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Numerical and experimental investigation of breakthrough features appearing in closed-flow transport experiments

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The investigation of solute transport with column outflow experiments can be carried out in a closed flow mode by recirculation of effluent solution to the solution supply vessel that feeds the column inflow. While the experimental effort is rather similar to standard column outflow approaches, the closed-flow mode allows to study physicochemical equilibration directly. Under defined boundary conditions, i.e. low volume of the solution supply vessel, the breakthrough furthermore exhibits an oscillation of concentration in the effluent and the solution supply vessel. Since each oscillation represents one cycling of tracer solution through the porous medium, interaction processes imprint on the whole data range of the breakthrough. As a consequence, the breakthrough shows additional characteristic and indicative features that permit further interpretation of involved processes and gives intrinsic control over boundary conditions. This reduces uncertainty of parameter fitting by generating smaller confidence intervals and elimination of indeterminacies/equifinality.

A numerical simulation of closed flow experiments is based on the coupling of a transport equation with the partial differential equation that describes the course of concentration in the solution supply vessel. This is especially interesting since the column influent is short-circuited to the effluent via the mixing process in the solution supply vessel, resulting in a dynamic boundary at the column inflow.

We present ways of implementation in an explicit and implicit euler scheme. Furthermore, we conducted a set of experiments to verify this numerical model. We show that a single tracer breakthrough can be used to determine the dispersion, the exact applied pumping rate and, depending on the tracer, the water content or the retardation.