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Modeling the oxygen mass transfer across the capillary fringe using a multiphase reactive transport code - numerical model construction and comparison with experimental data

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In the groundwater, the degradation kinetics of organic contaminants is highly dependent on the supply of electron donors and acceptors that are accessible to the microorganism. Aerobic metabolism, where dissolved oxygen is used as electron acceptor, yields the highest degradation rate. Therefore, investigating the reactive transport of oxygen over the capillary fringe is of vital importance to the understanding of oxygen supply for the groundwater remediation processes.

Recently, Haberer et al. (2010) have conducted a series of experiments. A quasi 2-D flow-through chamber, filled with glass beads, was set up and continuously flushed with oxygen-depleted groundwater from left to right. Groundwater gradient slowly developed and steady state was reached with a capillary fringe developed on top of the groundwater table. Oxygen was only allowed to enter the tank from the top, diffusing through the capillary fringe. The oxygen profile across the capillary fringe (i.e. both in the gas and aqueous phase and at the interface) was monitored using the optode technology. A good dataset is then available for the calibration and validation of multiphase reactive transport models.

In this context, the numerical modeling software OpenGeoSys (OGS) is further extended to simulate the above experiment. At each time step, the two-phase flow governing equations were first solved by the finite element method, producing the profile of gas and capillary pressures. Based on the calculation of Darcy velocities, mass transport equations were solved for each chemical component, i.e. the sum of oxygen concentrations both in the aqueous and gas phase is calculated. The results were further passed to the Biogeochemical Reaction Network Simulator (BRNS), which simulates the chemical reactions in the aqueous phase based on each node.

The simulated oxygen profile is compared against the measurement data. Both results show that the transport of oxygen over the groundwater table is controlled by transverse vertical dispersion in the aqueous phase, which is 3∼4 magnitudes lower than the value of pore diffusion in the gas phase. In general, the coupled code OGS-BRNS can reproduce the reaction of oxygen in the aqueous phase. However, the simulated OGS results tend to make an over-estimation of oxygen concentration around the capillary fringe. Analysis shows this behavior is mainly due to the quick change of saturation values at the groundwater table, which leads to a very high gradient and causes trouble for the numerical code.

Further strategies to improve the numerical model include using a smooth capillary fringe model to alleviate the numerical difficulties, or building component transport equations directly into two-phase flow equations and solve them monolithically. These works are currently underway.

Christina M. Haberer, Massimo Rolle, Sanheng Liu, Olaf A. Cirpka, Peter Grathwohl, 2010, A high-resolution non-invasive approach to quantify oxygen transport across the capillary fringe and within the underlying groundwater, Journal of Contaminant Hydrology, DOI: 10.1016/j.jconhyd.2010.10.006.