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Thermo kinetic modeling of microbially mediated redox reactions using batch experiments mixing soil and a treated sewage effluent

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Understanding the fate of metals and pollutants in soils and aquifers is of primary importance to insure and preserve the good quality of groundwater resources. Water quality changes are mostly related to microbial activities and redox conditions, and appropriate models which account for such processes are needed. This study uses experimental data to evaluate the potentiality of thermodynamic consistent kinetic rate laws and relevant thermodynamic database to simulate microbially catalyzed redox reactions.

A thermo-kinetic bio-geochemical modeling derived from Jin and Bethke's approach (2007) is implemented in the geochemical code Phreeqc v2.16 (Parkhurst and Appelo, 1999). It involves kinetic rate laws to study microbially mediated redox reactions and uses a modified version of the thermodynamic database Thermoddem (Blanc et al. 2009) where redox species are decoupled to prevent from fast chemical re-oxidation or reduction resulting from reaching equilibrium conditions that would not be realistic (Lindberg and Runnels 1984). Such approach allows maintaining redox disequilibrium in the aqueous system while a thermodynamic term is added in the kinetic rate laws to guaranty the consistency with thermodynamic considerations.

This modeling approach is constrained by experimental data from batch incubations mixing extracts of a Soil Aquifer Treatment (SAT) system with a treated sewage effluent under anoxic conditions. Batch solution is sampled weekly for the measurements of anions and cations by ion chromatography, of pH, Eh, T, dissolved O2 concentration, of dissolved inorganic and organic carbon contents, and of microbial counts of active population using the most probable number method for the denitrifying, manganic-, iron-, and sulfate- reductive communities.

Analytical results illustrate the succession of microbial activities usually proposed under anoxic conditions: denitrification, manganese, iron and sulfate reduction. Additionally, they reveal significant mobilization of manganese, up to 8.5 mg/L, while chemical compositions and changes in color of the incubated solutions highlight the occurrence of precipitation/dissolution reactions of metal minerals.

Modeling results reproduce well the experimental data, the redox disequilibrium and the succession of electron acceptors observed during the incubation. Simulated reductive dissolution of Mn-oxides and Fe-oxides, combined with precipitation of secondary minerals, including iron sulfides and carbonates, are in good agreement with the observations. The modeling approach and derived kinetic parameters will then be applied to simulate field-scale SAT system infiltrated with treated sewage effluent.

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References:
Blanc P., Lassin A., Piantone P. 2009. Thermoddem, a thermodynamic database for modelling the alteration of waste minerals, http://thermoddem.brgm.fr/.
Jin, Q., Bethke, C.M., 2007. The thermodynamics and kinetics of microbial metabolism. Am. J. Sc. 307, 643-677.
Lindberg R.D. and Runnels M.D. 1984. Ground water redox reactions: an analysis of equilibrium state applied to Eh measurements and geochemical modelling. Science. Vol. 225, 925-927.

Parkhurst, D.L., Appelo C.A.J., 1999. User's guide to PHREEQC (version 2): A computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations. U.S. Geological Survey Water-Resources Investigations Report 99-4259, 312 p.