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Imaging and image-based fluid transport modeling at the pore scale in geological materials: A practical introduction to the current state-of-the-art

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ABSTRACT

Fluid flow and mass transport in geological materials are crucial in diverse Earth science applications. To fully understand the behavior of geological materials in this context, the pore scale properties of these materials have to be investigated and related to effective material properties. Imaging techniques are becoming ever more valuable tools to characterize the microstructure (especially in three dimensions), while numerical models to calculate transport properties based on experimental images of the microstructure are quickly maturing. The results of image-based modeling studies depend crucially on both the employed model and the quality of the pore space image on which the model runs. Given the technicality and the cross-disciplinary nature of this matter, this review aims to provide a practical and accessible introduction to both the experimental and numerical state-of-the-art, intended for students and researchers with backgrounds in experimental geo-sciences or computational sciences alike.

Contents

Abbreviations: μ, linear X-ray attenuation coefficient; μXRF, micro-X-ray fluorescence spectroscopy; 2D, two-dimensional; 3D, three-dimensional; A, cross-sectional surface area; BGK, Bhatnagar–Gross–Cook approximation; BIB-SEM, broad ion beam scanning electron microscopy; BSE, backscattered electrons; CDI, coherent diffractive imaging; CFD, computational fluid dynamics; CT, computed tomography; DOHT, distance-ordered homotopic thinning; D-PNM, dual pore network model; EDS or EDX, energy-dispersive (X-ray) spectroscopy; EMP, electron-microprobe; ESRF, European Synchrotron Radiation Facility (France); eV, electron volt; FE-SEM, field-emission scanning electron microscopy; FIB, focussed ion beam; FIB-nt, focussed ion beam nanotomography; FLM, fluorescence light microscopy; G, shape factor; g_{ij}, conductivity from pore i to pore j; *I*, intensity; I_0, incident intensity; IFPEN, Institut Français du pétrol et des énergies nouvelles; keV, kilo electron volt; LB, lattice-Boltzmann; LG, lattice-gas; L_{ij}, distance between pores i and j; Micro-CT, micro-computed tomography; MIP, mercury intrusion porosimetry; MLA, mineral liberation analyzer; MRI, magnetic resonance imaging; MTF, modulation transfer function; P, perimeter length; P_c, capillary pressure; pc-micro-CT, phase contrast micro-CT; PEEK, polyether ether ketone (a type of polymer); P_i, pressure in pore i; Pixel, picture element; PNM, pore network model; PSD, pore size distribution; PSI, Paul Scherrer Institute (Switzerland); QEMSCAN, Quantitative Evaluation of Minerals by SCANning electron microscopy; q_{ij}, flux from pore i to pore j; r, radius; SAXS, small-angle X-ray scattering; SE, secondary electrons; SEI, secondary electron imaging; SEM, scanning electron microscopy; SPH, smoothed particle hydrodynamics; TOMCAT, the beamline for TOmographic Microscopy and Coherent rAdiology experimentTs at the Paul Scherrer Institute; Voxel, volume Element; XRD, X-ray diffraction; XRF, X-ray fluorescence spectroscopy; Z, atomic number; ϑ, contact angle; σ, interfacial tension.

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1. General introduction

Fluid flow and mass transport in geological porous media (e.g. rocks, sediments, soils) are crucial aspects of several important geological applications, e.g. hydrology, petroleum engineering, CO_2-sequestration, sub-surface storage of nuclear waste, geothermal energy generation and building stone performance. To reduce uncertainties related to these systems and to increase their efficiency, accurate predictions of their behavior over time have to be made. This is typically done by running large-scale numerical models (on the order of meters to kilometers), which use constitutive equations to describe the behavior of the geological materials in question. They therefore require the input of effective material properties such as porosity, permeability, and dispersivity, which are characteristic of the geological materials in which the processes take place. These materials are composed of minerals on the one hand and pores or fissures/cracks on the other hand. Properties of the pores and minerals, such as geometry, size, surface area, connectivity and distribution have a strong effect on the material's behavior. The internal microstructure, the chemical composition, and the macroscopic material properties are indeed strongly and directly related to each other. Therefore, understanding why and how the macroscopic features of the materials vary over space and time requires the examination of the material's microstructure. Given the complexity and the heterogeneity of many of these natural porous media, such a deep understanding is crucial, as it is often impossible to acquire and test all the relevant samples at all the relevant conditions (e.g. in the case of kilometer-sized geological reservoirs). Experimental measurements of transport properties in this context are often difficult, expensive and time-consuming, making models at the scale of the material's microstructure (typically termed "pore scale") an attractive tool to supplement direct measurements, to enhance the understanding of a material's behavior, and therefore to help interpolate and extrapolate effective material properties.

The different transport processes to be modeled in this context can be classified as single-component or multi-component flows (i.e. multiple chemical species may be mixed in the same fluid phase); single-phase and multi-phase flows (i.e. multiple immiscible or partially miscible fluids may be present) and non-reactive or reactive flows (i.e. fluids in the pore space may react with each other or with the solid minerals). In nature, these processes often take place simultaneously and may be strongly coupled. The behavior may be driven by several forces, including gravity, capillarity, thermal forces, entropy and applied hydraulic pressure. While the processes and driving forces may differ between different porous media applications (which are not limited to geological