

Geochemical studies with coupled THMCB processes in the context of energy geosciences for carbon neutrality

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Energy geosciences fields in the context of carbon neutrality include geological storage of carbon dioxide and green hydrogen, enhanced geothermal energy utilization, efficient shale oil and gas extraction, as well as high-level nuclear waste geological repository. It involves sandstone, carbonate rock, mudstone, salt rock, granite, basalt and other rocks. Such a geological system involves a wide nm- μ m scale pore size, various pore connectivity and wettability, in addition to the thermal-hydraulic-mechanical-chemical-biological (THMCB) coupled process of deep earth environments. Nano-petrophysics research includes the properties of rocks, fluids (formation water, liquid hydrocarbons, gases like hydrogen, supercritical CO₂), and the interaction between rocks and fluids.

This presentation focuses on the geochemical aspects of THMCB processes, such as diffusion and chemical transport, compounded by the pore structure characteristics (especially low pore connectivity, topological properties of pore structure) of various rocks. A series of complementary methods for quantifying pore connectivity and its effects on geochemical processes is developed, including mercury intrusion porosimetry, nuclear magnetic resonance, X-ray CT, focused ion beam-scanning electron microscopy, (ultra) small-angle neutron and X-ray scattering, hydrophilic and hydrophobic liquids and tracers followed by laser ablation-inductively coupled plasma-mass spectrometry tracer mapping. The tracers contained in brine and n-decane fluids have different molecular sizes and chemical reactivity. For example, two tracers in n-decane fluid have the narrower-sized 1-iododecane (1.393 nm $\times$ 0.287 nm $\times$ 0.178 nm) and wider trichlorooxobis rhenium (1.273 nm $\times$ 0.919 nm $\times$ 0.785 nm), and tracer diffusion into shale of these tracers indicate the limited accessibility (several millimeters from shale sample edge), connectivity, and tortuosity of nanopores in shales.

Some rocks may exhibit poor microscopic scale connectivity and corresponding abnormal diffusion characteristics, which will strongly affect macroscopic fluid flow and chemical transport and the application of various rocks to help achieve carbon neutrality. Through multi-approach experimental and theoretical research, applying a variety of micron-decimeter scale sample sizes and nano-micron scale characterization capabilities, this presentation demonstrates that the diffusion coefficient, adsorption coefficient, and chemical transport mechanism and parameters of geomedia with low pore connectivity can depend on the sample size of various rocks due to pore accessibility, reflecting the macroscopic fluid-medium interaction behavior emerging from the micropore structure mechanism.