniform triangulations $\mathcal{T}_h$ of meshsizes $h = 2^{-\ell}$, $\ell = 2, 3, \dots, 7$ (see Figure 3(a), (b)). The system is evolved according to the restriction (3.12), until $t = 0.01$. The errors between each component of the numerical solution $\phi_{1,h}, \phi_{2,h}, \phi_{3,h}, \mathbf{u}_h, p_h$, computed with a meshsize h , and the exact manufactured solution, are given by

$$e(\Phi) := \|\phi_{1,h} - \phi_{1,\text{ex}}\|_{L^1(\Omega)} + \|\phi_{2,h} - \phi_{2,\text{ex}}\|_{L^1(\Omega)} + \|\phi_{3,h} - \phi_{3,\text{ex}}\|_{L^1(\Omega)},$$

TABLE 2

Example 2 ($N = 2$): Minimum values of the solutions $\phi_{l,K}^n$, $l = 1, 2$, and maximum values of the solution ϕ_K^n obtained with the FVE and IRP-FVE schemes for different values of h , up to times $t = 0.5$ and $t = 1.5$, for domains Ω_θ with inclinations $\theta = 0^\circ$ and $\theta = 30^\circ$.

	h	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$
$\theta = 0^\circ$	FVE, $t = 0.5$				FVE, $t = 1.5$		
	5.00e-01	1.87e-02	2.40e-02	0.4750	-2.05e-03	2.26e-03	0.5601
	2.50e-01	1.23e-03	1.19e-02	0.5372	-1.22e-03	-3.04e-05	0.6001
	1.25e-01	-1.38e-03	1.89e-05	0.5865	-1.38e-03	-5.03e-03	0.6022
	6.25e-02	-1.16e-03	-1.71e-03	0.6002	-1.31e-02	-6.63e-03	0.6020
	IRP-FVE, $t = 0.5$				IRP-FVE, $t = 1.5$		
	5.00e-01	2.10e-02	2.45e-02	0.4657	6.05e-05	2.54e-03	0.5286
	2.50e-01	1.36e-03	1.20e-02	0.5098	2.03e-10	8.03e-05	0.5594
	1.25e-01	1.20e-06	9.74e-04	0.5416	1.83e-26	3.06e-09	0.5840
	6.25e-02	9.16e-15	4.86e-06	0.5724	3.87e-36	1.27e-13	0.5967
$\theta = 30^\circ$	FVE, $t = 0.5$				FVE, $t = 1.5$		
	5.00e-01	2.42e-02	2.43e-02	0.4735	-3.99e-04	2.27e-03	0.5651
	2.50e-01	8.94e-04	1.07e-02	0.5280	-5.06e-03	-1.80e-04	0.5988
	1.25e-01	-2.07e-03	3.01e-05	0.5863	-4.92e-03	-3.49e-03	0.6075
	6.25e-02	-6.16e-03	-3.48e-03	0.6012	-1.88e-02	-4.48e-02	0.6324
	IRP-FVE, $t = 0.5$				IRP-FVE, $t = 1.5$		
	5.00e-01	2.42e-02	2.51e-02	0.4622	4.28e-05	2.55e-03	0.5275
	2.50e-01	1.15e-03	1.11e-02	0.5075	3.34e-11	3.43e-05	0.5623
	1.25e-01	1.05e-06	8.11e-04	0.5402	1.47e-20	3.30e-08	0.5833
	6.25e-02	5.06e-13	1.65e-05	0.5708	5.29e-36	5.18e-13	0.5969

$$\mathbf{e}_0(\mathbf{u}) := \|\mathbf{u}_h - \mathbf{u}_{\text{ex}}\|_{0,\Omega}, \quad \mathbf{e}_1(\mathbf{u}) := \|\mathbf{u}_h - \mathbf{u}_{\text{ex}}\|_{1,h}, \quad \mathbf{e}_0(p) := \|p_h - p_{\text{ex}}\|_{0,\Omega}.$$

The rates of convergence associated with the numerical errors $\mathbf{e}$ and $\mathbf{e}'$ obtained using successive mesh sizes h and h' are defined as

$$\begin{aligned} r(\Phi) &:= \frac{\log(\mathbf{e}(\Phi)/\mathbf{e}'(\Phi))}{\log(h/h')}, & r_0(\mathbf{u}) &:= \frac{\log(\mathbf{e}_0(\mathbf{u})/\mathbf{e}'_0(\mathbf{u}))}{\log(h/h')}, \\ r_1(\mathbf{u}) &:= \frac{\log(\mathbf{e}_1(\mathbf{u})/\mathbf{e}'_1(\mathbf{u}))}{\log(h/h')}, & r_0(p) &:= \frac{\log(\mathbf{e}_0(p)/\mathbf{e}'_0(p))}{\log(h/h')}. \end{aligned}$$

