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Anisotropic diffusivity in porous rocks calculated by X-ray computed tomography-based random walk simulations

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Water molecules and contaminants migrate long distances in water-saturated porous strata by diffusion in systems with small Peclet numbers. Natural porous rocks possess the anisotropy for diffusive transport along the percolated pore space. An X-ray Computed Tomography (CT) based approach is presented to characterize anisotropic diffusion in porous rocks. The advantage of this method is that much less time is required to obtain a set of direction-dependent diffusion coefficients compared with the conventional method using diffusion cells and cut samples. High-resolution three-dimensional (3-D) pore images were obtained for a pumice and three sandstones by micro-focus X-ray CT and synchrotron microtomography systems. The cluster-labeling process was applied to each image set to extract the 3-D image of a single percolated pore cluster through which diffusing species can migrate a long distance. The non-sorbing random walk simulation was performed on the percolated pore cluster to obtain the mean-square displacement. The diffusion coefficient along each direction in the 3-D space was calculated by taking the time derivative of the mean-square displacement projected on the corresponding direction. A diffusion ellipsoid with three orthogonal principal axes was obtained for each rock sample. The 3-D two-point autocorrelation of the percolation pore cluster was computed to quantify the geometrical anisotropy of the pore shape; another ellipsoid fitting was applied to the domain with high-autocorrelation values. The autocorrelation ellipsoids were prolate or oblate in shape, presumably depending on the eruption-induced deformation of magma and regional stress during sandstone diagenesis, and the direction of the principal axes of the diffusion ellipsoids correlated well with those of the autocorrelation ellipsoids. This suggests that the anisotropy in the pore shape of the deformed rocks is responsible for the anisotropy in the diffusivity of non-sorbing fluid molecules in porous rocks. In particular, the calculated diffusion coefficients for pumice and Tako sandstone samples showed high anisotropy (the maximum to minimum diffusivity ratio was ~3). For these samples, the shape of the direction-dependent diffusion coefficients was no longer convex ellipsoidal, but rather, constricted in the direction of minimum diffusivity. Systematic calculations of the diffusion ellipsoids for synthetic 3-D rock pore images uniaxially elongated or compressed using an affine transformation suggested that the constriction is not particular to the two samples, but can occur for any rocks when the maximum to minimum diffusivity ratio of the diffusion ellipsoids exceeds ~1.5. This constriction derived from the inherent heterogeneity of porous media (i.e., arrangement of highly anisotropic impermeable solids) cannot be explained by the conventional diffusion tensor approach assuming a homogeneous medium. A new treatment must be developed to quantitatively analyze the diffusion in highly anisotropic porous media for which the conventional convex ellipsoid analysis breaks down phenomenologically.

Reference:

Nakashima, Y., Kamiya, S., and Nakano, T. (2008) Diffusion ellipsoids of anisotropic porous rocks calculated by X-ray computed tomography-based random walk simulations. Water Resources Research (in review).