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A numerical modeling approach to assess the impact of heterogeneity on bioavailability and total biodegradation

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Natural porous media like soils and aquifers are characterized by heterogeneities at various scales. While macro-scale heterogeneities can be resolved by REV-based models of the subsurface, heterogeneities at the scale of pore assemblies can not be resolved by such model approaches. As a consequence effective reaction rates used e.g. to describe the biodegradation of contaminants might be a function of such pore-scale heterogeneities. However, it is not known to which extent these heterogeneneities affect the bioavailability of chemical species to the microorganisms and thus the total biodegradation rates. The specific objective of this project is to assess and model these bioavailability effects and their impact on total contaminant biodegradation in porous media resulting from structural heterogeneity at the pore scale. By using a numerical modeling approach it is the aim to obtain a better and quantitative understanding of the bioavailability of biodegradable compounds in porous media, and to derive a quantitative link between pore scale heterogeneity of the medium and effective biodegradation rates.

Therefore, a reactive transport model for two-dimensional, water-saturated pore networks has been developed. The model is capable of simulating water flow, solute transport and biogeochemical reactions in pore structures of different heterogeneities. The intra pore bioavailability is defined by a linear exchange model making use of recent results from theoretical analyses of single pore systems. The bioavailability of biodegradable species and their effective degradation rates at the scale of pore networks is assessed for various spatially heterogeneous pore network realizations following a given pore size distribution and geo-statistical spatial correlation function.

Simulation results for homogeneous networks are in agreement with continuum scale modeling results considering the same intra pore bioavailability. For heterogeneous pore networks, simulation results indicate a decrease of bioavailability/effective biodegradation rates with increasing heterogeneity of the pore structure. This may lead towards finding effective rate laws for biodegradation as a function of the heterogeneity of a porous medium.

Keywords: *biodegradation, pore network, reactive transport models, bioavailability, pore-scale heterogeneity*