As observed in Table 1 and Figure 3(c), the scheme attains its optimal convergence rates in all variables, i.e., the concentration error $\mathbf{e}(\Phi)$ decays at rate two in the L^1 norm, the velocity error $\mathbf{e}_0(\mathbf{u})$ at rate two in the L^2 norm, while $\mathbf{e}_1(\mathbf{u})$ and $\mathbf{e}_0(p)$ decay at rate one, as expected for the nonconforming $\mathbb{P}_1^{\text{CR}}/\mathbb{P}_0$ pair.

4.2. Example 2: $N = 2$, effect of limiters. Here, we consider domains Ω_θ representing a rectangular vessel rotated by an angle $\theta \in \{0^\circ, 30^\circ, 45^\circ, 60^\circ\}$ with respect to the vertical axis along with $N = 2$ particle species with diameters $d_1 = 2.9 \times 10^{-3}$ m, $d_2 = 2.0 \times 10^{-3}$ m, $n_1 = n_2 = 4.6$, and $\mu_0 = 1000$. We set a maximum total concentration of $\phi_{\text{max}} = 0.6$ and the initial concentration profile $\Phi_0(\mathbf{x}) = (0.06, 0.02)^T$. At $t = 3$, Figure 4 shows that the settling efficiency of both particle species increases as the inclination angle is increased. In this test, we measure the quantities

TABLE 3

Example 2 ($N = 2$): Minimum values of the solutions $\phi_{l,K}^n$, $l = 1, 2$, and maximum values of the solution ϕ_K^n obtained with the FVE and IRP-FVE schemes for different values of h , up to times $t = 0.5$ and $t = 1.5$, for domains Ω_θ with inclinations $\theta = 45^\circ$ and $\theta = 60^\circ$.

	h	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$
$\theta = 45^\circ$		FVE, $t = 0.5$			FVE, $t = 1.5$		
	5.00e-01	2.44e-02	2.57e-02	0.4637	-2.03e-03	2.27e-03	0.5521
	2.50e-01	1.96e-03	1.31e-02	0.5170	-1.99e-03	-2.82e-06	0.5913
	1.25e-01	-3.71e-03	1.18e-03	0.5714	-3.71e-03	-3.71e-03	0.6015
	6.25e-02	-4.51e-03	-2.07e-05	0.6002	-4.51e-03	-7.43e-03	0.6300
		IRP-FVE, $t = 0.5$			IRP-FVE, $t = 1.5$		
	5.00e-01	2.44e-02	2.57e-02	0.4585	1.31e-05	2.65e-03	0.5298
	2.50e-01	1.92e-03	1.33e-02	0.5012	9.36e-11	5.59e-05	0.5606
	1.25e-01	9.60e-06	1.76e-03	0.5394	2.22e-20	2.64e-07	0.5855
	6.25e-02	2.35e-12	1.98e-05	0.5689	4.86e-35	4.84e-12	0.5967
$\theta = 60^\circ$		FVE, $t = 0.5$			FVE, $t = 1.5$		
	5.00e-01	2.01e-02	2.47e-02	0.4758	-8.28e-04	3.57e-03	0.5649
	2.50e-01	1.03e-03	1.22e-02	0.5358	-5.62e-03	-8.80e-06	0.6001
	1.25e-01	-2.09e-03	8.87e-05	0.5847	-4.57e-03	-5.98e-03	0.6079
	6.25e-02	-4.24e-03	-3.65e-03	0.6001	-6.29e-03	-1.20e-02	0.6360
		IRP-FVE, $t = 0.5$			IRP-FVE, $t = 1.5$		
	5.00e-01	3.34e-02	2.68e-02	0.4661	4.05e-04	7.45e-03	0.5289
	2.50e-01	9.52e-03	1.79e-02	0.5088	3.70e-09	1.63e-04	0.5570
	1.25e-01	3.50e-05	4.88e-03	0.5386	2.86e-20	2.69e-07	0.5845
	6.25e-02	1.00e-12	1.62e-05	0.5714	1.11e-33	4.43e-12	0.5967

$\underline{\phi}_l := \min_{K,n} \{\phi_{l,K}^n\}$, $l = 1, \dots, N$, and $\bar{\phi} := \max_{K,n} \{\phi_K^n\}$ to verify satisfaction of the IRP property. These values are presented in Tables 2 and 3 for the cases with and without the use of limiters, up to times $t = 0.5$ and $t = 1.5$. For the scheme without limiters it occurs that $\underline{\phi}_l < 0$ or $\bar{\phi} > \phi_{\max}$, while in the case of the scheme with limiters the numerical solution remains within $\mathcal{D}$ for all θ , as expected.

