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Modeling clay micro-structures and computation of their effective diffusion coefficients

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Due to almost zero hydraulic conductivity and high sorption capacity, compacted smectite clays such as bentonite are used as back-fill material in geological waste repositories. In such systems convection due to pressure gradients is negligible and the transport of ions and water takes place by molecular diffusion, which is a rather slow process. Owing to spatial variability and heterogeneity of clays at multiple scales, effective diffusion coefficients for macro-scale transport simulations must consistently be up-scaled from the molecular diffusion coefficient at the pore scale. In this work, we propose a novel technique for modeling clay micro-structures, which is further used for up-scaling molecular diffusion coefficients. Our model clay rock, with a size of the order of a millimeter, is composed of compacted grains of clay minerals. The space between the grain boundaries forms micro-pores. The grains are assumed to be smectites consisting of stacks of basic clay layers and inter-layers, which are aligned (roughly) along the grain's principle axis. To generate such structures, a kinetic Monte carlo method is employed on a grid to obtain closely packed grains of desired shapes, sizes and orientations. The grid nodes are initialized with random indexes; the total number of indexes is a simulation parameter. A grain is defined as a cluster of connected grid nodes having the same index. Each grid node is assigned an energy functional, which decreases, when its neighboring nodes have the same index. At every step, the simulation proceeds by randomly selecting a node and then randomly switching its index. The change is accepted, if the energy of the node decreases. Although simulation results are presented for regular grids, the method is general, and can easily be extended for complex unstructured grids. The resulting packed grains are then used to generate micro-pores between the grains and nano-pores (interlayer space in smectite particles, in this case) within the grains such that the sample has the desired porosity and connectivity. By assigning molecular diffusion coefficients obtained in atomistic simulations to the various types of pore space in the clay structure model we account for pore scale interaction of solvent and solutes with the surface of clay minerals. Finally, a random walk based mesh-less particle method is used to compute effective diffusion coefficients for the whole sample. The main results include the influence of clay micro-structure, with particular emphasis on grain size distribution and anisotropy, on effective diffusion coefficients.