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# Lattice Boltzmann Method for Reacting Flows in Porous Media

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**Abstract.** We review recent developments in lattice Boltzmann method for reacting flows in porous media. We present the lattice Boltzmann approaches for incompressible flow, solute transport and chemical reactions in both the pore space and at the fluid/solid interfaces. We discuss in detail the methods to update solid phase when significant mass transfer between solids and fluids is involved due to dissolution and/or precipitation. Applications in different areas are presented and perspectives of applying this method to a few important fields are discussed.

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**Key words**: Reactive flows, lattice Boltzmann method, porous media, pore scale.

## 1 Introduction

Reacting flows in natural and man-made porous media are ubiquitous, particularly in various energy, earth and environment systems. Examples include electrochemical energy conversion devices (fuel cells and batteries), stimulation of petroleum reservoirs, geologic storage of carbon dioxide and nuclear wastes, subsurface contaminant migration, bioremediation etc. In these examples, the inherently complex morphology of such porous media coupled with multi-physicochemical transport and interfacial processes over multiple length scales makes this problem notoriously difficult and consequently poses several open questions. On one hand, most of the key processes, including fluid mobility, chemical transport, adsorption and reaction, are ultimately governed by the pore-scale interfacial phenomena, which occur at scales of microns.

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On the other hand, because of the wide disparity in length scales, it is virtually impossible to solve the pore-scale governing equations at the scale of interest. As a result, a continuum formulation (macroscopic approach) of reactive transport in porous media based on spatial averages and empirical parameters is often employed. As the spatial averaging is taken over length scales much larger than typical pore and grain sizes, spatial heterogeneities at smaller scales are unresolved. These unresolved heterogeneities, together with the empirical parameters often unrelated to physical properties, lead to significant uncertainties in reactive flow modeling at the larger scale. Therefore, to reduce uncertainties in the numerical modeling of reactive transport processes at the scale of interest, it is imperative to better understand these processes at the pore scale and to incorporate pore-scale effects in the continuum scale [34,35].

The problem of reacting flows in porous media has been studied extensively at the pore scale using various approaches under different simplifying conditions [2,3, 8,10,12,17,20–23,25–28,43,53]. The lattice Boltzmann method (LBM), a relatively new numerical method in computational fluid dynamics [6,44], has undergone great advances and developed into a powerful numerical tool for simulating complex fluid flows and modeling physics in fluids in the past two decades. Owning to its advantage in handling nonequilibrium dynamics, especially in fluid flow applications involving interfacial dynamics and its ease to treat complex boundaries (geometries), the LBM offers a promising approach for investigating pore-scale phenomena involving reacting flows in porous media. In this article, we review recent developments in LBM for reacting flows in porous media. Earlier work on lattice gas and lattice Boltzmann methods and their applications in reaction-diffusion systems can be found in the excellent review by Chen et al. [5].

## 2 Lattice Boltzmann method for fluid flow

The flow of a single aqueous fluid phase in the pore space of a porous medium can be simulated by the following evolution equation (the so-called LBGK equation) [4,41]

$$f_\alpha(\mathbf{x}+\mathbf{e}_\alpha\delta t, t+\delta t) = f_\alpha(\mathbf{x},t) - \frac{f_\alpha(\mathbf{x},t) - f_\alpha^{\mathrm{eq}}(\mathbf{x},t)}{\tau}. \tag{2.1}$$

In the above equation, $\delta t$ is the time increment, $f_\alpha$ the distribution function along the $\alpha$ direction in velocity space, $f_\alpha^{\mathrm{eq}}$ the corresponding equilibrium distribution function and $\tau$ the dimensionless relaxation time. For the commonly used two-dimensional, nine-speed LB model (D2Q9) as shown in Fig. 1, the discrete velocities $\mathbf{e}_\alpha$ have the following form:

$$\mathbf{e}_\alpha = \begin{cases} 0, & \alpha = 0, \\ \left(\cos\frac{(\alpha-1)\pi}{2}, \sin\frac{(\alpha-1)\pi}{2}\right)c, & \alpha = 1-4, \\ \sqrt{2}\left[\cos\left(\frac{(\alpha-5)\pi}{2}+\frac{\pi}{4}\right), \sin\left(\frac{(\alpha-5)\pi}{2}+\frac{\pi}{4}\right)\right]c, & \alpha = 5-8, \end{cases} \tag{2.2}$$