



Pore-scale simulation of multicomponent multiphase reactive transport with dissolution and precipitation



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ABSTRACT

Multicomponent multiphase reactive transport processes with dissolution–precipitation are widely encountered in energy and environment systems. A pore-scale two-phase multi-mixture model based on the lattice Boltzmann method (LBM) is developed for such complex transport processes, where each phase is considered as a mixture of miscible components in it. The liquid–gas fluid flow with large density ratio is simulated using the multicomponent multiphase pseudo-potential LB model; the transport of certain solute in the corresponding solvent is solved using the mass transport LB model; and the dynamic evolutions of the liquid–solid interface due to dissolution–precipitation are captured by an interface tracking scheme. The model developed can predict coupled multiple physicochemical processes including multiphase flow, multicomponent mass transport, homogeneous reactions in the bulk fluid and heterogeneous dissolution–precipitation reactions at the fluid–solid interface, and dynamic evolution of the solid matrix geometries at the pore-scale. The model is then applied to a physicochemical system encountered in shale gas/oil industry involving multiphase flow, multicomponent reactive transport and dissolution–precipitation, with several reactions whose rates can be several orders of magnitude different at a given temperature. The pore-scale phenomena and complex interaction between different sub-processes are investigated and discussed in detail.

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1. Introduction

Multicomponent multiphase reactive transport processes in porous media are widespread in energy and environment sciences. Typical examples are proton exchange membrane fuel cells (PEMFC) [1], Liesegang phenomena [2], hydrocarbon recovery [3,4], porous media bio-filtration devices [5–7], solidification of metallic materials [8], geological storage of nuclear wastes [9], and carbon dioxide (CO₂) sequestration [10–14]. The coupled transport processes and multiphase phenomena, together with the dynamic evolutions of the solid matrix structures caused by dissolution–precipitation, make the situation even more complicated [12,13,15–17]. Usually the phenomena at the continuum-scale are of engineering interest; however they originate from the underlying pore-scale processes and interactions. For example, surface reactions taking place at the pore scale lead to the dissolution/precipitation of the solid phase, which in turn affect the fluid flow and

solute transport, thus altering the material properties such as porosity and permeability that determine the continuum-scale behaviors. Therefore, understanding the meso/microscopic phenomena and the complicated interactions between different processes is critical to achieving a better prediction of the related systems.

With the improvement of the computational resources, pore-scale simulation, in which the realistic porous structures are considered, has become a critical technique for exploring multiple physicochemical problems. To accurately simulate pore-scale multicomponent multiphase reactive transport processes with dynamic evolutions of the solid phases, where the topography of the evolving liquid–gas–solid interfaces is part of the required result, the numerical model must be able to handle the following four major fundamental issues. The first one is to capture the deformable liquid–gas interfaces which may stretch, break-up or coalesce. Available models for tracking the moving liquid–gas interface can be roughly classified in two groups: the diffusion interface model and the sharp interface model and one can refer to a recent review paper for more details [18]. The second fundamental issue is to track the moving fluid–solid interfaces due to dissolution–precipi-

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tation (or melting–solidification). The common feature of the problems with the evolutions of solid phases is that there is no fluid flow and mass transport in the solid phase, and flow at the solid–fluid interfaces is usually subjected to a no-slip condition as the dissolution–precipitation (or melting–solidification) is relatively slow in the practical systems [9,12,16,17]. The third one is to simulate mass transfer in the multiphase systems. The mass transfer processes in different phases, which are very important for understanding the reactive transport processes, pose a great challenge for simulation. In addition, the accompanying evolution of the liquid–gas–solid interfaces makes the inter-phase mass transfer more complicated [9,18]. The last one is the incorporation of homogeneous and heterogeneous reactions into the simulations [19].

