PORE-SCALE DETERMINATION OF MACROSCOPIC COEFFICIENTS FOR MACROSCALE MODELING OF REACTIVE TRANSPORT FLOW IN POROUS MEDIA

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The geo-sequestration of carbon dioxide is an attractive option to reduce the emission of greenhouse gases. Within carbonate reservoir, acidification of brine in place can occur during CO2 injection. This acidification leads to mineral dissolution which can modify the petrophysical properties of the porous media. Additionally, the macroscopic parameters governing the solute displacement, namely the solute velocity, dispersion and mean reaction rate are strongly controlled by the local mineral reaction and the fluid-flow. Thus, studying the evolution of CO2 propagation during a reservoir storage project is conditioned by the accurate determination of the aforementioned parameters, which are a key input data to reactive flow reservoir simulators.
In order to achieve an accurate, physically based description of mass transfer occurring during the mineral dissolution, the numerical model has to account for the local heterogeneity of the porous media. Many approaches exist to investigate reactive flow through porous media depending on its representation. In a detailed geometry of porous media consisting of void and solid voxels, the local equations describing the reactive transport phenomena are usually resolved in a direct way by random walk, finite difference or lattice Boltzmann numerical methods. However, those approaches are time consuming and a limited pore volume can be addressed. An alternative approach is the pore-scale network modeling (PNM) where the void space of the porous medium is described as a network of nodes (pores) and bonds (throats) with idealized geometry (cylindrical channel with circular, square or triangular cross section). The network can be a three-dimensional regular or irregular lattice structure. The reactive transport flow properties of channels and pores are determined by solving analytically the macroscopic transport equation, assuming an asymptotic behaviour of the concentration. The results are incorporated in the network to compute the effective properties at the core scale. As the approach solves the physics of reactive transport in non-detailed way and uses a simplified representation of the pore structure, it can be used to describe the physical situation for a wide range of pores (several thousands of pores) with affordable computational resources.
The objective of this work is firstly to validate the ability of the PNM approach to model the reactive transport flow in porous media. The assumption of an asymptotic evolution of the concentration at pore level is established from locale and macroscopic equations by solving the time dependency of the concentration by a numerical scheme based on a finite difference formulation. Secondly, two-case studies depending on the way of building the pore network of the considered carbonate sample (well core data) are subjected to reactive flow. In one case, the representative network is constructed by regular lattice of pores connected by throats that reproduce the basic petrophysical properties of the sample. In the other case, the network is built from actual 3D images of rocks captured by the Computed Micro Tomography (CMT) facility.
The mean solute velocity, dispersion and reactive apparent coefficient are presented and discussed for both networks. Their dependency to the pore structure, fluid flow and the surface reaction is brought into light. It is observed that those coefficients can vary up to one order of magnitude

compared to the ones of non surface reactive flow. For instance, when kinetics is limited by mass transport (fast reaction compared to the transport characteristic time), a low flow rate leads to a greater chemical disequilibrium in pore-body than in pore-throat and a fast flow rate leads to a repartition of disequilibrium over the porous media flow paths. In the latter case, the solute velocity can be significantly higher than that of the flow. Finally, a sensitivity study on reactive and flow regimes has been conducted in terms of dimensionless number.