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Effect of medium permeability anisotropy on the morphological evolution of two non-uniformities in a geochemical dissolution system

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SUMMARY

The morphological evolutions of chemical dissolution fronts have attracted increasing interest in the field of the geological sciences and in industrial applications. Extensive research based on numerical simulations has been conducted to understand how various mechanisms and processes influence the morphological evolution of chemical dissolution fronts within geological media. Most researchers in previous studies have assumed the medium permeability to be isotropic for developing numerical models, despite isotropic geological media being uncommon in the real world. This study investigates the effect of medium permeability anisotropy on the morphological evolutions of two non-uniformities with higher permeability in a geochemical dissolution system. A series of numerical simulations are performed to evaluate the effect of medium permeability anisotropy on the morphological evolution of a chemical dissolution front. The simulation results indicate that the patterns of the dissolution reaction front are substantially affected by medium permeability anisotropy. An increase in the permeability anisotropy ratio, which is defined as the ratio of the permeability in the transverse direction to that in the longitudinal direction, enhances the dominance of the flow-focusing effect over the stabilizing or merging effect induced by diffusion/dispersion mechanism. Therefore, an increase in the permeability anisotropy ratio can increase the fingering length of the dissolution front or cause the dissolution front to have a more unstable pattern. By contrast, a reduction in the permeability anisotropy ratio will weaken the flow-focusing effect, thereby reducing the fingering length of the dissolution front or changing the front morphology such that it has a more stable status. The effect of the permeability anisotropy ratio on the morphological evolution tends to decrease when the Zhao number (negative dimensionless upstream pressure gradient) of the system increases. The consideration of medium permeability anisotropy in the geochemical dissolution model renders the simulation of the morphological evolutions of dissolution reaction fronts more realistic.

1. Introduction

When groundwater flows through a geological medium, mass transfer between aqueous and solid phases occurs because of various heterogeneous chemical reactions. Among such heterogeneous chemical reactions, the dissolution and precipitation reactions are the most important; these two reactions cause appreciable mass transfer between solid and aqueous phases, and also alter both the porosity and permeability of the geological medium.

If small non-uniformities with high permeability, which are common in real geological media, exist initially in a real geological medium, groundwater preferentially flows through these high-permeability zones. The increased groundwater flow causes a faster local dissolution, which in turn enhances the porosity and permeability of the zones. Consequently, flow in low-permeability zones is laterally captured to these high-permeability zones, resulting in a flow-focusing effect (Fig. 1). The flow-focusing effect tends to amplify non-uniformities and causes them to develop into unstable fingering reaction fronts. Molecular diffusion/mechanical dispersion resulting from a concentration gradient may inhibit the flow-focusing effect, preventing the unstable fingering reaction front from elongating indefinitely (Chadam et al., 1986; Ortoleva et al., 1987a,b; Zhao et al., 2008a,c; Zhao, 2014).

The morphological evolution of chemical reaction fronts induced by a dissolution reaction was initially investigated by

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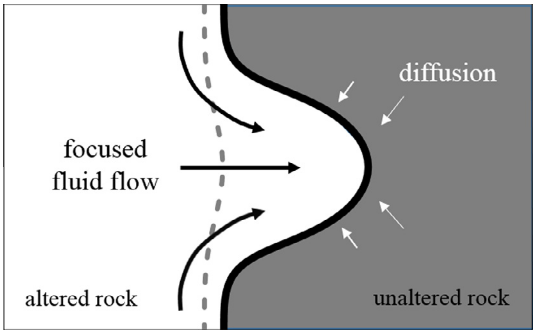

Fig. 1. Competition of flow-focusing mechanism with diffusion. The gray dashed line represents the initial position of chemical dissolution front.

Ortoleva and his coauthors in the late 1980s (Chadam et al., 1986; Ortoleva et al., 1987a,b). Chadam et al. (1986) performed a numerical simulation to demonstrate such a dissolution-induced fingering reaction front phenomenon by numerically solving a set of fully coupled nonlinear governing partial differential equations for groundwater flow, chemical species transport and porosity change induced by mineral dissolution. However, Zhao et al. (2008a) noticed that some governing equations derived by Chadam et al. (1986) were incorrect due to two conceptual mistakes: including (1) the confusion between the average linear velocity and Darcy velocity for a fluid-saturated medium and (2) the neglect of the dissolved mineral shape, and they re-derived the governing equations to correct those errors. After Zhao et al. (2008a) corrected these two conceptual mistakes, they have conducted extensive and pioneering research, both theoretically and numerically, to investigate how several factors such as reactive surfaces of particles (Zhao et al., 2008b), mechanical dispersion (Chen et al., 2009a; Zhao et al., 2010a), mineral dissolution ratios (Zhao et al., 2010b), medium/fluid compressibility (Zhao et al., 2012a,b), the permeability–porosity relationships (Lai et al., 2014) and temperature effect (Zhao et al., 2015a,b) affect the morphological evolution of reaction fronts within geological media in the field of the emerging computational geosciences (Zhao et al., 2009). As a result, the first monograph on this topic was published in the world (Zhao, 2014), indicating that a complete theoretical framework has been established on the chemical dissolution-front instability in porous media. In addition, the relevant numerical simulations have also conducted by others (Chen et al., 1990, 2009b; Ortoleva, 1994; Renard et al., 1998; Chen and Liu, 2002, 2004; Zhao et al., 2013b).