Different numerical methods have been developed to investigate pore-scale fluid flow and transport processes, including the direct numerical simulation method (DNS) [16], pore-network model (PNM) [20], lattice Boltzmann method (LBM) [2,12–15,19,21–24], and smoothed particle hydrodynamics [25,26]. Each of these methods has its own advantage and disadvantages. Little work has been done on the development of pore-scale reactive transport models with dissolution–precipitation because of the difficulty of handling the coupled physicochemical processes and directly capturing the complex structural evolutions. Single-phase fluid flow and reactive transport with dissolution–precipitation was studied by Kang et al. [21,22] in which the LBM was used to simulate transport processes and the Volume of Pixel (VOP, a method for tracking fluid–solid interfaces) was adopted to update the solid structures. They predicted the relationship between permeability and porosity under different Pe (Peclet number, representing the relative strength of convection to diffusion) and Da (Damköhler number, representing the relative strength of reaction to diffusion). Later, Kang et al. [19] extended their model to multicomponent systems and used the model to study reactive transport processes associated with geological CO_2 sequestration [12]. For multiphase reactive transport with moving solid–fluid interfaces, the numerical studies are scarce in the literature [9,24]. Recently, Parmigiani et al. [24] used the LBM to study the injection process of a non-wetting fluid into a wetting fluid coupled with dynamic evolution of the solid geometries. In their study the change of solid phase was caused by melting only. Very recently, Chen et al. [9] constructed a pore-scale model based on the LBM and the VOP to simulate multiphase reactive transport with phase transition and dissolution–precipitation processes [9]. Their pore-scale model can capture coupled non-linear multiple physicochemical processes including multiphase flow with phase separation, mass transport, chemical reaction, dissolution–precipitation, and dynamic evolution of the pore geometries. The model was used to study the thermal migration of a brine inclusion in a salt crystal [9]. However, in their model, the two-phase system is a single-component water–vapor system and only the transport of a single solute was considered [9]. From the above review, it can be seen that currently there are no pore-scale studies of multicomponent multiphase reactive transport processes with dissolution–precipitation.

The objective of the present study is to develop a pore-scale model which can handle multiphase flow involving multicomponent homogenous and heterogeneous reactions. Specific goals include (i) constructing a two-phase multi-mixture model based on the LBM, (ii) simulating multiple physicochemical processes including multiphase fluid flow, multicomponent mass transport, homogeneous reactions in the bulk fluid and heterogeneous reactions at the fluid–solid interfaces, and dissolution and precipitation of the solid phases at the pore-scale, and (iii) investigating the complex interplay between different sub-processes. We base our model on the LBM, which is well suited for solving fluid flow in complex geometries and has been successfully used in the study

of flow in porous media. Furthermore, the kinetic nature of the LBM enables it to conveniently represent microscopic interactions between different fluids, thereby facilitating the automatic tracking of the fluid–fluid interfaces in a multiphase system [27]. The fluid–solid interactions can also be implemented conveniently in the LBM without including additional complex kernels [28]. To the best of our knowledge, there has been no such a pore-scale model reported in the literature. The specific physicochemical problem considered in this study stems from a novel unconventional oil recovery process involving multicomponent multiphase reactive transport with dissolution and precipitations. However, readers with background in PEMFC, micro-reactors, oil recovery, and geological storage of CO_2 and nuclear wastes may find potential applications of this model.

The rest of this paper is organized as follows. In Section 2 the physicochemical problem considered is briefly introduced. In Section 3 the multicomponent multiphase pseudopotential LB model proposed by Shan and Chen and the mass transport LB model are introduced. Then a two-phase multi-mixture model, in which the pseudopotential LB model, the mass transport LB model and a front-tracking method for liquid–solid interface are incorporated, is developed in Section 4. In Section 5, the two-phase multi-mixture model is adopted to simulate the physicochemical problem introduced in Section 2 and investigate the complex interactions between different processes. Finally some conclusions are presented in Section 6.

2. Physicochemical problem

The physicochemical system considered in this study is encountered during the development of a novel unconventional oil recovery technology, whose viability relies heavily on a better understanding of the pore-scale processes. The reactions involved are as follows



Reaction R1 and R3 are homogeneous reactions in the bulk fluid, while the remaining two are heterogeneous reactions at the liquid–solid interface. The physicochemical processes are generalized as follows (shown in Fig. 1). Initially, the system contains an aqueous component $A_{(aq)}$, a gas component $C_{(g)}$ and a primary solid phase $D_{(s)}$. Then due to chemical disequilibrium, $A_{(aq)}$ is

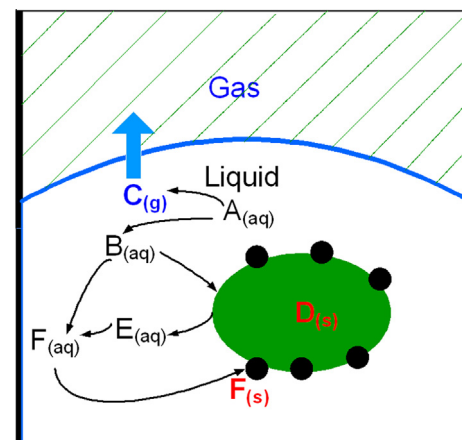


Fig. 1. Schematic of the multicomponent multiphase reactive transport processes.

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