Commun. Comput. Phys.
doi: 10.4208/cicp.201009.271010s

Vol. **9**, No. 5, pp. 1165-1178
May 2011

Contact Angle Determination in Multicomponent Lattice Boltzmann Simulations

Sebastian Schmieschek[1,2] and Jens Harting[2,1,*]

[1] *Institute for Computational Physics, University of Stuttgart, Pfaffenwaldring 27, 70569 Stuttgart, Germany.*
[2] *Department of Applied Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands.*

Received 20 October 2009; Accepted (in revised version) 27 October 2010

Available online 14 January 2011

Abstract. Droplets on hydrophobic surfaces are ubiquitous in microfluidic applications and there exists a number of commonly used multicomponent and multiphase lattice Boltzmann schemes to study such systems. In this paper we focus on a popular implementation of a multicomponent model as introduced by Shan and Chen. Here, interactions between different components are implemented as repulsive forces whose strength is determined by model parameters. In this paper we present simulations of a droplet on a hydrophobic surface. We investigate the dependence of the contact angle on the simulation parameters and quantitatively compare different approaches to determine it. Results show that the method is capable of modelling the whole range of contact angles. We find that the a priori determination of the contact angle is depending on the simulation parameters with an uncertainty of 10% to 20%.

PACS: 47.55.D-, 47.11.-j

Key words: Lattice Boltzmann, Shan-Chen model, contact angle, droplets, hydrophobic surface.

1 Introduction

During the last few decades the miniaturization of technical devices down to submicrometric sizes has made considerable progress. In particular, during the 1980s, so-called microelectro-mechanical systems (MEMS) became available for chemical, biological and technical applications leading to the rise of the discipline called "microfluidics" in the 1990s [1]. In microfluidic devices the surface to volume ratio of a fluid can be large and thus a good understanding of the behavior of the fluid close to the surface is mandatory. However, the behavior of a fluid close to a solid interface is very complex and involves

*Corresponding author. *Email addresses:* sschmie@icp.uni-stuttgart.de (S. Schmieschek), j.harting@tue.nl (J. Harting)

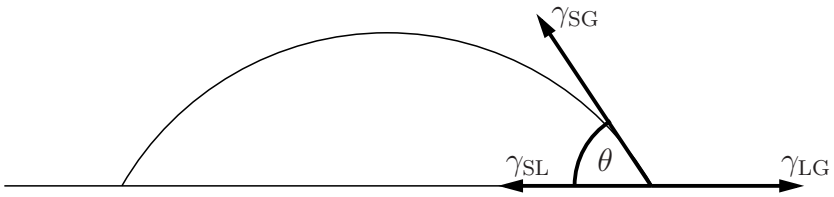

Figure 1: Definition of the contact angle as given by Young's equation.

the interplay of many physical and chemical properties. These include the wettability of the solid, the shear rate or flow velocity, the bulk pressure, the surface charge, the surface roughness, as well as impurities and dissolved gas.

A common concept to quantify the wettability of a surface is the so called contact angle. The contact angle is the angle at which the interface between a liquid and a gas or vapor meets a solid surface. If the contact angle is larger than 90°, the surface is called non-wettable (hydrophobic if the liquid is water) and if the angle is smaller than 90°, it is said to be wettable (hydrophilic). Superhydrophobic surfaces are surfaces with contact angles larger than 150°. Here, almost no contact between droplet and surfaces can be observed and the effect is often referred to as "Lotus effect". Regardless of the amount of wetting, the shape of the drop can be approximated by a truncated sphere.

For a droplet on an idealised smooth surface, the contact angle θ can be computed using the surface tensions between liquid and gas γ_{LG}, liquid and surface γ_{LS} and surface and gas γ_{SG} as given by Young's equation [2] (see Fig. 1),

$$\cos\theta = \frac{\gamma_{SG} - \gamma_{SL}}{\gamma_{LG}}. \tag{1.1}$$

The model of Young was extended by Wenzel [3] as well as Cassie and Baxter [4] in order to take the influence of surface roughness into account. While Wenzel describes a state where the surface is completely covered by the liquid, Cassie and Baxter describe a state where gas bubbles are enclosed between the liquid and the rough surface. Both states have been observed experimentally and in simulations [5, 6]. The transition between the Wenzel and the Cassie-Baxter state leads to the phenomenon of contact angle hysteresis as observed for droplets on a tilted surface where one has to distinguish between the advancing and the receding contact angle [7–9]. In particular the state proposed by Cassie and Baxter is of technological interest since it can be used to significantly increase the contact angle in order to generate superhydrophobic surfaces with $\theta > 150°$ [10–12]. Such surfaces can be utilized to increase the flow velocity and thus the mass flux in microchannels [13, 14].

While both molecular dynamics and lattice Boltzmann methods (LBM) have been employed to simulate systems with wetting properties, only LBM allow to reach experimentally relevant time- and length scales. Therefore, the method has become very popular to simulate typical problems occurring in microfluidics. A particular advantage of the