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Single-Field Numerical Modeling of Gas-Liquid Mass Transfer

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Extended Abstract

Mass transport and its transfer at interfaces in multiphase systems is a key aspect of numerous natural phenomena and industrial processes, ranging from geochemical reactions to chemical engineering applications. It is therefore essential to develop numerical modeling of such phase interactions to better understand or optimize these processes and applications. In this research, we focus on diffusion-driven phase change flows in a two-phase system, characterized by a dense phase and a dispersed phase. More precisely, the dispersed phase is a pure gaseous phase whose species dissolves into the dense liquid phase. Depending on the properties of the solution, in terms of undersaturation or supersaturation of the solute, the dispersed phase decreases or increases in volume, thus generating dissolution/precipitation phenomena. As solute transport limits the kinetics, the interface is at thermodynamic equilibrium and is characterized by a concentration jump.

Few studies in the literature have addressed the numerical modeling of dissolution and precipitation phenomena, with even fewer focusing on precipitation. This complexity arises from two major challenges: accounting for phase volume variations induced by mass transfer while maintaining the concentration discontinuity at interfaces, and incorporating the mass volume changes that occur when species transfer between dense and dispersed phases. Two types of modeling approaches have been developed to address this challenge, based respectively on single-field and two-field formulations of the species conservation equation. Rather than solving separate advection/diffusion equations for each phase, the single-field formulation uses a unified approach that incorporates the principles of species flux conservation, in the bulk and at the interface, into one global equation. It refers in the literature as the Continuous Species Transfer (CST) model and, more recently, the Compressive Continuous Species Transfer (C-CST) model.

In this study, we implemented a single-field CST formulation in the Notus open-source CFD software, utilizing an algebraic Volume of Fluid (VOF) approach based on the Compressive Interface Capturing Scheme for Arbitrary Meshes (CICSAM). While accurate predictions of dissolution phenomena were obtained with the literature-standard methods, the simulation of precipitation phenomena did not yield accurate results, particularly regarding the discontinuity in the species concentration at the interface. To overcome this limitation, we developed the velocity extension algorithm, typically used in the two-field formulation, to discretize the source terms governing the phase volume change in both the mass conservation and VOF equations.

First, the validation of these new numerical developments within the single-field framework is demonstrated through the case of gaseous phase precipitation for different Henry's coefficients (from 0.01 to 1) in 1D, 2D, and 3D configurations. These results have not been obtained in the literature. Validation was carried out by comparing the concentration profiles and phase volume change kinetics with exact solutions specifically developed in this study. Secondly, the 3D dynamic simulation of the growth of a rising bubble exhibits the relevance of the velocity extension algorithm in solving precipitation phenomena with the one-field approach.