Geophysical Research Abstracts
Vol. 18, EGU2016-13757, 2016
EGU General Assembly 2016

Analysis of sequential reactive transformations using stable isotope analysis: a theoretical assessment

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Stable isotope methods have been establish as powerful tools for the analysis of reactive transformation in the subsurface with applications ranging from the field of contaminant hydrology to biogeochemical cycling. While the link between single transformations based on stable isotope signatures and their changes is commonly well understood and allows for qualitative and – in case certain requirements are met – also quantitative analysis, the interpretation of sequential reactive transformations, e.g. decay chains, is more complicated. In the latter case isotope signature changes of individual reactive compounds are affected by more than one transformation which challenges the interpretation of these changes.

In recent years, some methods have been proposed (e.g. isotope mass balance approaches) which allow at least for a qualitative or semi-quantitative estimation of sequential reactive transformation processes. However, a systematic assessment of the validity of these estimation methods is missing so far and the accuracy of these methods – in general and for specific conditions encountered in the field – is not fully validated. In this presentation we use a combination of mathematical analyses and numerical modeling to test the validity of the proposed estimation methods and to determine the limits of their applicability. Results recommend modifications of existing theoretical estimation approaches and identify sorption processes as potential limitation of their applicability.