A Quantitative Comparison of Physical Accuracy and Numerical Stability of Lattice Boltzmann Color Gradient and Pseudopotential Multicomponent Models for Microfluidic Applications

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Abstract. The performances of the Color-Gradient (CG) and the Shan-Chen (SC) multicomponent Lattice Boltzmann models are quantitatively compared side-by-side on multiple physical flow problems where breakup, coalescence and contraction of fluid ligaments are important. The flow problems are relevant to microfluidic applications, jetting of microdroplets as seen in inkjet printing, as well as emulsion dynamics. A significantly wider range of parameters is shown to be accessible for CG in terms of density-ratio, viscosity-ratio and surface tension values. Numerical stability for a high density ratio $\mathcal{O}(1000)$ is required for simulating the drop formation process during inkjet printing which we show here to be achievable using the CG model but not using the SC model. Our results show that the CG model is a suitable choice for challenging simulations of droplet formation, due to a combination of both numerical stability and physical accuracy. We also present a novel approach to incorporate repulsion forces between interfaces for CG, with possible applications to the study of stabilized emulsions. Specifically, we show that the CG model can produce similar results to a known multirange potentials extension of the SC model for modelling a disjoining pressure, opening up its use for the study of dense stabilized emulsions.

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1   Introduction

The numerical modeling of multiphase/multicomponent fluids is still a challenge and the Lattice Boltzmann Method (LBM) has shown great potential in this field [1]. Several models for simulating multiphase/multicomponent flows using the LBM have been proposed over the last three decades, including the color gradient (CG) model [2], the pseudopotential model [3], the free-energy model [4] and the mean-field model [5]. In the current work the CG model – based on a two-species variant of the lattice gas automata model introduced in [6] – is compared to the classical pseudopotential model developed by Shan and Chen (SC) and first introduced in [3]. The aim of comparing the two models is to quantitatively characterize how well each model performs in the context of realistic flow problems involving challenging interface dynamics, where e.g. surface tension and disjoining pressure play a crucial role in the breakup of fluid ligaments and in the coalescence of droplets. Specifically, our main focus is to investigate the feasibility and limitations of each of the two models for accurately simulating the jetting of microdroplets [7], a challenging industrial application where accurate modeling of multicomponent fluids is essential. During a typical jetting cycle, the ejected droplet is usually followed by a long attached tail/ligament. This ligament can either contract and coalesce with the main droplet or detach from the main droplet and contract into one or more detached satellite droplets. The droplet(s) formed during a jetting cycle will oscillate to some degree with a frequency that is analytically known [8]. Besides LBM based models, there are several other popular approaches that could be considered to simulate such a jetting system, among which the front-tracking method [9], the volume-of-fluid (VOF) method [10] and the level-set method [11]. These methods are based on solving the macroscopic Navier-Stokes equations alongside with a technique to track the interface between different phases and apply interfacial tension [12]. In the front-tracking method interface breakup does not automatically arise from numerical modeling of the interface, which necessitates manually rupturing the interface, according to an *ad hoc* criterion, e.g. as described in [13], in order to model interface breakup physics. On the contrary, both VOF and level-set methods naturally capture breakup and coalescence of interfaces. The VOF method requires interface reconstruction for determining and applying the proper surface tension, which can be a computationally expensive operation and may not always be physically consistent [14]. It has also been shown in [15] that both VOF and level set methods suffer from numerical instability around the interface when complex geometries are considered in combination with interfacial tension being the dominant force.

LBM based multiphase/multicomponent models have the advantage that coalescence and breakup events naturally arise from solving the mesoscopic level equations and no