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A molecular collision based Lattice Boltzmann method for simulation of homogeneous and heterogeneous reactions

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ABSTRACT

A novel molecular collision based Lattice Boltzmann model at mesoscale was extended for representing hydrodynamics and concentration field of three typical reactive systems: (a) a reactive flow in a catalytic pore, (b) a fluid flow in a rectangular channel with a homogeneous reaction in the bulk and (c) a fluid flow that passes a reactive cylindrical obstacle in a channel. For detailed comparison of the performance of the model, all problems were solved by conventional reactive Lattice Boltzmann models. Also, three Damkohler numbers including advection-based and diffusion-based were derived using dimensional analysis. For the numerical validations, the results of collision model showed a good agreement with finite element method and demonstrated the ability of the proposed model for capturing different reaction problems especially heterogeneous reactions.

1. Introduction

Reactive flows are omnipresent in many academic and industrial researches such as bioengineering (Adam et al., 2012; Bornscheuer et al., 2012), fuel cell (Proietti et al., 2011), hydrogen generation devices (Karunadasa et al., 2010), combustion (Yamamoto et al., 2002), etc. Therefore, several authors have conducted numerical studies on reaction and relevant issues (Danish et al., 2008; Li Puma and Yue, 2003; Yamamoto et al., 2010; Zheng et al., 2013). Numerical models for reaction problems can summarized into four major categories: macroscopic (Eymard et al., 2010; Ten Thije Boonkkamp and Anthonissen, 2011), mesoscopic (Li et al., 2015), microscopic (Levchenko et al., 2010) and multiscale models (Hellander et al., 2012). Microscopic methods such as molecular dynamics investigate the interactions between single atoms and molecules. Therefore, because of computational cost limitations, studies about hydrodynamics and transport of species using microscopic methods are restricted to smaller ranges of time and space compared to other categories. On the other hand, conventional numerical methods at the macro scale, such as finite volume (FV), finite element (FE) and finite difference (FD), which are implicit solvers of discretized Navier–Stokes equations become complicated when applied to the reactive processes. An important reason is that under practical conditions, reactions usually occur in complex domains with liquid–solid or vapor–solid interfaces and complex boundary conditions, so the solver needs to solve many partial differential equations including momentum, energy, and concentration equations. Moreover, due to continuum nature of these schemes, it is difficult to accurately capture gas–liquid–solid interfaces and related parameters.

Lattice Boltzmann method (LBM) is a mesoscopic method and a powerful alternative tool for physical and physicochemical investigation of reactive systems. In addition, LBM is an efficient method for momentum, energy and mass transport analysis in simple and complicated geometries (He et al., 1997). Due to the kinetic background of LBM, it can easily deal with complicated geometries and boundary conditions (He et al., 1998; Peng, 2013). Consequently, there are many works published based on LBM in porous media (Chen et al., 2015; Falcucci

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et al. 2017; Guo and Zhao, 2005; Sullivan et al., 2005; Tong et al., 2014; Xin et al., 2013; Yoshino and Inamuro, 2003; Zhao et al., 2010). Furthermore, LBM is an explicit approach with high capability of parallel computing which is the major advantage of this method in comparison with the conventional Navier–Stokes solvers. These features of this method cause tendency to the use of LBM in reactive flow problems in complex structures that was reviewed by Kang et al. (2010) and other applications in complex flows studied by Aidun et al. (2010).

One of the first efforts in the simulation of reactive systems with LBM was performed (Ponce Dawson et al., 1993) that implemented Lattice Boltzmann technique to simulate diffusive systems with homogeneous reactions. (Qian and Orszag, 1995) utilized LBM to study dynamics of a special kind of pattern formation in diffusion–reaction systems. He et al. (2000) proposed a model for simulation of diffusion–convection problems coupled with surface reaction. Succi and Gabrielli (2001) accomplished a study of hydro-chemical phenomena in catalytic devices. Kang et al. (2006a) developed a general multicomponent pore scale LBM for simulating reactive transport in porous media. An LBM based model was constructed by Kamali et al. (2012) to reproduce a one-dimensional simulation of the Fischer–Tropsch reactor. Chen et al. (2013) investigated multiphase flow with heat transfer, dissolution, precipcitation and surface chemical reaction. Li et al. (2014) used an LBM based model to simulate the multicomponent flow and heat transfer with catalytic reactions. A higher order accuracy LBM model was employed by Zhang and Yan (2014) for bimolecular autocatalytic diffusion–reaction systems. Simulation of the geochemical reactive transport in fractured reservoirs was carried out by Tian et al. (2016).

