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Stochastic upscaling of porous media transport: from pore-scale particle tracking simulations to larger scale velocity based correlated CTRW models

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Understanding pore-scale flow and transport is key for the upscaling of dispersion, mixing, and reaction processes from the pore to the Darcy scale. We present a detailed study of particle transport in the flow through a pore geometry obtained from x-ray microtomography of a Berea sandstone sample, [1]. Flow is solved numerically using OpenFOAM, while transport is simulated using particle tracking. We focus on transport measurables such as propagators, breakthrough curves (BTCs), and evolution of the mean squared displacement (MSD). We observed anomalous transport through the early arrivals, the long tailing of the BTC, and the nonlinear growth of the mean squared displacement. In order to characterize and understand the cause of these non-Fickian characteristics, we study the tortuosity, constrictivity, and the correlation between the length of a streamline and its average velocity. We also compute the full Eulerian and Lagrangian velocity statistics inside the sample, which we use in the further upscaling of the transport process. All these characteristics depend on whether a uniform or flux weighted injection condition is used.

We propose a new representative elementary volume (REV) definition based on the stationarity and ergodicity of the velocity process, namely a sample will be considered an REV if the velocity distribution experienced by the particles becomes stationary within the size of the domain and if it is ergodic, [2]. Note that unlike the usual definitions of REV, which imply that transport in an REV is Fickian, this allows for anomalous transport. Since, according to this definition, our sample is an REV where ergodicity is achieved, its characteristics are valid at larger scales, and we can thus upscale the transport through a stochastic model based on the velocity statistics. This leads us to two upscaled one-dimensional correlated continuous time random walk (cCTRW) models based on the velocity statistics obtained from the particle tracking simulation, [2]. The first cCTRW is based on the full velocity transition matrix while the second one relies on an Eulerian velocity PDF and a Bernoulli process parametrized by the correlation length of the rock sample, [3]. The results of these models' simulations are then compared with the particle tracking simulations. Both CTRW models reproduce well the growth of the MSD and the slope of the breakthrough curve, the first one being slightly more accurate at the expense of a slight increase in computational cost. This accuracy difference can be explained by the fact that one is parametrized by the full transition matrix while the other accepts as its only parameter the velocity correlation scale. These approaches allow for an efficient upscaling of pore-scale transport and give a new meaning to the concept of the REV.

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