Upscaling multi-component reactive transport using multi-rate mass transfer

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Heterogeneity in hydraulic conductivity leads to incomplete mixing. Upscaling using the dispersion tensor in the advection-dispersion equation overestimates mixing. Modelling multi-component reactive transport using upscaled dispersion we overestimate reaction rates and overall reactions. Multi-rate mass transfer was shown previously to better represent mixing. But it is still unclear under what conditions.

We compare here explicit multi-component transport in heterogeneous aquifers for the example of calcite-dissolution. We compare different types of heterogeneity from intermediatly well connected (multigaussian) fields to very well connected fields. The fundamental difference stems from their connectivity structure. We observe for the well connected field different dominating channels with an almost uniform advective velocity while the multigaussian fields show dominating channels with a varying advective velocity. Then, we compare our results with an effective reactive mass transfer model where the distribution of exchanges rates or the memory function are derived from information of the hydraulic conductivity field only.

We see that reactive multi-rate models show a good agreement for the well connected fields where the connected channels are more or less homogeneous and the immobile inclusions are of more or less equal size. In these types of fields a reactive mass transfer model describes well the mixing in the heterogeneous aquifer and predicts well reaction rates and overall reactions. For the multigaussian fields the results are less good. We conclude that heterogeneity within the more connected channels, as well as the different overall advective time of the individual channels lead to a bad prediction of mixing and reaction-rate for these fields. We conclude that a more complex model allowing for different adevection time should be used to properly upscale multi-component reactive transport in such an aquifer.