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## Impact of microstructure on anion exclusion in compacted clay media

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### Abstract

The sensitivity of ion concentration distribution models to three key model assumptions, the pore-size distribution of clay media, the distance of closest approach of ions to the clay surface, and the accessibility of sub-nanometer-wide clay mineral interlayer spaces to anions, was explored by solving the Poisson-Boltzmann equation for swelling and non-swelling clay materials. Our calculations show that all three model assumptions significantly impact values predicted for the anion accessible porosity. As a consequence, macroscopic measurements of anion exclusion in clay media cannot be used to test any of the three model assumptions independently of the two others. Information gained at the nanoscale, in particular, a detailed characterization of pore size distribution, is necessary to develop accurate predictive models of the anion accessible porosity of clay media.

**Keywords:** clay, illite, montmorillonite, anion exclusion, Poisson-Boltzmann, microstructure, molecular dynamics.