

## Lattice Boltzmann Simulations of Thermocapillary Motion of Droplets in Microfluidic Channels

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**Abstract.** Our recently developed lattice Boltzmann model is used to simulate droplet dynamical behaviour governed by thermocapillary force in microchannels. One key research challenge for developing droplet-based microfluidic systems is control of droplet motion and its dynamic behaviour. We numerically demonstrate that the thermocapillary force can be exploited for microdroplet manipulations including synchronisation, sorting, and splitting. This work indicates that the lattice Boltzmann method provides a promising design simulation tool for developing complex droplet-based microfluidic devices.

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**Key words:** Lattice Boltzmann method, thermocapillary force, droplet manipulation, microfluidics.

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## 1 Introduction

Droplet-based microfluidics has recently emerged as a promising, versatile platform for biological and chemical processes due to its advantages such as cost and time savings, improved analysis sensitivities, efficiency and accuracy. Unlike continuous-flow-based microfluidics, droplet-based microfluidics that creates discrete volumes with the use of immiscible fluids, allows for independent control of each droplet, thereby generating

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droplet microreactors that can be individually processed for transportation, mixing and analysis [1]. Since reagents and samples can be confined in the droplets, it eliminates the issues associated with Taylor dispersion and surface adsorption, which can cause sample dilution and cross-contamination [2]. Droplet microfluidics offers great potential for performing a large number of reactions without increasing system size or complexity [3]. In addition, several studies [4,5] demonstrated that droplet microfluidics has the ability to implement simple Boolean logic functions, a critical step towards the realisation of a microfluidic computer.

Exploiting the benefits of droplet-based microfluidics efficiently, thus facilitating a wide range of applications, requires manipulation of droplets with high precision and flexibility. The most commonly encountered droplet manipulations include droplet generation, fission, fusion, mixing and sorting. Diverse mechanisms have been used for these droplet manipulations, including hydrodynamic stress, electrowetting, magnetic force, optical forces, thermocapillary force, surface acoustic waves, and dielectrophoresis [6]. Among these, thermocapillary force becomes increasingly attractive because it can be generated easily by means of substrate embedded microheaters [7,8] or by laser heating [9,10], which allows contactless, reconfigurable, and real-time control of multiple droplets without the need for any special microfabrication or moving parts. To date, the thermocapillary force has been combined with the geometry of the microchannel to realise various droplet manipulations including mixing, sorting, fission, fusion, sampling and switching [11,12].

Experimental studies have helped to understand thermocapillary flows in microfluidic devices, but it is still very difficult to conduct precise experimental measurements of the local temperature and flow fields during the transport process of a droplet. Thus, current applications of microfluidics are very largely done by experimental trial and error. Numerical modelling and simulations can complement experimental studies, providing an efficient pathway to enhance our understanding of dynamical droplet behaviour at the microscale. However, it is challenging to use traditional CFD (computational fluid dynamics) methods, e.g., the volume-of-fluid (VOF) [13] and level-set (LS) [14] methods, for simulating thermocapillary flows in microchannels because of numerical instability arising at the interface region when the interfacial tension becomes a dominant factor in microdroplet behavior [15]. Also, minimising the spurious velocities at the interface still remains a major challenge for these methods. In addition, a suitable slip model with slip length at the molecular scale has to be introduced to avoid stress singularities at the moving contact-line. Microscopically, the interface between different phases and the contact-line dynamics on the solid surface are due to interparticle interactions [16]. Thus, mesoscopic level models are expected to describe accurately the thermocapillary flows in a microchannel.

Recently, the lattice Boltzmann method (LBM) has developed into a promising alternative to traditional CFD methods for simulating complex fluid flow problems. LBM is a pseudo molecular method based on particle distribution functions that performs microscopic operations with mesoscopic kinetic equations and reproduces macroscopic