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Lattice Boltzmann Method for Simulating Phase Separation of Sheared Binary Fluids with Reversible Chemical Reaction

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Abstract. A lattice Boltzmann method is utilized for governing equations which control phase separation of binary fluids with reversible chemical reaction in presence of a shear flow in this paper. We first present the morphology modeling of sheared binary fluids with reversible chemical reaction. We then validate the model by taking the unsheared binary fluids as an example. It is found that the results fit well with the references. The paper shows structures of the sheared system and gives the detailed analysis for the morphology of sheared binary fluids with reversible chemical reaction. The phase separation of the domain structures with different chemical reaction rates is discussed. Through simulations of the sheared binary fluids, two interesting phenomena are observed, which do not exist in a binary mixture without reversible chemical reaction. One is that the same results appear in both low and high viscosity, and the other is that the domain growth exponent with both low and high viscosities presents wave due to the competition of the viscosity and phase separation. In addition, we find that the finite size effects resulting in the growth exponent decreasing appear faster than that of the unsheared blend at a large time when the size of domains is comparable with the lattice size.

AMS subject classifications: 76D06, 76D07

Key words: Phase separation, reversible chemical reaction, lattice Boltzmann method, sheared binary fluids.

1. Introduction

The effects of a shear flow imposed on the fluid blends have been researched through numerical simulations in the last years. And the investigation indicates that when a fluid blend is quenched from a disordered state to a segregate system, phase separation and morphology of the fluid blends are strongly influenced by different sheared flows [1–5]. In the case of fluid mixtures subjected to a simple shear flow, the structures of domains are always aligned along the flow direction [6–9]. Taking the report written by Lamura and

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Gonnella [8] for example, we can see how the interplay between disordering tendencies of the shear and phase separation leads to a state of dynamic equilibrium where domains are broken up and reformed.

However, among the above reports, the investigated objects are just some simple sheared blends without the chemical reaction. In fact, on one hand, the blends with chemical reaction are of significant importance for industrial engineering and our daily life. On the other hand, Xie et al. [10, 11] show that a shear flow can greatly affect the phase evolution of the multi-component mixtures with the chemical reaction blends by the rheological method. Therefore, it is necessary to investigate the morphology and phase separation of complex sheared mixtures coupling chemical reaction through the numerical simulation. Based on the idea that is from simple to difficult, two-component blends with reversible chemical reaction is researched in this paper.

Moreover, taking existing references into consideration, we find that there is little investigation for phase separation of the sheared binary mixtures with the reversible chemical reaction. It is note that [12, 13] performed early work using numerical method and revealed that many interesting patterns can be obtained in the binary systems with the reversible chemical reaction. So the main purpose of this paper is to see how the shear flow affects the complex binary mixtures with reversible chemical reaction through the numerical simulation.

Based on our target, lattice Boltzmann method (LBM) is utilized in this paper. Lattice Boltzmann method [14–18] originating from the lattice gas automata (LGA) [19–21] has been applied to computational fluid dynamics since 1980s. Compared with traditional macroscopic numerical methods, LBM possesses a lot of advantages including easy-coding, simple handing boundary, natural parallelism and clear physical picture. Furthermore, in the light of its microscopic nature and mesoscopic characteristic, we may truly simulate hydrodynamic effects on phase separation and morphology of complicated fluids. Due to both the above reasons and in absence of research about the shear flow on phase separation with reversible chemical reaction, we utilize LBM to investigate this problem.

2. Model

2.1. Determining the morphologies: governing equations

In this paper, for the sake of simulating the structural evolution of a binary A/B fluids system, we adopt the LBM to model the phase separation in reversible chemical reaction. Here, we characterize our system by one order parameter named φ, which is defined as

$$\varphi = \varphi_A - \varphi_B,$$

where $\varphi_A$and φ_B are the local volume fractions of A and B components.

We chose a free energy function [13, 22]

$$F(\varphi) = \int d\mathbf{r} \left[-\frac{\tau}{2}\varphi^2 + \frac{g}{4}\varphi^4 + \frac{\kappa}{2}(\bigtriangledown\varphi)^2 + \frac{\rho \ln \rho}{3} \right]. \tag{2.1}$$