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Gas Transport and Mass Transfer within the vadose Zone: Tracer Experiments, 1-D analytical and 2-D numerical Modeling

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Based on the working hypothesis that **small-scale heterogeneity** of the hydraulic conductivity determines flow and transport of the near-surface groundwater and that this heterogeneous boundary condition could be the **"driver" for the high variability of the soil gas and emission pattern,** a test site was equipped in the Fuhrberger Feld (scale 6.5m$\times$2.5m, 20 groundwater sampling wells, 5m under ground surface (GS); approx. 30 soil air sampling points in 3 horizons, 30, 60, 90 cm under GS) and characterized with standard methods. The pedotransfer-functions, precipitation, water table fluctuation, depth-dependent dissolved gases (N_2O, O_2, CO_2, CH_4) and the corresponding soil gases were measured over a one-year period [1].

For transient modeling, i.e. under transient boundary conditions (measured groundwater fluctuations, dissolved N_2O-distribution), the geochemical complex-model MIN3P (*Richards* equation, saturation dependent diffusion [2]) was used. The small-scale heterogeneous permeability- and tortuosity fields were produced using conditional *Gaussian* simulation. The data base consists of geological profiles, EC-Logs, sieve curve analyses, small-scale pumping tests and injection-Logs.

In this paper we present 1D- and 2D-simulations of gas transport through the unsaturated zone (0.5 – 1.5m under GS). For realistic model predictions in-situ measurements of effective diffusion coefficients are a necessary requirement. We carried out a series of combined SF_6-N_2O-tracer tests at the field site. This combination has the main advantage that SF_6 behaves like a conservative tracer (H_{SF6}= 108) , whereas N_2O behaves like a tracer with equal partitioning (H_{N2O}= 1.1). For parameter estimation the Marquardt-Levenberg-algorithm (Mathematica 6.0) was used. As fit function we use the finite-size solution (i.e. the initial gas concentration is concentrated within a sphere of a radius R) with R and D_{eff} as fit parameters. For the SF_6-breakthrough curves at depths of 0.3 and 0.6m (injection point 0.9 m under GS) we found excellent agreement. In contrast we found significant deviations between the experimental and theoretical retardation coefficient ($R_{exp} < R_{theor}$) for the N_2O-breakthrough curves (only the retardation coefficient was used as fit parameter). These experimental results raise the question: Under which physical conditions the local equilibrium approach (LEA) is appropriate? This is of central importance, since all present standard models – like MIN3P, HYDRUS, STOMP, TOUGH2 – use LEA for describing the mass transfer between the gaseous and aqueous phase. It is well-known that the main critical point concerning LEA is that the instantaneous mass transfer overestimates the effective water phase diffusive transport, especially, if there are hydraulic barries with complete water saturation, and therefore LEA can cause an unphysical “smoothing” of local gas concentration pattern, usually observed at the test site.

We propose an exact 1D-analytical solution of a kinetic, two-phase model that describes the mass transfer between a gas phase and an immobile water phase (spherical water saturated aggregates). The model takes into account both gas phase diffusion and convection. This solution is an inverse solution of the kinetic model given in [3]. At the conference we present the results of a sensitivity analysis and answer the question: Under which physical conditions LEA holds? Based on this we critically discuss our 2D-simulations of gas transport and gas emission at the Fuhrberg test site.

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