Commun. Comput. Phys.
doi: 10.4208/cicp.OA-2016-0211

Vol. **23**, No. 4, pp. 1116-1130
April 2018

Wetting Boundary Condition in an Improved Lattice Boltzmann Method for Nonideal Gases

Qin Lou*, Mo Yang and Hongtao Xu

School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, P.R. China.

Received 18 November 2016; Accepted (in revised version) 20 July 2017

Abstract. A numerical scheme capable of modeling fluid behavior on wetting surfaces is developed based on an interface-capturing lattice Boltzmann equation model [Q. Lou and Z. Guo, Phys. Rev. E 91,013302 (2015)], which has not yet been applied to wetting problems. With the proposed numerical scheme, the spurious densities near the solid surfaces can be eliminated and a wide range of equilibrium contact angles can also be reproduced. Further, the equilibrium contact angle on the solid surface, as a simulation parameter, can be given in advance according to the wettability. Numerical tests, including the dynamics behavior of a liquid drop spreading on a smooth surface and the capillary intrusion, demonstrate that the proposed numerical scheme performs well and can eliminate the spurious densities near the solid surface.

AMS subject classifications: 76T10, 76M25, 76D45, 82C40

Key words: Interface-capturing lattice Boltzmann equation model, wetting boundary condition, surface interactions.

1 Introduction

Wetting phenomena have received increasing attention owing to the prevalence in many industrial processes and in everyday applications, for example, the falling rain droplets along a window pane, the spray coating process, the fabrication of composite materials, the oil recovery process, and so on. However, some aspects, such as the interaction among different phases, complex surface properties, and the movement of contact lines, make the understanding and modeling of wetting phenomena both challenging and rewarding. In the past several decades, although the wetting phenomena have been studied by a variety of numerical methods, including the diffusive interface method [1], the phase field method [2, 3], the spectral boundary element method [4–6], the level set

*Corresponding author. *Email addresses:* louqin560916@163.com (Q. Lou), glxybgs@usst.edu.cn (M. Yang), htxu@usst.edu.cn (H. Xu)

method [7], and the molecular dynamics method [8–10], now it is still a challenging problem in developing a more efficient and more accurate numerical approach for such complicated wetting phenomena.

Over the past two decades, the lattice Boltzmann equation (LBE) method has attracted considerable attention in modeling multi-phase flows. As a mesoscopic numerical approach based on the Boltzmann equation, this method focuses on the particle distribution function, and the macroscopic quantities (e.g., density and velocity) can be obtained from the moments of the distribution functions. The LBE method can easily simulate the multi-phase flows without tracking the interface between immiscible phases, and for this reason, it has also been widely employed to study multi-phase flow problems [11–22]. As a relatively new numerical method, the LBE model borrows many of the concepts from other approaches. For example, the wetting phenomena are also studied for the multiphase LBE methods by implementing a wetting boundary condition.

Generally, there are two types of wetting boundary conditions in the LBE models. The first one originates from the work of Martys and Chen [23]. In their work, the wetting properties of the solid were described by a fluid-solid interaction, and different contact angles could be obtained through adjusting interaction strength. Inspired by the idea, some other forms of fluid-solid interactions were also proposed in the literature [24,25]. Initially, this type of wetting boundary condition was introduced into the pseudopotential LBE model, but later, it was also used for other LBE models [26,27]. The most distinct advantage of this type of wetting boundary condition is that it can be extended easily to other LBE models. However, in this type of wetting boundary condition, the equilibrium contact angle cannot be viewed as an input simulation parameter, and must be determined through an additional simulation. Moreover, the fluid densities or density gradients in this kind of wetting boundary condition are constants at the solid wall. At the equilibrium state, hence, a transition region with a distance of order l is necessary to vary the density from its value at the surface to that in the bulk phase. As a result, a "film" with the thickness of l is formed, creating spurious densities at the solid surface. Although the magnitude of l is usually at a molecular scale [28,29], the interface width obtained by the LBE model, as one of the diffusive interface method, is many orders of magnitude thicker than the real physical interface. So when modeling macroscopic flow in micro pore, the pore may be filled with the "film", and this type of wetting boundary condition will lose its applicability.

The second type of wetting boundary condition was developed based on the surface energy method, and was first proposed for the free energy LBE model by Briant *et al.* [30]. In this method, the wetting behavior of non-ideal gases at a solid surface is controlled by a wall free energy function which describes the interaction at the surface between the solid and the fluids. In general, the wall free energy function can be expanded in a power series of a variable related to the fluid density. In the framework of LBE method, Briant *et al.* [30–32] first used a linear form of the wall free energy function, and later it was also used in the kinetic theory-based LBE model by Lee *et al.* [33]. The main advantage of this type of wetting boundary condition is that the equilibrium contact angle can be