For the simulation of homogeneous reactions coupled with fluid flow and studying physical and physicochemical parameters of a system, most of the reaction models used a source term in mass transport equation representing chemical reaction rate (Chen et al., 2014; Kang et al., 2007; Yamamoto et al., 2005). This source term originates from Arrhenius model that is a macroscopic description of reaction rate imported into mesoscopic mass transport equation of LBM which is not as accurate as using a mesoscopic approach. However, to the best of our knowledge, there are a few attempts that did not use a macroscopic approach for the reaction computing. Mishra and De (2013) established a stochastic kinetic Monte Carlo (MC) technique for the simulation of homogeneous chemical reaction. In their work, a microscopic reaction simulator was coupled with LBM which is a mesoscopic solver for hydrodynamics and scalar transport field. The capability of the proposed model was shown in solving a typical problem with a laminar flow in a 2-D rectangular domain where an elementary chemical reaction takes place in a square block in the middle. The model showed a good performance but it should be noted that fluctuations were observed in the prediction of species distribution in the reactive sites essentially arised from the stochastic nature of Monte Carlo scheme. In addition, computational time of MC–LBM model obviously increases compared with the conventional reactive models. In another study, Bresolin and Oliveira (2012) executed a fully mesoscopic model based on reaction kinetic theories to investigate 1-D diffusion–reaction systems. The presented model was evaluated with a binary diffusion in a cylindrical pore with a first-order homogeneous chemical reaction and results demonstrated a good agreement with the analytical solution.

The objective of the present paper is to extend the mesoscopic algorithm for the homogeneous chemical reaction modeling presented by Bresolin and Oliveira (2012) in order to investigate two-dimensional advection–diffusion–reaction problems that are very pervasive in reaction engineering. Also, to examine the capability of this model in other kinds of reactions, the developed model was used to simulate heterogeneous reactions. To illustrate the ability of the methodology, three different cases were studied. In case (a), a reactive diluted flow in a catalytic pore was examined in which the dominant phenomenon was molecular diffusion. Case (b) was a laminar solvent flow consisting of solute species that streams between two parallel plates. An elementary chemical reaction occur in the bulk and in contrast with case (a), advection is the paramount phenomenon. Finally, a laminar flow around a reactive cylindrical obstacle in a rectangular channel was studied in case (c). For the comparison of the presented model with the conventional reactive LBM models from the accuracy and computational point of view, all problems were simulated with conventional reactive LBM equations. Furthermore, proper dimensionless numbers have been addressed in each case using dimensional analysis.

The remainder of the paper is arranged as follows. In Section 1, we characterize three cases investigated in this work from the computational domain, governing equations and boundary conditions viewpoints. In Section 2, dimensionless numbers are derived in three cases. Also, we describe the details of LBM formulation for fluid flow, capture hydrodynamics of the system, explain relations between macroscopic and mesoscopic variables and present two different models of LBM for reactive solute transport including a new model of reaction algorithm and its kinetic foundation, collision model, and the conventional reaction model, i.e. macro model in Section 3. Simulation results of two LBM models in three cases are presented and discussed in Section 4. Finally, in Section 5, a brief conclusion of the paper is presented.

2. Numerical method

2.1. Lattice Boltzmann method for fluid flow

Lattice Boltzmann equation is derived from the discretization of Boltzmann equation. Using statistical mechanics, Boltzmann equation can be written as (Wolf-Gladrow, 2000),

$$\frac{\partial f}{\partial t} + \vec{\xi}.\nabla f = Q(f,f). \tag{1}$$

where f is the Particle Distribution Function (PDF), $\vec{\xi}$ is the velocity of the particle and Q is the collision term. The term f refers to the probability of the presence of the particles with a certain speed, at a given time and position. In order to simplify and linearize the collision term, some theories have been introduced in the literature. A well-known method is Bhatnagar, Gross and Krook (BGK) (Bhatnagar et al., 1954) which introduced a simplified model for collision operator as:

$$Q(f,f) = \frac{1}{\tau}(f^{eq} - f) \tag{2}$$

where τ is relaxation time and f^{eq} is defined as the equilibrium Particle Distribution Function. Because Lattice Boltzmann method is extended at the cradle of Lattice-Gas Cellular Automata (Wolf-Gladrow, 2000), similar to LGCA, lattices with a specific structure in the LBM are used to discretize Eqs. (1) and (2) in the sense of velocity and space. Interested readers are referred to D'Humieres and Lallemand (1987) and Frisch et al. (1986) for more details about LGCA method and its applications. The conventional lattice structure used for isothermal two-dimensional problem for the velocity vectors is a two-dimensional 9-speed model (D_2Q_9) that has the form,

$$\vec{e}_\alpha = \begin{cases} (0,0) & \alpha = 0 \\ c\,(\cos[(\alpha-1)\pi/2], \sin[(\alpha-1)\pi/2]) & \alpha = 1-4 \\ \sqrt{2}\,c\,(\cos[(\alpha-5)\pi/2+\pi/4], \sin[(\alpha-5)\pi/2+\pi/4]) & \alpha = 5-8 \end{cases} \tag{3}$$

The term c is defined as $\frac{\Delta x}{\Delta t}$ which is supposed to be 1 in this implementation. As mentioned, f is a function of particles speed, so in Eq. (1), the velocity can be replaced by $\vec{e}_\alpha$ which is also a function of the location of particles. As a result:

$$f(\vec{\zeta}, x, t) \rightarrow f_\alpha(x,t) \tag{4}$$

The next important step is to relate the intangible mesoscopic probabilities to more familiar macroscopic expressions