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Geostatistical analysis of 3D microCT images of porous media for stochastic upscaling of spatially variable reactive surfaces

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The 3D imaging of porous media through micro tomography allows the characterization of porous space and mineral abundances with unprecedented resolution. Such images can be used to perform computational determination of permeability and to obtain a realistic measure of the mineral surfaces exposed to fluid flow and thus to chemical interactions. However, the volume of the plugs that can be analysed with such detail is in the order of 1 cm^3, so that their representativity at a larger scale, i.e. as needed for reactive transport modelling at Darcy scale, is questionable at best. In fact, the fine scale heterogeneity (from plug to plug at few cm distance within the same core) would originate substantially different readings of the investigated properties. Therefore, a comprehensive approach including the spatial variability and heterogeneity at the micro- and plug scale needs to be adopted to gain full advantage from the high resolution images in view of the upscaling to Darcy scale.

In the framework of the collaborative project H2STORE, micro-CT imaging of different core samples from potential H_2-storage sites has been performed by partners at TU Clausthal and Jena University before and after treatment with H_2/CO_2 mixtures in pressurized autoclaves.

We present here the workflow which has been implemented to extract the relevant features from the available data concerning the heterogeneity of the medium at the microscopic and plug scale and to correlate the observed chemical reactions and changes in the porous structure with the geometrical features of the medium.

First, a multivariate indicator-based geostatistical model for the microscopic structure of the plugs has been built and fitted to the available images. This involved the implementation of exploratory analysis algorithms such as experimental indicator variograms and cross-variograms. The implemented methods are able to efficiently deal with images in the order of 1000^3 voxels making use of parallelization. Sequential Indicator Simulations are then employed to generate equi-probable realizations of microscopic structures with varying mineral proportions and porosity but constrained to the spatial variability observed in the plugs. The statistics computed on the ensemble of realizations (essentially the distribution of mineral reactive surfaces exposed to porous space) is integrated at a larger, Darcy scale. In a further step, the analysis of the microscopic changes in the plugs after exposure to reactive solution establishes the correlations betweens amount of chemical reactions and changes in the spatial models, thus deriving some effective correlations which can be injected into the reactive transport modelling.

In this contribution, we demonstrate the implemented workflow on a series of images obtained from plugs from a german depleted gas field exposed to H_2 and CO_2-charged brines. The geostatistical evaluation of microscale variability of the porous media contributes to the upscaling of relevant variables and helps estimating - if not reducing - the uncertainty due to the heterogeneity across scales of the natural systems.