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Application of the rhizosphere model RhizoMath for modelling the reactive transport of arsenic in the rhizosphere

K. Szegedi (1,3), D. Vetterlein (1,3), H.-U. Neue (2) and R. Jahn (3)

(1) Helmholtz Centre for Environmental Research - UFZ, Department of Soil Physics and (2) Department of Soil Chemistry, Halle (Saale), Germany, (3) Institute of Soil Science and Plant Nutrition, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany (krisztian.szegedi@ufz.de)

The transfer of nutrients and contaminants from bulk soil to roots and into plants depends on many plant and soil processes. The RhizoMath approach for modelling co-occurring processes in the rhizosphere, including speciation in the soil solution, is based on coupling the mathematical package MATLAB with the geochemical code PHREEQC. RhizoMath has a built-in initialization module that performs calibration against experimental data. Its greatest advantage is that different geochemical models (with and without charge balance) and geometries (planar and radial) are already included (Nye and Marriott, 1969; Nietfeld, 2001). Moreover, due to its graphical user interface the tool can be applied without changing the source code or a complex input file.

A compartment system experiment was conducted as this setup enables the collection of soil solution with increasing distance from the root surface and with time (Vetterlein & Jahn, 2004). Nine compartment systems were set up with application of goethite in increasing amounts to an artificial quartz substrate spiked with known amounts of nutrients and arsenate as described in Vetterlein et al. (2007) and planted with corn (*Zea Mays*), one plant per pot. Soil matric potential was continuously measured by microtensiometers with increasing distance from the centre of the root compartment. Soil solution samples were collected with micro suction cups assembled according to

Göttlein et al. (1996) and installed horizontally with a spatial resolution of 6 mm. The weight of the compartment system and the sand bed was continuously registered in order to determine the evapotranspiration rate.

The initialization module of RhizoMath was used to determine the number of surface binding sites and values of the equilibrium constants of corresponding stoichiometric equations describing the surface complexation of As(V) on goethite at the beginning of compartment system experiments reported by Vetterlein et al. (2007). Concentration values derived from soil solution samples of compartment systems without goethite were used as initial values for systems containing 1 or 4 g kg^{-1} goethite. Equilibrium phases were defined according to saturation indices. The applied minteq.dat database was modified to exclude nitrification and extended with the sorption of carbonate according to Appelo et al. (2002). Initial numbers (e.g., starting values for the optimization) of weak and strong surface binding sites of hydrous ferric oxide were estimated according to Tretner (2002). Initial values of the equilibrium constants of the surface binding reactions were taken from Dzombak and Morel (1990). The optimized parameter set enabled PHREEQC to describe the initial soil solution composition of the compartment system experiments with 1 and 4 g kg^{-1} goethite.

Compartment system experiments, involving more complex speciation, were modelled using the transport module of RhizoMath. Values of sorption parameters were determined with the initialization module. The model was able to qualitatively describe the effects observed after two weeks of citrate exudates on the simultaneous transport of arsenate and phosphate that compete for surface binding sites with each other and with other oxyanions such as citrate. A better quantitative agreement between modelled and experimental results required a further refinement of the transport module such as including interactions among nutrients and contaminants during root uptake (competition for transport proteins) and a more sophisticated plant growth model.

Szegedi et al. 2008. The New Tool RhizoMath for Modeling Coupled Transport and Speciation in the Rhizosphere, Vadose Zone Journal, Special Issue “Vadose Zone Modeling”, *In press*

Vetterlein et al. 2007. Competitive mobilisation of phosphate and arsenate associated with goethite by root activity. Journal of Environmental Quality 36, 1811-1820.

Other citations are available in the two references above.