4.3. Example 3: $N = 2$, trapezoidal geometry. This example is motivated by an experiment performed in a vessel with downward-facing inclined walls [27], see Figure 5(a). The parameters and initial condition are the same as in Example 2, but we set $\mu_0 = 100$. The quantities $\underline{\phi}_l$ for $l = 1, 2$ and $\bar{\phi}$, with and without the use of limiters, are presented in Table 4, up to $t = 1$. Without the scaling limiters, some computations yield $\underline{\phi}_l < 0$ or $\bar{\phi} > \phi_{\max}$, while in the case of the scheme with limiters the numerical solution remains within $\mathcal{D}$. Figure 6 displays the evolution of the total concentration and the fluid velocity field, where we observe clear-liquid interfaces together with the recirculation pattern induced by the downward-facing inclined walls.

4.4. Example 4: $N = 4$, reflux classifier geometry. We consider the geometry of a reflux classifier taken from [24], see Figure 5(b). (A reflux classifier is an advanced gravity separation device that combines a vertical fluidized bed with a set of parallel inclined lamella plates to sort fine particles based on their density and size. The applied fluidization in- and outflows and the parallel plates are, however,

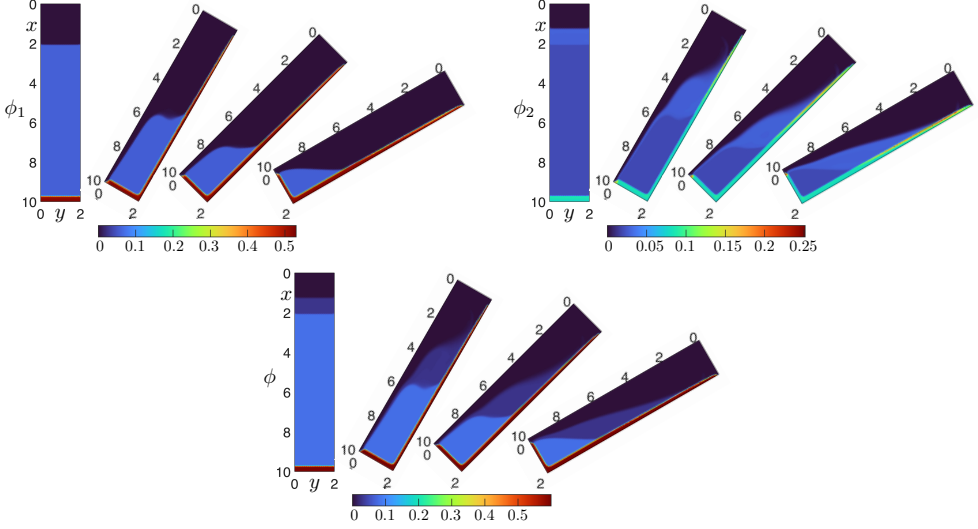


FIG. 4. Example 2 ($N = 2$): concentrations ϕ_1 , ϕ_2 (top) and total concentration ϕ (bottom) at $t = 3$ computed with the IRP-FVE scheme in the rotated vessels Ω_θ for $\theta = 0^\circ, 30^\circ, 45^\circ, 60^\circ$ (left to right), with 11.896 triangles and 18.036 control volumes for all domains.

