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Reactive Transport Modeling in Carbonate Rocks: A Single Pore Model

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Abstract : Calcite is the main mineral found in carbonate rocks, which form significant hydrocarbon reservoirs and subsurface repositories for CO2 sequestration. The injected CO2 mixes with the reservoir fluid and disturbs the geochemical equilibrium, triggering calcite dissolution. Different combinations of fluid chemistry and injection rate may therefore result in different evolution of porosity, permeability and dissolution patterns. To model the changes in porosity and permeability Kozeny-Carman equation K∝□(□)□^n is used, where K is permeability and □ is porosity. The value of n is mostly based on experimental data or pore network models. In pore network models, this derivation is based on accuracy of relation used for conductivity and pore volume change. In fact, at a single pore scale, this relationship is the result of the pore shape development due to dissolution. We have prepared a new reactive transport model for a single pore which simulates the complex chemical reaction of carbonic-acid induced calcite dissolution and subsequent pore-geometry evolution at a single pore scale. We use COMSOL Multiphysics package 5.3 for the simulation. COMSOL utilizes the arbitary-Lagrangian Eulerian (ALE) method for the free-moving domain boundary. We examined the effect of flow rate on the evolution of single pore shape profiles due to calcite dissolution. We used three flow rates to cover diffusion dominated and advection-dominated transport regimes. The fluid in diffusion dominated flow (Pe number 0.037 and 0.37) becomes less reactive along the pore length and thus produced non-uniform pore shapes. However, for the advection-dominated flow (Pe number 3.75), the fast velocity of the fluid keeps the fluid relatively more reactive towards the end of the pore length, thus yielding uniform pore shape. Different pore shapes in terms of inlet opening vs overall pore opening will have an impact on the relation between changing volumes and conductivity. We have related the shape of pore with the Pe number which controls the transport regimes. For every Pe number, we have derived the relation between conductivity and porosity. These relations will be used in the pore network model to get the porosity and permeability variation.

Keywords : single pore, reactive transport, calcite system, moving boundary
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