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An upscaled two-equation model of transport in porous media through unsteady-state closure of volume averaged formulations

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We focus on a theoretical analysis of nonreactive solute transport in porous media through the volume averaging technique. Darcy-scale transport models based on continuum formulations typically include large scale dispersive processes which are embedded in a pore-scale advection diffusion equation through a Fickian analogy. This formulation has been extensively questioned in the literature due to its inability to depict observed solute breakthrough curves in diverse settings, ranging from the laboratory to the field scales. The heterogeneity of the pore-scale velocity field is one of the key sources of uncertainties giving rise to anomalous (non-Fickian) dispersion in macro-scale porous systems.
Some of the models which are employed to interpret observed non-Fickian solute behavior make use of a continuum formulation of the porous system which assumes a two-region description and includes a bimodal velocity distribution. A first class of these models comprises the so-called “mobile-immobile” conceptualization, where convective and dispersive transport mechanisms are considered to dominate within a high velocity region (mobile zone), while convective effects are neglected in a low velocity region (immobile zone). The mass exchange between these two regions is assumed to be controlled by a diffusive process and is macroscopically described by a first-order kinetic. An extension of these ideas is the two equation “mobile-mobile” model, where both transport mechanisms are taken into account in each region and a first-order mass exchange between regions is employed.
Here, we provide an analytical derivation of two region “mobile-mobile” meso-scale models through a rigorous upscaling of the pore-scale advection diffusion equation. Among the available upscaling methodologies, we employ the Volume Averaging technique. In this approach, the heterogeneous porous medium is supposed to be pseudo-periodic, and can be represented through a (spatially) periodic unit cell. Consistently with the two-region model working hypotheses, we subdivide the pore space into two volumes, which we select according to the features of the local micro-scale velocity field. Assuming separation of the scales, the mathematical development associated with the averaging method in the two volumes leads to a generalized two-equation model. The final (upscaled) formulation includes the standard first order mass exchange term together with additional terms, which we discuss. Our developments allow to identify the assumptions which are usually implicitly embedded in the usual adoption of a two region mobile-mobile model. All macro-scale properties introduced in this model can be determined explicitly from the pore-scale geometry and hydrodynamics through the solution of a set of closure equations. We pursue here an unsteady closure of the problem, leading to the occurrence of nonlocal (in time) terms in the upscaled system of equations. We provide the solution of the closure problems for a simple application documenting the time dependent and the asymptotic behavior of the system.