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Three-Dimensional Numerical Simulation of Droplet Evaporation Using the Lattice Boltzmann Method Based on GPU-CUDA Accelerated Algorithm

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Abstract. The three-dimensional (3D) single component multiphase Shan-Chen lattice Boltzmann (LB) model is implemented with the GPU-accelerated algorithm based on the CUDA platform for the simulation of droplet evaporation. It is found that the speed-up of the GPU-accelerated 3D LB model with respect to the CPU-based 3D LB model increases with the computational node number. The maximum speed-up is higher than around 300 when the computational domain is composed of 256^3 computational nodes. Regarding the calculations performed using the GPU-accelerated 3D LB model that incorporates the operation of data output through CPU, the percentage of computational time consumed by CPU for executing the sequential tasks increases with the computational node number. The model validations are carried out through the comparisons of the simulations with Laplace's law and the D^2 law. Then, the GPU-accelerated 3D LB model is applied to simulate the evaporation phenomena of a droplet laying on smooth and rough solid surfaces. It is shown that the contact angle of the evaporating droplet on a smooth solid surface almost remains stable during the evaporation process. For the evaporating droplet sitting on a rough solid surface, however, the time evolution of the contact angle displays obvious oscillations. The simulated morphology evolution of the evaporating droplet sitting on a rough solid surface demonstrates that the oscillations of the contact angle are governed by the stick-slip movement, namely, depinning and receding, of the liquid-gas-solid contact line. This can be attributed to the large hysteresis of the droplet displaying the wetting Wenzel state.

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Key words: Lattice Boltzmann modeling, GPU computing, evaporation, contact angle.

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1 Introduction

The evaporation phenomenon of droplets on solid surfaces is ubiquitous in the natural world and plays an important role in many applications, such as inkjet printing, surface coating and heat transfer enhancement [1]. When a droplet evaporates, the associated mass loss at the liquid-gas interface leads to droplet shape readjustment that is strongly influenced by the liquid-solid interaction. This is because the movement of the liquid-gas-solid contact line that determines the droplet shape can be significantly affected by the topographical structures of the solid surface [2–5]. In addition, the liquid-gas interface is receding simultaneously as the droplet evaporation proceeds. Consequently, the dynamic wetting state of the evaporating droplet on a solid surface, e.g., the dynamic evolutions of contact angle and droplet shape, is rather complicated and difficult to be sufficiently understood.

Owing to the rapid development of computational science, numerical modeling has become an effective tool for understanding the interfacial wetting phenomena in the liquid-gas-solid coexisting systems [6–8]. Among the various numerical models, the multiphase lattice Boltzmann (LB) models, e.g., the pseudopotential and the phase-field multiphase LB models, have attracted a lot of attentions due to the feature of LB models without the need to explicitly track the interfaces [9,10]. In particular, the multiphase LB models can automatically describe the movement of the liquid-gas-solid contact line and the evolution of droplet shape for simulating the evaporation process of droplets on a solid surface [11–18]. Li et al. [11] simulated the evaporation process of droplets on the smooth substrates using a two-dimensional (2D) free-energy LB model by adding the evaporation source term in the LB equation to indicate the mass loss in the liquid-gas interface. The simulation results show that the wetting diameters of the evaporating droplets decrease while the contact angles remain almost constant. The pattern of a droplet during evaporation is governed by the motion of the liquid-gas-solid contact line. Li et al. [12] simulated the self-propelled motion of Leidenfrost droplets on ratchet surfaces using a 2D LB model with liquid-vapor phase change. It is found that the vapor flows caused by the droplet evaporation play an important role in the motion of the self-propelled Leidenfrost droplets. Laghezza et al. [13] conducted three-dimensional (3D) LB simulations of multi-droplet evaporation on the smooth solid surface. The simulation results showed that the evaporation dynamics of each droplet is deeply impacted by its assigned position with respect to the surrounding droplets. Ledesma-Aguilar et al. [14] performed 3D LB simulations of sessile droplet evaporation on smooth solid surface chemically patterned with hydrophilic and hydrophobic stripes. The time evolutions of contact angle and droplet size displayed the oscillating characteristics due to the stick-slip movement of the liquid-gas-solid contact line during evaporation. Moradi et al. [15] employed the 3D LB models to study the wetting behavior of small droplets on rough solid surfaces during evaporation. It was demonstrated that for the droplet with a size comparable to the roughness scale of the rough solid surface, the droplet shape is strongly affected by the substrate geometry. Other LB simulations concerning droplet evaporation can be