Geophysical Research Abstracts
Vol. 12, EGU2010-4502, 2010
EGU General Assembly 2010

Modelling chemical and biological reactions during unsaturated flow in silty arable soils

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Ion dynamics in arable soils are strongly affected by the chemical and biological transformations triggered by fertilizer input. Hydrogeochemical models may improve our understanding of underlying processes. Our objective was to test the ability of the hydrogeochemical model PHREEQC2 in combination with the parameter optimization programme PEST to describe and predict chemical and biological processes in silty soils triggered by fertilizer application or acidification and to investigate the usefulness of different parameterization approaches. Three different experiments were carried out using undisturbed columns of two topsoils (0-25 cm) from Germany (Göttingen, GO) and from the Oman (Qasha', QA). The columns were irrigated at 10 oC with 3 mm day-1 for one year using 1 mM HCl (HCl experiment) and two fertilizer solutions with low (0.1 to 0.9 mmol L-1) and high concentrations (1.3 to 14.7 mmol L-1) of N (as NH4NO3), K, Ca and Mg. In the fertilization experiments (Fert1, Fert2), the columns were alternately irrigated with the two different solutions for variable time periods. One-dimensional transport and homogenous and heterogenous reactions were calculated using PHREEQC2. The Fert1 experiment was used for calibration. The models were validated using the Fert2 and HCl experiments. The models tested were model variant m1 with no adjustable parameters, model variant m2 in which nitrate concentrations in input solutions and cation exchange capacity were optimized for Fert1, and m3 in which additionally all cation exchange coefficients and ion concentrations in the initial solution were optimized. Model variant m1 failed to predict the concentrations of several cations for both soils (modelling efficiencies (EF) ≤ 0), since N dynamics were not considered adequately. Model variants m2 and m3 described (Fert1 treatment) and predicted (Fert2 and HCl treatment) pH, cation and NO3- concentrations generally more accurately for both soils. For nutrient cations, EF values for prediction for GO ranged from 0.44 (K) to 0.99 (Ca), for QA from 0.21 (K) to 0.96 (Ca). After optimization, PHREEQC2 was able to predict NO3- concentrations in both soils (EF ≥ 0.57). Model variant m3 indicated that between 54 (QA) and 72 % (GO) of the exchange sites were involved in cation exchange reactions. Our results show the importance of the inclusion of nitrogen species when modelling cation dynamics in arable soils from different climate regions. The hydrogeochemical model PHREEQC2 in combination with PEST was useful to describe and predict ion dynamics in silty soils under unsaturated conditions.