# Investigation of the pore heterogeneity effect on reactive transport processes in porous media

張, 雨田

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氏　　名　：Yutian Zhang　ウデン　チョウ

論 文 名：**Investigation of the pore heterogeneity effect on reactive transport processes in porous media**
（多孔質媒体の不均質性が反応性輸送プロセスに与える影響評価）

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# 論 文 内 容 の 要 旨

Reactive transport processes in porous media play a vital role in a wide range of science and engineering applications, including carbon dioxide capture and storage, enhanced oil and gas recovery, fuel cells, and environmental remediation. Heterogeneous reactions (i.e., phase change occurrence) are crucial because the pore geometry and physical properties (e.g., transport properties) of reservoir rock change under mineralization/dissolution conditions. The transport process involving heterogeneous reactions is determined by two dimensionless parameters: Péclet (Pe) and Damköhler (Da) numbers. Pore space heterogeneity also plays an important role in heterogeneous reactive transport processes in porous media. However, the quantitative investigating the role of pore heterogeneity on reactive transport is rarely studied. For exploring the relationship between the pore heterogeneity and the reactive transport process, this study uses a stochastic approach to simulate the process of sedimentary rock growth and generate porous models with different heterogeneity. The lattice Boltzmann (LB) method is adopted to simulate fluid flow and solute transport. Our simulation work successfully models the rock dissolution processes in the heterogeneous porous media. To monitor the dissolution process via electromagnetic monitoring, furthermore, the finite element method is applied to calculate electric current flow in porous media during the dissolution process. This numerical study enables us to understand the effect of pore heterogeneity on dissolution regimes, hydraulic permeability, and electrical conductivity evolution quantitatively.

Chapter 1 describes the research motivation and reviews the importance of studying the reactive transport processes in porous media, major engineering applications at the subsurface, and previous studies relating to the effect of pore space heterogeneity on heterogeneous reactions at the pore scale, existing approaches for quantitatively modeling pore heterogeneity, and the common methods for producing stochastic porous structures in a controllable manner. Furthermore, the major objectives of this thesis and the main numerical methods applied in this study are presented. In addition, a brief structure of this dissertation is presented.

Chapter 2 numerically explores the influence of pore heterogeneity on dissolution patterns and hydraulic permeability evolution under diverse hydrodynamic conditions in a two-dimensional system. A topological invariant (i.e., Euler Characteristic) was first proposed to characterize pore space heterogeneity at dissolution processes on a pore scale. A linear Boolean model is employed to generate porous medias with apparently different Euler characteristics. The lattice Boltzmann method (LBM) with dual particle distribution functions is adopted to compute the fluid flow, solute transport, and interface heterogeneous chemical reactions in complex geometry structures (i.e., porous media).

A more specific classification of dissolution patterns was observed for a wide range of Pe and Da numbers in the three Boolean microstructures. These results indicate that the dissolution patterns are sensitive to pore heterogeneity when both the Pe and Da numbers are high. Further, a novel approach based on statistics was developed to quantitatively identify dissolution regimes. Four normalized porosity¬permeability curve types were observed, and they were strongly related to the dissolution patterns, and rate at which the solid grains disappeared. These permeability evolution types are highly sensitive to pore heterogeneity under high Da conditions. In addition, three zones (i.e., nonlinear, linear, and weak zones) of the effects of pore heterogeneity at the rate of permeability change in terms of Pe and Da were also observed. Further, these results suggest that, in CCS and EOR projects, the dissolution process and permeability evolution can be estimated before the injection of a CO2/acid solution.

Chapter 3 numerically investigates the effect of pore heterogeneity on the transport property evolution of porous rock induced by mineral dissolution in a three-dimensional system. Both topological measurement and statistical analysis are adopted to quantify the pore space complexity; their highly consistent results indicate that both approaches are effective for pore heterogeneity characterization. Different heterogeneous artificial porous rocks are generated by three-dimensional linear Boolean models; their main deviation includes the variance of a solid grain radius size distribution. An extended-LB model that involves an interface chemical reaction boundary is developed to mimic the solute transport and mineral dissolution processes in a 3D porous rock; an LB-BGK (Bhatnager-Gross-Krook) solver was applied to compute the single-phase fluid velocity field in a three-dimensional discrete domain. The finite element method (FEM) combined with a minimum energy approach was employed to simulate the electrical current as well as electrical conductivity in binary porous rocks. Three typical dissolution patterns were reproduced by adjusting the Pe and Da numbers for all 3D microstructures to consider diverse hydrodynamic conditions. Both normalized porosity–permeability and porosity–conductivity relationships are highly sensitive to pore heterogeneity in all mineral dissolution patterns. The largest deviation of the permeability evolution rate in all porous media occur in the wormhole dissolution regime. A novel empirical formula with a quantitative pore heterogeneity influence is proposed to predict the permeability from electrical conductivity data (i.e., formation factor).

This thesis systematically and quantitatively investigates the influence of pore heterogeneity on the dissolution patterns and transport property evolution of porous media. Our results find that the wormhole dissolution patterns are affected by the pore heterogeneity characterized by Euler Characteristic when Pe and Da are high ($\in$ [1,10]). Furthermore, both hydraulic and electrical conductivities evolution on a mineral dissolution condition is affected by pore space heterogeneity, especially to the wormhole dissolution patterns. These results and findings suggest that the Euler Characteristic is an effective descriptor for porous medium heterogeneity in both 2D and 3D systems. The novel permeability–formation factor relationships under mineral dissolution conditions can be applied to formation rocks, which are described by a linear Boolean model. Further, the chemical dissolution reaction is a general one, which indicates that the findings of this study may be applicable to wider applications.