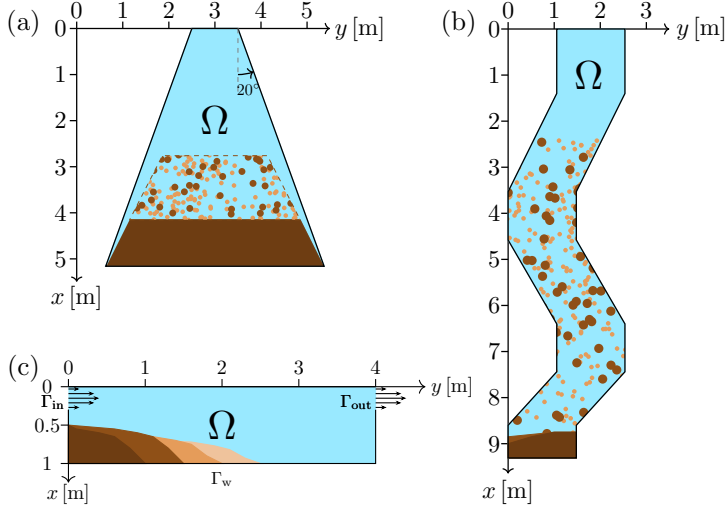


FIG. 5. Examples 3 to 5: (a) roof-shaped domain (Example 3), (b) polygonal domain shaped as a reflux-classifier vessel (Example 4), (c) rectangular tank whose boundary is subdivided into an inflow part Γ_{in} , an outflow part Γ_{out} , and zero-flux solid walls Γ_w (Example 5).

not considered here.) We set $N = 4$ and $d_1 = 2.9 \times 10^{-3} \text{ m}$, $d_2 = 2.5 \times 10^{-3} \text{ m}$, $d_3 = 2.0 \times 10^{-3} \text{ m}$, and $d_4 = 1.3 \times 10^{-3} \text{ m}$ along with the vector of initial concentrations $\Phi_0(\mathbf{x}) = (0.05, 0.05, 0.05, 0.05)^T$. In this test we vary the mixture viscosity through the parameter μ_0 and the exponents of hindered settling functions. The remaining parameters are set as in Example 2. Figure 7 shows the four components of the concentration vector, the total concentration, and the fluid velocity field at

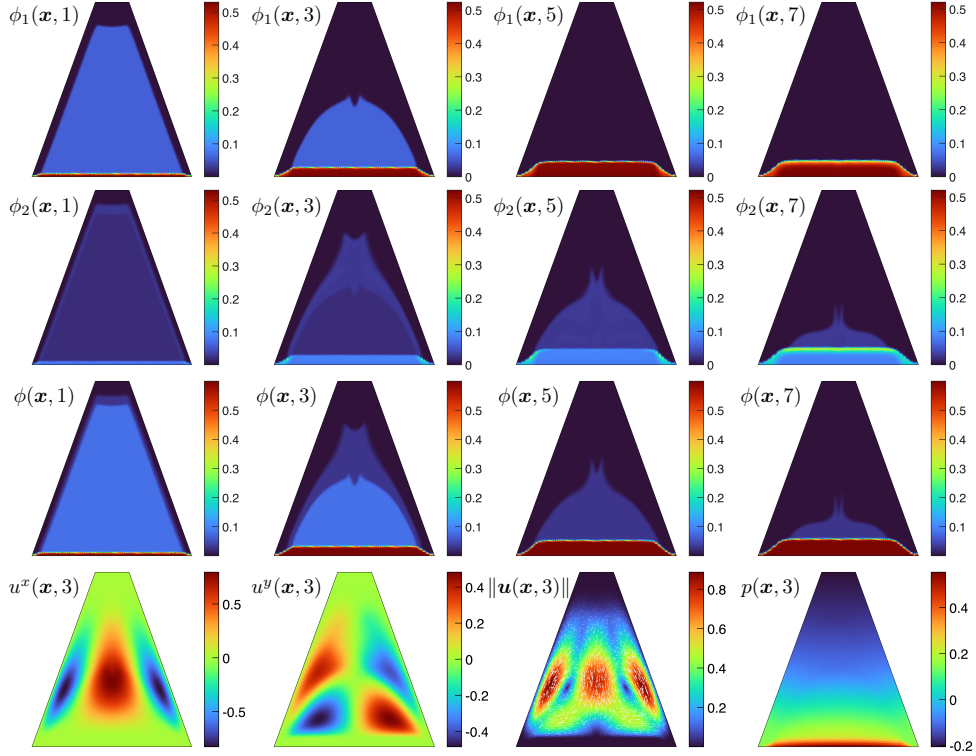


FIG. 6. *Example 3* ($N = 2$): Top three rows: concentrations ϕ_1 , ϕ_2 and total concentration ϕ at $t = 1, 3, 5, 7$ (left to right). Bottom row: velocity components u^x and u^y , speed $\|\mathbf{u}\|$, and pressure p at $t = 3$ with 3.840 triangles and 5.844 control volumes.

