

Nanometer to centimeter scale analysis and modeling of pore structures in geologic CO₂ storage formations and caprocks

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The microstructure and evolution of pore space in rocks is a critically important factor controlling fluid flow. The size, distribution and connectivity of these confined geometries dictate how fluids migrate into and through these micro- and nano-environments, wet and react with the solid. (Ultra)small-angle neutron scattering and autocorrelations derived from BSE imaging provide a method of quantifying pore structures in a statistically significant manner from the nanometer to the centimeter scale. These methods were used to characterize the pore features of a variety of potential CO₂ geological storage formations such as the shallow buried quartz arenites from the St. Peter Sandstone and the deeper Mt. Simon quartz arenite in Ohio as well as the Eau Claire shale and mudrocks from the Cranfield MS CO₂ injection test. For example, analyses of experimental and natural samples of St. Peter sandstone show total porosity correlates with changes in pores structure including pore size ratios, surface fractal dimensions, and lacunarity. These new data suggest that microporosity is more prevalent in nominally coarse-grained sandstone and may play a much more important role than previously thought in fluid/rock interactions. The preliminary results from shale and mudrocks indicate there are dramatic differences not only in terms of total micro- to nano-porosity, but also in terms of pore surface fractal (roughness) and mass fractal (pore distributions) dimensions as well as size distributions. Information from imaging and scattering data can also be used to constrain computer-generated, random, three-dimensional porous structures. The results integrate various sources of experimental information and are statistically compatible with the real rock. This allows a more detailed multiscale analysis of structural correlations in the material.

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Iron oxides in copper mining environments: Transformation and reactivity

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The formation, transformation and surface chemistry of iron mineral oxides is of geological significance in surface waters polluted with acid mine drainage (AMD). Geochemical behaviour of these iron oxides controls the availability and mobility of contaminants in these highly polluted systems. The acidic pH values, together with the presence of high amounts of sulphate, will favour the formation of schwertmannite which is a metastable iron oxide that will be transformed to goethite under oxic conditions [1]. However, in copper mining environments co-precipitation of iron and copper ions is expected and therefore the surface chemistry of the iron oxides present in these systems may be different. AMD precipitates have been found to be very effective scavengers of contaminants, although changes in the AMD conditions may result in the release of metals or other contaminants to surface waters.

Several iron oxide samples have been prepared in the presence of high concentrations of sulphate and different copper concentrations in order to simulate copper-rich mining environments. Long-term transformation experiments were conducted in order to study the mineral oxide stability and surface chemical changes produced over a fifteen months period. Schwertmannite particles are found to be formed initially, but throughout the experiment a release of sulphate, iron and copper ions was observed at the more acidic pH values, which lead to the formation of goethite-like particles. Reactivity of the different mineral phases against arsenate shows that the major adsorption capacity is found in the initial schwertmannite-like particles and arsenate mobility increases in the more stable iron mineral phases that are formed during the transformation experiment.

[1] Bingham, Schwertmann, Traina, Winland & Wolf (1996), *Geochim. Cosmochim. Acta* **60**, 2111-2121.