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A Lattice Boltzmann Study of Phase Separation in Liquid-Vapor Systems with Gravity

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Abstract. Phase separation of a two-dimensional van der Waals fluid subject to a gravitational force is studied by numerical simulations based on lattice Boltzmann methods implemented with a finite difference scheme. A growth exponent $\alpha = 1$ is measured in the direction of the external force.

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1 Introduction

Phase ordering in fluids is an important process that still needs to be completely understood in many cases of practical relevance. When a fluid is quenched from an initial disordered state into a regime of two-phase coexistence below the spinodal line, domains of the two phases are formed and grow with time. The typical size R of domains follows the power law $R \sim t^{\alpha}$ with the growth exponent α being *universal* in the sense that it does not depend on the microscopic details of the fluid, assuming only a few values related to the physical mechanism operating during phase separation [1]. Hydrodynamics is in general relevant and the coupling with the velocity field can change the value of the growth exponent α from that of purely diffusive growth [2, 3].

In this paper we consider the ordering of a liquid-vapor system subject to an external field mimicking the effects of gravity. The role of gravity on phase ordering has been

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more studied in binary systems. In critical quenches, after an initial diffusive growth with exponent $1/3$, there is a viscous growth characterized by $\alpha=1$ followed by an inertial regime with $\alpha=2/3$ [4]. Gravity becomes relevant when heavy domains resting on top of light ones become gravitationally unstable, thus accelerating the domain growth [5]. This occurs at late stages making inertial growth difficult to observe. A theoretical analysis neglecting hydrodynamical contributions suggests an exponent $\alpha_z=1$ for the size of domains in the vertical direction [6]. There are few studies of phase separation for liquid-vapor systems. In two-dimensional simulations the values $\alpha=1/2$ for high viscosity fluids and $\alpha=2/3$ for low-viscosity fluids have been found [2,7]. We are not aware of simulations made on a liquid-vapor system subject to gravity, where the growth exponent is measured.

We address this problem by applying the lattice Boltzmann method (LBM) to simulate a van der Waals fluid described by the Navier-Stokes and the continuity equation. LBM have been proved successful in studying fluids with mesoscopic structures (liquid-vapor interfaces in our case) on large time scales, as it is needed for phase separation [2,4,8–12]. In our approach, the thermodynamic description is based on a free-energy functional where interfaces are described at a coarse-grained level. The free-energy interface cost is expressed, as usual in van der Waals-Landau models, in terms of gradients of the density field. Locally, the fluid satisfies the van der Waals state equation. A finite difference version of LBM is implemented where the relationship $c=\delta s/\delta t$ among the lattice speed c and the space and time steps δs and δt does no longer hold, as in standard *collision - streaming* LBM [8–12]. The rejection of this condition has two advantages. First, this allows one to further consider multicomponent fluid systems where the masses of the component particles, as well as the lattice speeds, may be no longer identical [13, 14]. Second, higher order numerical schemes (including flux limiter schemes) may be considered in order to reduce unphysical effects like the spurious velocity and the numerical viscosity [7, 13–18]. The use of high order numerical schemes in finite difference LBM helps further to improve the numerical stability and accuracy [7, 17] while providing a convenient alternative to interpolation supplemented LBM [19, 20].

Our main results is that the sedimentation process induced by gravity is characterized by an exponent $\alpha=1$ independently on the values of viscosity and gravity.

The paper is organized as follows. Our LBM approach is described in Section 2; numerical results are shown in Section 3 and conclusions will be drawn in Section 4.

2 Description of the model

In this paper, we use the D2Q9 isothermal finite difference lattice Boltzmann model in two dimensions, which is well known in the literature [9–11, 15, 21]. This model relies on the following set of $\mathcal{N}=9$ evolution equations for the non-dimensionalized distribution functions $f_i(\mathbf{r},t)$, $i=0,1,\cdots,\mathcal{N}-1$, defined in the nodes $\mathbf{r}=(x,y)$ of a lattice with $\Lambda_x\times\Lambda_y$