TABLE 4

Example 3 ($N = 2$): Minimum values of the solutions $\phi_{l,K}^n$, $l = 1, 2$, and maximum values of the solution ϕ_K^n obtained with the FVE and IRP-FVE schemes for different values of h up to time $t = 1$, for the roof-shaped domain.

h	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$	$\underline{\phi}_{,1}$	$\underline{\phi}_{,2}$	$\bar{\phi}$
	FVE, $t = 1$			IRP-FVE, $t = 1$		
5.00e-01	2.092e-04	6.865e-03	0.54500	3.601e-04	6.966e-03	0.51791
2.50e-01	-7.512e-04	1.421e-04	0.58050	3.864e-06	1.062e-03	0.53733
1.25e-01	-5.535e-03	-3.175e-04	0.60024	1.309e-12	1.946e-05	0.57438
6.25e-02	-5.487e-03	-5.601e-03	0.62836	1.300e-28	6.561e-10	0.59294

$t = 4$. Panels (a) and (b) correspond to $\mu_0 = 100$, with $n_l = 4.6$ for $l = 1, \dots, 4$ in panel (a) and $(n_1, n_2, n_3, n_4) = (3.1, 3.5, 4.0, 4.6)$ in panel (b). Panel (c) corresponds to $\mu_0 = 1000$ and $n_l = 4.6$ for $l = 1, \dots, 4$. The results show size-driven segregation of the four species and its sensitivity to the Richardson–Zaki exponents n_l and the mixture viscosity in the reflux classifier.

4.5. Example 5: $N = 4$, vessel with continuous inflow and outflow. In this final example we employ the FVE scheme in a regime where suspension is fed into

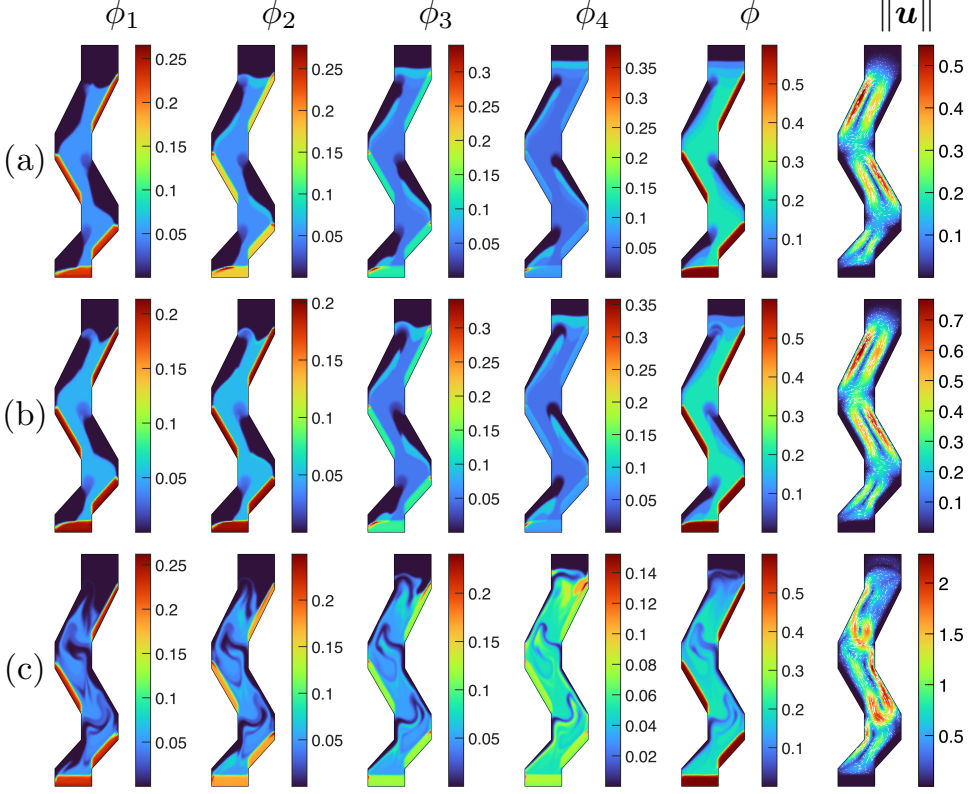


FIG. 7. *Example 4* ($N = 4$): reflux classifier at $t = 4$. Concentrations $\phi_1, \dots, \phi_4$, total concentration ϕ , and velocity magnitude $\|\mathbf{u}\|$ for (a) $\mu_0 = 100$ and $n_l = 4.6$ for $l = 1, \dots, 4$; (b) $\mu_0 = 100$, $n_1 = 3.1$, $n_2 = 3.5$, $n_3 = 4.0$, and $n_4 = 4.6$; and (c) $\mu_0 = 1000$ and $n_l = 4.6$ for $l = 1, \dots, 4$. All cases use a mesh with 8.652 triangles and 13.170 control volumes.

