On diffusively corrected multispecies kinematic flow models*

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Abstract

This presentation provides a survey of some recent results related to efficient numerical methods for the numerical solution of convection-diffusion systems of the form

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}\boldsymbol{f}(\Phi) = \frac{\partial}{\partial x}\left(\boldsymbol{B}(\Phi)\frac{\partial \Phi}{\partial x}\right), \quad x \in \Omega \subset \mathbb{R}, \quad t \geq 0, \tag{1}$$

where t is time, $x \in \Omega$ is spatial position where Ω is a bounded interval, $\Phi = (\phi_1, \dots, \phi_N)^{\mathrm{T}}$ is the vector of unknowns that usually denote the partial density or concentration of one of the N species that make up the disperse phase, $\boldsymbol{f}(\Phi) = (f_1(\Phi), \dots, f_N(\Phi))^{\mathrm{T}}$ is a flux vector where $f_j(\Phi) = \phi_j v_j(\Phi)$ for specified velocity functions $v_j(\Phi)$, and $\boldsymbol{B}$ is matrix that expresses a diffusive correction of the first-order model $\partial\Phi/\partial x + \partial \boldsymbol{f}(\Phi)/\partial x = \mathbf{0}$.

Models of this kind arise as one-dimensional models of the flow of one (disperse) substance through a continuous fluid. Applications include the settling of polydisperse suspensions of solid particles in a viscous fluid [1, 2, 3, 6], multiclass vehicular traffic under the effect of anticipation distances and reaction times [4, 5], the settling of dipersions and emulsions [7], and chromatography [8]. In many of these applications it is assumed that $\boldsymbol{B}(\Phi) = \mathbf{0}$ on a Φ-set of positive N-dimensional measure, so that (1) becomes strongly degenerate, and moreover $\boldsymbol{B}$ may depend discontinuously on Φ. For the numerical solution of (1) along with initial and boundary conditions that depend on the appliction under study these properties pose a number of difficulties whose partial solution will be addressed. For instance, it is well known that implicit-explicit (IMEX) numerical scheme that are based on discretizing the convective and diffusive parts of (1) are a potentially suitable tool to avoid the severe time step limitation associated with fully explicit discretization of (1). However, their implementation relies on the efficient numerical solution of the nonlinear systems of algebraic equations arising from the discretization of (1), which can not be achieved by standard Newton-Raphson techniques when $\boldsymbol{B}$ depends discontinuously on Φ. A combined smoothing and line search technique [5] solves the problem of solving the corresponding nonlinearly implicit equations. Alternatively, this problem can be avoided by the construction of so-called linearly implicit methods [2] that are slightly less accurate, but noticeably more efficient than their nonlinearly implicit counterparts.

The main collaborators in this research are Pep Mulet (Universitat de València, Spain) and Luis Miguel Villada (Universidad del Bío-Bío, Concepción).

*This work was partially supported by CONICYT-Chile through BASAL project CMM, Universidad de Chile; Fondecyt project 1170473; CRHIAM, project CONICYT/FONDAP/15130015; and by Centro de Investigación en Ingeniería Matemática (CI^{2}MA), Universidad de Concepción.

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