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Modelling of Water Flow and Solute Transport in Double Porosity Unsaturated Media: Theory, Two-scale Computations and Experiments

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"Multi-scale, multi-components, multi-phases" are the key words that characterize the double porosity media, like fissured rocks, aggregated soils or composite geomaterials, subject to environmental conditions. In relation to this context an integrated upscaling approach to the modelling of water flow and solute transport under unsaturated conditions in double porosity media, is presented. The proposed approach combines three issues: theoretical, numerical and experimental, and enables to relate the macroscopic behaviour to the microscopic features, like microphysics and microstructure.

In the theoretical part, the macroscopic models are derived by applying the asymptotic homogenization method. It is assumed that the microstructure of the medium is composed of two porous domains, showing contrasted hydraulic conductivities, and named macro- and micro-porosity. It can be shown that this situation leads to the local non equilibrium of water capillary pressure and solute concentration, which has to be taken into account during the transient phase of the process. In case of water capillary and gravitary flow, the macroscopic model consists of two coupled nonlinear equations [1]. Compared to the phenomenological models, the model obtained by homogenization offers a complete description of the problem, including the definition of the effective parameters (in a general case anisotropic) and the domain of validity of the model. By the latter term we understand a set of underlying assumptions on the microstructure of the medium, the considered spatial and time scales, and the relations between the local hydraulic parameters and the forces driving the flow. All these assumptions are explicitly introduced via the estimation of the dimensionless parameters and the formulation of the appropriate boundary and interface conditions at the microscopic scale. For practical purposes the generalized water flow model was formulated, in order to take into account all possible situations (and the appropriate individual models) that can occurs during a single flow process (local equilibrium/local non-equilibrium). In case of solute transport (in unsaturated conditions), a twoequation model was developed [2], in which a coupling between dispersion - convection in the macro-porosity and diffusion in the micro-porosity domain, can be seen. As in the case of water flow, the macroscopic parameter (dispersion tensor) can be calculated from the solution of the local boundary value problem. Finally, the domain of validity of

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the modeling is given. It is based on observations and measurements of the orders of magnitudes of characteristic quantities involved in the process.

The numerical implementation of the double-porosity models requires a particular strategy, allowing for two-scale simultaneous computations. This class of models is currently under intensive development because of growing interest of taking into account the microstructure of the porous medium (and its evolution). In order to implement the water flow model a Fortran code was developed for the case of (macroscopically) two-dimensional (axi-symmetric) conditions, coupled with the (microscopically) one dimensional conditions (spherical flow) [3]. The general idea of the numerical model is to associate with each macroscopic "point" a period representing the microstructure. The code is based on the Finite Volume Method and the mass conservative mixed formulation. The transport model was implemented by using the commercial code Comsol Multiphysics (Finite Element Method) for the case of (macroscopically) one dimensional problem, coupled with the (microscopically) one dimensional problem [2]. In this case the coupling strategy is different and required the domain transformation.

The experimental validation of the double-porosity models presented in this study follows the logic "from micro towards macro". Therefore, an a priori knowledge of the microstructure of the medium and the local physical parameters, is necessary. It is possible in the case of artificially created media in the laboratory conditions (physical models). Only a very few such studies are reported in the literature and they concern very simple geometry. We present a series of experiments on a physical model that mimics the behaviour of the double porosity medium [3], [4]. The model is a three dimensional periodic structure, composed of sintered clay spheres embedded in Hostun sand HN38. The unsaturated water flow experiments were carried out under different flow conditions: infiltration or drainage, and in different macroscopic geometrical conditions: one or two-dimensional axi-symmetrical case. During the experiments the capillary pressure, the water content and the outlet water flux, were measured. As to the transport problem, a series of one-dimensional dispersion experiments of the NaCl tracer under unsaturated steady-state water flow conditions, was performed [2]. Here, the inlet and outlet concentration, the water content and the fluxes, were measured. Two different types of inlet boundary condition were applied: step-wise and pulse-wise. In all cases very good agreement between measurements and numerical simulations can be observed, which provides a proof of predictive capacity of the developed models.

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