a rectangular vessel Ω whose boundary is split into three mutually disjoint relatively open parts $\bar{\Gamma}_{\text{in}} \cup \bar{\Gamma}_{\text{out}} \cup \bar{\Gamma}_{\text{w}} = \partial\Omega$, where Γ_{in} is the feed (inlet) section, located on the upper part of the left wall, Γ_{out} is the discharge (outlet) section, located on the upper part of the right wall, and $\Gamma_{\text{w}} := \partial\Omega \setminus (\bar{\Gamma}_{\text{in}} \cup \bar{\Gamma}_{\text{out}})$ collects the impermeable walls (see Figure 5(c)). This configuration is of interest for continuously operated solid-liquid separation equipment [12]. The problem is closed with the boundary conditions

$$\begin{aligned} \mathbf{u} &= \mathbf{0}, & (f_l(\Phi)\mathbf{k}) \cdot \mathbf{n} &= 0 & \text{on } \Gamma_{\text{w}}, \\ \mathbf{u} &= \mathbf{u}_{\text{in}}, & \Phi &= \Phi_{\text{in}} & \text{on } \Gamma_{\text{in}}, \\ \mathbf{u} &= \mathbf{u}_{\text{out}}, & \partial_{\mathbf{n}}\Phi &= 0 & \text{on } \Gamma_{\text{out}}, \end{aligned}$$

where the boundary data satisfy the following compatibility condition

$$\int_{\Gamma_{\text{in}}} \mathbf{u}_{\text{in}} \cdot \mathbf{n} \, ds + \int_{\Gamma_{\text{out}}} \mathbf{u}_{\text{out}} \cdot \mathbf{n} \, ds = 0.$$

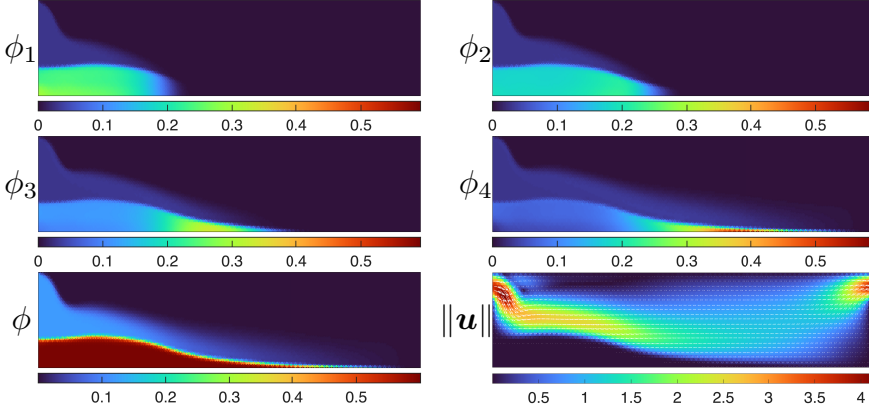


FIG. 8. *Example 5* ($N = 4$): concentrations $\phi_1, \dots, \phi_4$, total concentration ϕ and velocity magnitude $\|\mathbf{u}\|$ at $t = 4.25$ for the vessel with continuous inflow and outflow of Figure 5(c), with 9.600 triangles and 14.590 control volumes.

