Reactive transport upscaling of small reactive heterogeneities for regional modelling

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Abstract Sedimentary deposits often contain small heterogeneities in the form of intercalated lenses. These elements can affect both the transport of species and the biogeochemical reactions that the transported species undergo. The particular geometry of these frequently clayey lenses, extremely thin in comparison with the large lateral dimensions, would require very fine gridded models in order to accurately model the transport and reaction processes taking place. Therefore, the simulations would require a very large computational effort. On top, an exhaustive description of the sedimentary deposits would be necessary to accurately describe the physicochemical properties of these porous media. We develop a practical approach to infer the global effect of the small lens-shaped heterogeneities for the transport and reaction of species without having to model these features in detail. In particular, our goal is to characterize the effect of the small heterogeneities on reactive transport at a regional scale. We develop an upscale algorithm to reproduce the breakthrough curves of a model with local small scale heterogeneities by using an equivalent homogenous model, hereby relating the upscaling mechanism with the statistical properties of the field.

Key words groundwater; modelling; heterogeneity; reactivity upscaling; regional reactive transport model