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Dispersive transport across interfaces

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Experiments demonstrating asymmetrical dispersive transport of a conservative tracer across interfaces between different porous materials have recently been performed. Here, this phenomenon is studied numerically on the pore scale. The flow field is derived by solving the Stokes equation. The dispersive transport is simulated by a large number of particles undergoing random walks under the simultaneous action of convection and diffusion. Two main two-dimensional configurations are studied; each consists of two segments (called coarse and fine) with the same structure, porosity, and length along the main flow, but different characteristic solid/pore sizes. One structure consists of two channels containing cavities of different sizes, and the second of square "grains" of different sizes. At time t=0, a large number of particles is injected (as a pulse) around a given cross-section. The corresponding breakthrough curves (BTCs) are registered as functions of time at six different cross sections. Calculations are made twice; in the first case (CtoF), particles are injected in the coarse side and are transported towards the fine one; in the second one (FtoC), the opposite case is studied. These calculations are performed for various Péclet numbers (Pe). Comparison of the resulting BTCs shows features that are similar to experimental observations, but with qualitative and quantitative differences. The influences of the medium, of the injection and observation planes, and of Pe are detailed and discussed. A BTC for pulse injection can be characterized by its maximum M(t_M) and the time t_M at which it occurs. The observed differences for channels bounded by cavities are very small. However for the granular structures, M(t_M) is always larger for FtoC than for CtoF ; t_M depends on all the parameters, namely Pe, the size ratio between the large and small grains, the injection and the observation planes. The numerical results are systematically compared with solutions of one dimensional convection-dispersion equation (coupled or not with a stagnant zone).