# Simulation of Multiphase Multicomponent Reactive Flow in the Capillary Fringe

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**Abstract:** The capillary fringe(CF) is the zone immediately above the water table where the water content remains at or close to saturation. In recent years, considerable effort has been undertaken to deepen the understanding of the CF and how it may influence mass transfer between the vadose and the saturated zone. Component transport across the CF is relevant for many geochemical and microbial processes. We developed a numerical simulator for multiphase multicomponent flow in porous media including phase exchange and chemical reactions as required for understanding the dynamic behavior of the CF.

Many simulators for reactive multiphase flow use a global implicit approach with full upwinding of convective terms. A full implicit scheme produces numerical dispersion in the component transport which results in an overestimation of reaction rates. In order to reduce the numerical dispersion and to prevent the overestimation of the phase exchange and the reaction, we have chosen a splitting approach. Operator splitting allows us to discretize each operator with different numerical method and therefore a large amount of numerical diffusion for the component transport can be reduced using higher order methods.

The balance equations are reformulated into a multiphase flow part, a component transport part and a reaction part such that operator splitting techniques can be applied. The multiphase flow part is discretized with cell-centered finite volumes method in space and fully-implicit fully-coupled in time. The transport part is treated with explicit higher order finite-volume methods in order to minimize numerical dispersion while the reaction part can be treated with standard ODE solvers. Nonlinear equations are solved by a Newton-Algebraic Multigrid algorithm. Parallel simulation techniques are applied to the coupled problem.

Results from two-dimensional and three-dimensional simulations in the CF are presented. Various simulations show the capability of the developed model to incorporate phase disappearance and to reduce numerical diffusion in the transport part.

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