Simulating three-dimensional non-Fickian transport across arbitrary Péclet regimes using training trajectories

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Transport in natural porous media shows non-Fickian characteristics. From the Lagrangian perspective this leads to skewed and heavily tailed particle arrival time distribution. The skewness is triggered by the particles’ memory of velocity and direction, both of which persist over a specific characteristic length. Capturing this process memory is essential to represent non-Fickianity appropriately.

Classical non-Fickian models (e.g., CTRW models) simulate the effects of memory but not the mechanisms that leads to process memory. CTRWs have been applied successfully in many studies but nonetheless they have drawbacks. In classical CTRWs, each particle makes a spatial transition for which each particle adapts a random transit time. Consecutive transit times are drawn independently from each other, and this is only valid for sufficiently large spatial transitions. If we want to simulate non-Fickian transport on smaller scales than that, we have to implement the mechanisms behind memory into the simulation. Recent CTRW methods use transitions matrices to simulate correlated transit times derived from direct numerical simulation (DNS).

We present an alternative transition metric by mimicking the characteristic flow path of particles through the porous medium. A particle’s flow path incorporates all aspects of non-Fickian transport. Our hypothesis is that by realistically mimicking a particle's flow path, we inherently represent process memory so that we are capable of simulating non-Fickian transport in 3D.

Overall, we generate particle trajectories by a segment-wise resampling of DNS-based particle trajectories. The most obvious property of particle trajectories is that the change of velocity and the change of direction along a trajectory is smooth and therefore it is the smoothness that we target. We account for smooth transitions by merging trajectory segments with similar component-wise velocities at the intersection of consecutive segments. We achieve this by a nearest neighbor search in an archive of trajectory segments in order to find the best fit regarding the x-, y-, and z-velocities at the current segment’s end. By doing so, we guarantee that the velocity at the current segment end is similar to the beginning of the next segment. This results in relatively smooth transitions between segments regarding direction and velocity.

As the upcoming trajectory segment only depends on the current segment, our model forms a spatial Markov process. For parameterization, we determine the correlation lengths for speed and direction via the autocorrelation of the particles’ velocity and directional motion in DNS. The former defines the segment length and incorporates memory of speed. The latter defines the averaging scale of the component-wise velocity at the end of each segment. This incorporates memory of direction.

The modelling scheme that we present does not require a transition matrix to represent process dependence. This is advantageous as filling a nine-dimensional matrix, as required for a 3D transport simulation, is computationally expensive and valid only for the Péclet regime under consideration. By manipulating the advective displacement of our DNS-based training trajectories, we are able to scale the transport process across a range of Péclet regimes.

Altogether, we present a data-driven simulation approach for a non-Fickian, finite-Péclet transport process in porous media that is capable of scaling transport across Péclet regimes.