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Comparison of Lattice Boltzmann, Finite Element and Volume of Fluid Multicomponent Methods for Microfluidic Flow Problems and the Jetting of Microdroplets

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Abstract. We show that the lattice Boltzmann method (LBM) based color-gradient model with a central moments formulation (CG-CM) is capable of accurately simulating the droplet-on-demand inkjetting process on a micrometer length scale by comparing it to the Arbitrary Lagrangian Eulerian Finite Element Method (ALE-FEM). A full jetting cycle is simulated using both CG-CM and ALE-FEM and results are quantitatively compared by measuring the ejected ink velocity, volume and contraction rate. We also show that the individual relevant physical phenomena are accurately captured by considering three test-cases; droplet oscillation, ligament contraction and capillary rise. The first two cases test accuracy for a dynamic system where surface tension is the driving force and the third case is designed to test wetting boundary conditions. For the first two cases we also compare the CG-CM and ALE-FEM results to Volume of Fluid (VOF) simulations. Comparison of the three methods shows close agreement when compared to each other and analytical solutions, where available. Finally we

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demonstrate that asymmetric jetting is achievable using 3D CG-CM simulations utilizing asymmetric wetting conditions inside the jet-nozzle. This allows for systematic investigation into the physics of asymmetric jetting, e.g. due to jet-nozzle manufacturing imperfections or due to other disturbances.

AMS subject classifications: 76-XX

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1 Introduction

Simulating the droplet-on-demand (DoD) inkjetting process on a micrometer length scale can be challenging as the method must be numerically stable for a two-fluid system with realistic ink and air properties, as might be used in industrial applications, including a high density ratio $\mathcal{O}(1000)$ and specific viscosity and surface tension values. Apart from these fluid properties, wetting boundary conditions in and around the nozzle, from which droplets are ejected, play an important role and should give physically realistic results for relevant contact angles. In the jetting case presented in this paper, the interior of the nozzle is highly dewetting, with contact angle $\theta_{CA} = 10^\circ$. Many multi-phase/multi-component models for the lattice Boltzmann method (LBM) are either not numerically stable for the parameter ranges required for realistic jetting and/or surface tension is not independently tunable from the density ratio [1]. We show that the color-gradient model with central moments formulation (CG-CM) is capable of accurately simulating the jetting process, with realistic parameters, by comparing the results to the more established Arbitrary Lagrangian Eulerian Finite Element Method (ALE-FEM) [2–4] and Volume of Fluid (VOF) method [5–10] wherever possible. Specifically, we consider three validation test-cases, after which a full jetting simulation is presented. The cases are: (1) droplet oscillation, (2) ligament contraction and (3) capillary rise. The first two cases show the accuracy for a dynamic system where surface tension is the driving force. Simulation results are compared to an analytical solution for the droplet oscillation case and an analytical approximation for the ligament contraction case. The third case of capillary rise is designed to test wetting boundary conditions by measuring the rate of rise of the meniscus inside a capillary as a function of the contact angle applied at the capillary wall. Again, results are compared to an analytical solution, namely Washburn's law [11]. For the CG-CM simulation we use a color-gradient specific wetting boundary condition where a contact angle is directly imposed by altering the color-gradient field, see section 2.1.2. This method does not suffer from unphysical mass transfer along solid boundaries which occurs using the conventional fictive-density wetting boundary condition often used for LBM [11]. Finally, a full jetting cycle is simulated where ink is pushed out through a nozzle and droplet formation takes place. For this simulation we compare CG-CM and ALE-FEM results quantitatively. For the CG-CM and ALE-FEM codes we