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A new numerical benchmark for variably saturated variable-density flow and transport in porous media

Carlos Guevara and Thomas Graf

Leibniz Universität Hannover, Instituts für Strömungsmechanik und Umweltphysik im Bauwesen, Hannover, Germany (guevara@hydromech.uni-hannover.de)

In subsurface hydrological systems, spatial and temporal variations in solute concentration and/or temperature may affect fluid density and viscosity. These variations could lead to potentially unstable situations, in which a dense fluid overlies a less dense fluid. These situations could produce instabilities that appear as dense plume fingers migrating downwards counteracted by vertical upwards flow of freshwater (Simmons et al., Transp. Porous Medium, 2002). As a result of unstable variable-density flow, solute transport rates are increased over large distances and times as compared to constant-density flow. The numerical simulation of variable-density flow in saturated and unsaturated media requires corresponding benchmark problems against which a computer model is validated (Diersch and Kolditz, Adv. Water Resour, 2002).

Recorded data from a laboratory-scale experiment of variable-density flow and solute transport in saturated and unsaturated porous media (Simmons et al., Transp. Porous Medium, 2002) is used to define a new numerical benchmark. The HydroGeoSphere code (Therrien et al., 2004) coupled with PEST (www.pesthomepage.org) are used to obtain an optimized parameter set capable of adequately representing the data set by Simmons et al., (2002). Fingering in the numerical model is triggered using random hydraulic conductivity fields. Due to the inherent randomness, a large number of simulations were conducted in this study. The optimized benchmark model adequately predicts the plume behavior and the fate of solutes. This benchmark is useful for model verification of variable-density flow problems in saturated and/or unsaturated media.