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Application of a flexible lattice Boltzmann method based simulation tool for modelling physico-chemical processes at different scales

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Often, especially in the disciplines related to natural porous media, such as for example vadoze zone or aquifer hydrology or contaminant transport, the relevant spatial and temporal scales on which we need to provide information is larger than the scale where the processes actually occur. Usual techniques used to deal with these problems assume the existence of a REV. However, in order to understand the behavior on larger scales it is important to downscale the problem onto the relevant scale of the processes. Due to the limitations of resources (time, memory) the downscaling can only be made up to the certain lower scale. At this lower scale still several scales may co-exist – the scale which can be explicitly described and a scale which needs to be conceptualized by effective properties.

Hence, models which are supposed to provide effective properties on relevant scales should therefor be flexible enough to represent complex pore-structure by explicit geometry on one side, and differently defined processes (e.g. by the effective properties) which emerge on lower scale.

In this work we present the state-of-the-art lattice Boltzmann method based simulation tool applicable to advection-diffusion equation coupled to geochemical processes. The lattice Boltzmann transport solver can be coupled with an external geochemical solver which allows to account for a wide range of geochemical reaction networks through thermodynamic databases. The applicability to multiphase systems is ongoing.

We provide several examples related to the calculation of an effective diffusion properties, permeability and effective reaction rate based on a continuum scale based on the pore scale geometry.