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Doctor thesis outline:

Study of solute transport mechanism in porous media

「多孔質内での溶質分散現象研究 」

In this work, a state-of-the-art column-scale tracer dispersion experimental system is designed with the aid of micro-focused X-ray computer tomography (CT) to investigate the underlining mass transport mechanism. With the real-time imaging technique, the solute transport phenomenon is deciphered in three dimension (3D) for saturated and partially saturated porous media. In parallel, pore-scale lattice Boltzmann simulations were performed to study the fluid flow and solute transport behavior in the digital porous media samples at resolutions of tens of micrometers. The results can be used to illucidate the transport mechanism in porous media from the column to pore scale. The rest of the thesis is organized as follows:

In Chapter 2, we investigated the solute transport mechanism in saturated porous media. With the aid of non-destructive micro-focus X-ray CT, we performed three-dimensional (3D) tracer (NaI) dispersion experiments on unconsolidated packed particle beds saturated with NaCl solvent. The experimental apparatus and procedure will be thoroughly described, followed by image processing and a 3D visualization of the solute plume. Based on the theoretical analysis, the dispersion coefficient will be obtained by Brenner's method of moment[69]. Finally, the *Pe* number (or saturation) dependent dispersion coefficients would be fitted by Sahimi's empirical correlation curves[70] and compared with the up-to-date published results.

In Chapter 3, we studied the solute transport mechanism in partially saturated porous media. The solute transport process was non-destructively visualized under a stablized two-phase flow condition within a 3D packed particle bed by a state-of-art experimental system equipped with micro CT. The steady-state two-phase flow field was achieved by a continuous co-injection of the two-phase fluids: the sodium chloride (NaCl) solvent and pump oil. The co-injected flow was modelled by the Buckley–Leverett theory, such that the designated NaCl saturation S_w could be implicitly determined by the fractional flow rate f_w of the NaCl solvent. The experiment was conducted over a range of the NaCl solvent S_w and *Pe*, which have been varied from 0.09 to 0.44, and from 18.1 to 271.3, respectively. Then, the statistical moments, the dispersion coefficient, the dilution index, and the mean scalar dissipation rate are thoroughly investigated to describe the mixing state. The results can be used to elucidate the solute transport behavior in a two-phase system.

In Chapter 4, we utilized the lattice Boltzmann method (LBM) to simulate the coupled process of single/two-phase flow and the solute transport in 3D digital porous structures reconstructed from CT images. The proposed numerical-scheme is validated against the classic problem of Taylor-Aris dispersion in a pipe flow and the dispersion of a Gaussian plume in a linear shear flow. The down-scale porous medium used for the numerical simulation is a subset of that prepared for the experimental work as stated in in chapter 2 and chapter 3. The resolution for the CT image is about 100 μm, and the total size of the computational domain is in millimetre scale such that the resulting porosity and permeability are matched with the experimental results. The pore-scale simulation results can be used to explain the column-scale experimental results.

In Chapter 5, the significance of the porous medium heterogeneity on the solute transport will be comprehensively studied. One aspect of pore structure heterogeneity lies in the existence of stagnant zones, for example, dead-end pores, recirculation, vortices, and thinfilm layers, which are impermeable for fluid flow. Here, to elucidate the influence of stagnant zones on solute transport behavior, we performed direct computational fluid dynamics simulations on three-dimensional pore scale rock samples obtained from high resolution micro-CT, namely, randomly packed glass beads and four consolidated sandstones with an increasing level of heterogeneity: Fontainebleau, Berea, Takoh, and Shirahama sandstones. A multi-relaxation-time lattice Boltzmann method approach with Flekkøy's mass transfer scheme is employed to simulate the fluid flow and unidirectional miscible solute displacement process at the pore-scale. The justification of Fick's law for describing the solute transport phenomenon is evaluated. For heterogeneous porous media, however, early arrivals and late time tailing effects are observed from the residence time distribution. The dispersion coefficient is calculated using method of time moment, and the scalar dissipation rate is resolved to characterize the mixing state. It indicates convective transport dominates solute transport along the preferential flow path, whereas molecular diffusion plays a critical role in stagnant zones. Finally, on the basis of the local concentration field, the mass transfer coefficient between the mobile zones and stagnant pores was evaluated in terms of Damhöhler number.

Finally, some conclusions and prospects for future research are presented in Chapter 6.