Solution of direct and inverse problems for infiltration and contaminant adsorption in partially saturated porous media

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We discuss the numerical modelling of unsaturated-saturated flow in porous media and contaminant transport with adsorption in 1D. We develop an efficient numerical approximation which is a good candidate for solving inverse problems involving the determination of model parameters (hydraulic and geochemical).

Mathematical model for unsaturated flow is based on Richard's nonlinear and degenerate equation expressed in terms of effective saturation and head using Van Genuchten-Mualem ansatz with soil parameters. Flow in fully saturated sub region is governed by Darcy's equation. Adsorption (in whole porous media) is modelled by means of sorption isotherms and kinetic rate coefficient. Determination of hydraulic parameters (soil parameters) and geochemical model data (sorption isotherms and kinetic coefficient) are subjects for determination. Additionally, the mass diffusion through the boundary of porous media (contact solid-liquid) is shortly discussed, too. Here, the adsorption/desorption process is realized only at the boundary of solid.

To obtain required information for inverse problem, some measurements along the infiltration process must be collected. The acceleration can be achieved by using centrifugation where the flow driving force is much higher as by gravitational. In our presentation we will focus to the determination of sorption isotherms, kinetic rate coefficient and to the solution of direct problem for mass transfer on the boundary of solid/liquid contact. Determination of soil parameters under centrifugation we have discussed in our previous contributions -see [1], [2]. There, only simple measurements of global characteristics as: evolution of centrifuge force; amount of infiltrated and expelled water from the sample have been used. Also here at the determination of sorption isotherms and kinetics coefficient we will measure just amount of infiltrated water at some contaminant concentration and expelled mass of contaminant in some time moments.

Determination of model parameters is realized in an iterative way where the discrepancy of measured and computed global characteristics is minimized (using some common algorithms as Levenberg-Marquardt, or "fminsearch" available, e.g., in MATLAB library).


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