For this example, $\Gamma_{\text{in}} = (0, 0.3) \times \{0\}$ and $\Gamma_{\text{out}} = (0, 0.3) \times \{4\}$ and the inlet and outlet velocities are Poiseuille-type parabolic profiles given, for $x \in (0, 0.3)$, by

$$\mathbf{u}_{\text{in}}(x, 0) = 6\bar{\mathbf{u}}_{\text{in}} \cdot \frac{x}{\ell_{\text{in}}} \left(1 - \frac{x}{\ell_{\text{in}}}\right) (-\mathbf{n}), \quad \mathbf{u}_{\text{out}}(x, 4) = 6\bar{\mathbf{u}}_{\text{out}} \cdot \frac{x}{\ell_{\text{out}}} \left(1 - \frac{x}{\ell_{\text{out}}}\right) \mathbf{n},$$

where $\ell_{\text{in}} = m(\Gamma_{\text{in}})$, $\ell_{\text{out}} = m(\Gamma_{\text{out}})$, and $\bar{\mathbf{u}}_{\text{in}} = \bar{\mathbf{u}}_{\text{out}} = 2.5$. In addition, we employ $\Phi_{\text{in}} = (0.03, 0.03, 0.03, 0.03)^T$, $\mu_0 = 100$, $n_l = 4.6$, for $l = 1, \dots, 4$ and the remaining parameters are set as in Example 4. The vessel is initially filled with clear fluid, that is, $\Phi_0(\mathbf{x}) = (0, 0, 0, 0)^T$ so that the entire solids content of the vessel at time $t > 0$ originates from the feed through Γ_{in} . We simulate until $t = 4.25$ and the results are shown in Figure 8 where we observe the formation of a sediment layer at the bottom of the vessel. Specifically, the larger particles tend to settle onto the bottom close to the inlet while the second and third largest and the smallest particles are carried to more distant positions, as should be expected since they have smaller settling velocities.

5. Conclusions. We have introduced an invariant-region-preserving finite volume element scheme for the coupled transport-flow system (1.1) posed on a polygonal domain. The construction rests on two meshes: the Stokes system (1.1b), (1.1c) is discretized by nonconforming Crouzeix-Raviart elements with a jump stabilization on a primal triangulation, while the concentration equations (1.1a) are discretized by a finite volume scheme on the dual diamond mesh. The key structural ingredient is the local discrete divergence-free property (2.3), which is inherited by the dual mesh and makes the discrete velocity field compatible with the flux balance on each control volume. On this basis we proved in Theorem 2.1 that the first-order LLF scheme preserves the invariant region $\mathcal{D}$ under the CFL condition (2.10), and in Theorem 3.1 that the second-order MUSCL reconstruction equipped with a pair of linear scaling limiters retains this property under a more restrictive condition (3.12).

The numerical experiments confirm the optimal convergence rates for all variables and the preservation of region $\mathcal{D}$ in various vessel geometries. Future work will focus on increasing the spatial order beyond two while retaining the IRP property, either through central WENO (CWENO) reconstructions [10, 13] on the dual mesh or through a discontinuous Galerkin discretization of the transport part, in both cases

combined with the same scaling-limiter strategy. In addition, we are interested in the inclusion of sediment compressibility, which transforms (1.1a) into a strongly degenerate convection-diffusion system [5] and calls for an IRP analysis of the corresponding implicit or IMEX discretization of the diffusive term.

Another open issue is the inclusion of particle species that differ not only in size, but also in density. In fact, the original MLB model is based on the assumption that particles of species l have diameter d_l and density ρ_l . If we define the solid-fluid density difference $\bar{\rho}_l := \rho_l - \rho_f$, the vector $\bar{\rho} := (\bar{\rho}_1, \dots, \bar{\rho}_N)^T$ and $\bar{\rho}_l(\Phi) := \bar{\rho}_l - \bar{\rho}^T \Phi$, then the MLB velocity of particle species l is given by

$$(5.1) \quad v_l(\Phi) = \tilde{\mu}_{\text{sed}} (\delta_l \bar{\rho}_l(\Phi) V_l(\phi) - (\delta_1 \phi_1 \bar{\rho}_1(\Phi) V_1(\phi) + \dots + \delta_N \phi_N \bar{\rho}_N(\Phi) V_N(\phi))),$$

for $l = 1, \dots, N$. This equation is more general than (1.8) since (5.1) reduces to (1.8) in the equal-density case $\rho_1 = \dots = \rho_N = \rho_s$. However, for different-density particles ($\rho_l \neq \rho_j$ for at least one choice of $l \neq j$), the system (1.1a) with $v_l(\Phi)$ given by (5.1) is in general not hyperbolic on $\mathcal{D}$, as is shown in [9] (see also [7]), at least unless further restrictions on the particle sizes and densities and $\phi_{\max}$ and other parameters are introduced. Since the present numerical approach is based on the hyperbolicity of (1.1a) (or equivalently, that of (1.6)), it remains to establish under which conditions it may handle different-density systems using (5.1) as well.

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