Researchers in previous studies have often assumed the medium permeability to be the same in all direction (i.e., isotropic) for developing numerical models, despite the permeability commonly being anisotropic in real geological media. An anisotropic medium means that the permeability at a point varies in different directions. In general, medium permeability anisotropy is caused in real geological media because of (1) preferential lithological and crystal alignments; (2) irregularly shaped particles; (3) stress-induced effects; (4) aligned cracks; and (5) size, geometry, roughness, and circularity of soil pores. In a sedimentary medium, which comprises several layers with various thicknesses and permeabilities, the equivalent vertical and horizontal permeabilities can be easily computed mathematically if each layer is considered to be individually isotropic and homogeneous (Zhao et al., 2013a). The ratio of equivalent horizontal permeability to equivalent vertical permeability typically ranges from 2 to 10. Therefore, we can theoretically assume that the sedimentary medium is anisotropic. A numerical model that assumes the medium permeability isotropy may not be appropriate for correctly simulating the morphological evolutions of chemical dissolution fronts if medium permeability anisotropy is common in the real world.

More recently, Lai and Chen (2011) and Zhao et al. (2013a) found that medium permeability anisotropy can affect the morphological evolutions of a dissolution pattern. Zhao et al. (2013a) were the first to derive an analytical solution and establish a theoretical criterion for a critical condition, which is used to determine if the chemical dissolution front can become unstable. They also modified their numerical model used in previous studies by considering medium permeability anisotropy to investigate how medium permeability anisotropy affects the morphological development of a planar chemical dissolution front in a two-dimensional fluid-saturated porous medium. Their theoretical and numerical results indicated that a reduction in the medium permeability anisotropy ratio, which is defined as the ratio of the principal permeability in the transverse direction to that in the longitudinal direction (i.e. in the pore-fluid flow direction), can stabilize the chemical dissolution front, implying that it is more difficult for a planar reaction front to evolve into unstable fingering front patterns in a geochemical dissolution system.

Chen and Liu (2004) simulated the interaction of two non-uniformities in a chemical dissolution system and reported that the two non-uniformities developed into a stable planar front, unstable single-fingering front, and unstable double-fingering front at a low Zhao number (which is defined as the minus value of the dimensionless upstream pressure gradient at the entrance of the chemical dissolution system), medium Zhao number, and high Zhao number, respectively. They used primary and secondary critical Zhao numbers to explain the dependence of morphological patterns on the upstream pressure gradient. Note that since the Zhao number is a dimensionaless number, which can be used to represent the three major controlling mechanisms (i.e. pore-fluid flow, mass transport and chemical reactions) simultaneously taking place in a chemical dissolution system (Zhao et al., 2013a), it has a clear physical meaning and therefore can be used to replace the upstream pressure gradient.

Thus, to obtain further insight into the morphological evolution of a dissolution reaction front, we extended the study of Chen and Liu (2004) to investigate how permeability anisotropy of an aquifer influences the temporal development of two non-uniformities in a geochemical dissolution system. The permeability anisotropy was included in the coupled governing equation system for describing the porosity change induced by a dissolution reaction, groundwater flow, and reactive solute transport, and a numerical model was constructed. Subsequently, a series of numerical simulations were performed to illustrate the effects of the permeability anisotropy on the morphological development of the chemical dissolution front. We further demonstrated the physical basis of the development of reactive dissolution fronts subjected to various permeability anisotropy values by quantitatively analyzing the advective, diffusive/dispersive, and the resultant chemical species flux. Crucial conclusions based on simulation results were drawn.

2. Mathematical model

This section presents a brief description of the numerical model that is used to evaluate the impact of the aquifer permeability anisotropy on the morphological evolution of the two non-uniformities. The numerical model is developed on the basis of nonlinear partial differential equations for describing the dynamics of changes in medium porosity in relation to the mineral dissolution reaction, groundwater flow and transport of chemical species in a fluid-saturated porous medium. The underlying assumptions are summarized as follows (Zhao et al., 2008a; Zhao, 2014): (1) a single solid component and a single aqueous chemical species in