Geophysical Research Abstracts
Vol. 15, EGU2013-5542, 2013
EGU General Assembly 2013

Modeling the impact of pore-scale mass transfer on microbially-induced isotope fractionation.

Falk Hesse (1), Vladislav Prykhodko (1,3), Sabine Attinger (1,2), and Martin Thullner (1)

(1) Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany, (2) Institute of Geoscience, University of Jena - FSU, Jena, Germany, (3) Faculty of Computer Science, Mathematics and Natural Sciences, Leipzig University of Applied Sciences, Leipzig, Germany

Compound Specific Stable Isotope Analysis (CSIA) has become an established tool for monitoring biodegradation employed as a clean-up strategy at a polluted site. A necessary prerequisite for a successful application of CSIA is the knowledge of the fractionation factor, which furthermore must be constant under the conditions prevailing at the site. Recent studies have shown that these conditions are not always met, especially if mass-transfer limitations affect the biodegradation process.

In case of biodegradation rates, the impact of mass-transfer on different scales – including the pore scale – has already been demonstrated. In this study we therefore investigate if pore-scale mass transfer may similarly affect the observed fractionation factor and if a quantitative assessment of this impact is feasible. For this purpose we use high-resolution numerical simulations of biodegradation and the associated stable isotope fractionation in a simple pore geometry. Obtained concentrations and stable isotope signatures are then interpreted by the well-known Rayleigh model in order to derive the observed isotope fractionation factors affected by pore-scale mass transfer. These numerically derived fractionation factors are compared to an analytical approach previously reported in the literature, which uses a linear-exchange model to explicitly account for the mass transfer.

Our results show that this analytical approach provides a good prediction of the observed fractionation factor even in cases where pore-scale mass transfer strongly affected the results. We could furthermore derive a constant estimate for the unknown mass-transfer coefficient. This overall agreement between the numerical and analytical results was tested and confirmed for broad parameter intervals showing the robustness and applicability of the formula. Furthermore, we describe a scenario, where, in addition to microbially-induced isotope fractionation, the mass transfer was fractionating as well. Finally, we discuss the potential of our approach to use the observed isotope fractionation factor as a predictor of the relevance of mass-transfer for effective biodegradation rates and possible other phenomena.