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Multiscale modeling of porosity, permeability, diffusivity and reactive surface changes during dissolution.

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Meshed models in which equations are solved assuming that constant effective macroscopic properties can be defined in each cells are essential tools for predicting reservoir properties changes triggered by mineral dissolution (or precipitation) due to CO_2 injection. However, the parameterization of the dissolution–precipitation problem and their feedback effects on the flow field are still challenging. The problem arises from the mismatch between the scales at which averaged parameters and parameters relationships (such as the porosity-permeability heuristic relation) are defined and the scale at which chemical reactions occur according to the pore scale fluid concentration and flow heterogeneities and modify the pore network geometry.

Here, we investigate the links between the dissolution mechanisms that control the porosity changes and the related changes of the effective macroscopic value of the reactive surface area, permeability and diffusivity (or diffusional tortuosity) by means of numerical modeling at pore scale. The porous structure (pore space and mineral matrix) is spatially discretized in voxels. It is issued from either numerical generation or from processed X-ray microtomography images. Flow, reactant transport and matrix dissolution is modeled by solving iteratively the Stokes equation with no-slip boundary condition at the rock-pore interface and the advection-diffusion equation using Time Domain Random Walk (TDRW). In the examples presented here, the reaction is a first order kinetic dissolution reaction which allows a simple parameterization of the problem using the average Peclet and the Damkohler numbers characterizing the local diffusion-to-advection and the reaction-to-advection characteristic times. Depending on these parameters that are related to the reactant concentration, the reaction kinetic and the macroscopic pressure drop across the domain, effective relations between the porosity, permeability and diffusivity are obtained, showing a large range of behavior that can be directly compared to those obtained from laboratory scale experiments. The results emphasize the large influence of the initial heterogeneity. In the case of heterogeneous dissolution, i.e. when mass transfer localization occurs and heterogeneity is created by the dissolution itself (for example for high Da values) the effective parameters are scale dependent and cannot be used directly in macroscale models.