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Implicit-Explicit Methods for the Efficient Simulation of the Settling of Dispersions of Droplets and Colloidal Particles

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Abstract. Techniques for the efficient approximate solution of systems of convection-diffusion partial differential equations modelling the sedimentation of droplets of different sizes in a viscous fluid are introduced. These techniques comprise the use of Polynomial Viscosity Matrix (PVM) methods for the convective numerical fluxes and implicit treatment of the nonlinear diffusion terms. Numerical examples based on [A. Abeynaike et al., Chem. Eng. Sci., 79 (2012), pp. 125–137] are presented.

AMS subject classifications: 35K59, 35L65, 65L06, 65M06, 65M08, 76T20

Key words: Sedimentation of droplets, convection-diffusion system, polynomial viscosity matrix, implicit-explicit method.

1 Introduction

1.1 Scope

The settling of a dispersion of droplets [1, 24] or that of a suspension colloidal solid particles [14] dispersed in a fluid can be modelled by systems of convection-diffusion equations of the form

$$\partial_t \Phi + \partial_x \boldsymbol{f}(\Phi) = \partial_x \big(\boldsymbol{B}(\phi) \partial_x \Phi \big), \quad 0 < x < L, \quad t > 0, \tag{1.1}$$

where t is time, x is depth, $\Phi(x,t) = (\phi_1(x,t), \cdots, \phi_N(x,t))^{\mathrm{T}}$ is the sought unknown, namely the vector of volume fractions of droplets or particles of class i, and $\phi = \phi_1 + \cdots + \phi_N$ is the

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total volume fraction of the disperse phase. Here we assume that particles of class i have diameter d_i, where $d_1 > \cdots > d_N$. Thus, the corresponding settling velocities v_i of individual particles of class i in an unbounded fluid satisfy $v_1 > v_2 > \cdots > v_N$. Moreover, we assume that the flux vector $\boldsymbol{f}(\Phi)$ is of the form

$$\boldsymbol{f}(\Phi) = V(\phi)(v_1\phi_1,\cdots,v_N\phi_N)^{\mathrm{T}}, \tag{1.2}$$

where $V(\phi)$ is a given function and that $\boldsymbol{B}(\phi)$ is a given diffusion matrix that depends on ϕ. We assume that $\boldsymbol{B}$ is a positive semidefinite $N\times N$ matrix and explicitly allow that $\boldsymbol{B}=\mathbf{0}$ on ϕ-intervals of positive length.

The settling of a dispersion of initial composition Φ^0 in a column of depth L is now described by the system (1.1) together with the zero-flux boundary conditions

$$\boldsymbol{f}(\Phi) - \boldsymbol{B}(\phi)\partial_x\Phi\big|_{x=0} = \mathbf{0}, \quad \boldsymbol{f}(\Phi) - \boldsymbol{B}(\phi)\partial_x\Phi\big|_{x=L} = \mathbf{0}, \tag{1.3}$$

and the initial condition

$$\Phi(x,0) = \Phi^0(x), \quad 0 \le x \le L, \tag{1.4}$$

where Φ^0 is the initial composition. This paper is focused on new methods for the efficient numerical solution of the model (1.1)-(1.4) including a high-resolution discretization of the convective term.

Explicit numerical schemes for (1.1) on a uniform Cartesian grid of meshwidth Δx and time step Δt are easy to implement but are associated with a Courant-Friedrichs-Lewy (CFL) stability condition that requires the proportionality $\Delta t \sim \Delta x^2$, which makes long-term simulations of (1.1)-(1.4) on a uniform grid unacceptably slow. A well-known remedy consists in handling the diffusive term in (1.1) by an implicit discretization. The resulting semi-implicit or implicit-explicit (IMEX) schemes (cf. e.g., [3,13]) are associated with an acceptable CFL condition $\Delta t \sim \Delta x$ but the case that $\boldsymbol{B}$ depends discontinuously on ϕ needs to be handled by special nonlinear solvers [10] or by solving linear problems in each time step that arise from carefully distinguishing between stiff and nontiff unknowns in the discretized version of $\partial_x(\boldsymbol{B}(\phi)\partial_x\Phi)$ (see [4]). These variants will be addressed as *nonlinearly implicit* (NI-IMEX) and *linearly implicit* (LI-IMEX) schemes, respectively. On the other hand, so-called polynomial viscosity matrix (PVM) methods [11, 15] have turned out as efficient high-resolution schemes for the approximation of solutions of the first-order system of conservation laws $\partial_t\Phi + \partial_x\boldsymbol{f}(\Phi) = 0$ for models akin to (1.2) (see [9]). It is the purpose of this work to demonstrate that the combination of PVM methods with NI-IMEX and LI-IMEX discretizations provides an efficient solver for the model (1.1)-(1.4). Moreover, we present a linearized stability analysis, based on a scalar, linearized version of the problem under study, that reconfirms that stability of the particular IMEX-RK method advanced herein is subject to a CFL condition of the type $\Delta t \sim \Delta x$.