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One Hundred Ways to be Non-Fickian - A Rigorous Multi-Variate Statistical Analysis of Pore-Scale Transport

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Fickian transport in groundwater flow is the exception rather than the rule. Transport in porous media is frequently simulated via particle methods (i.e. particle tracking random walk (PTRW) or continuous time random walk (CTRW)). These methods formulate transport as a stochastic process of particle position increments. At the pore scale, geometry and micro-heterogeneities prohibit the commonly made assumption of independent and normally distributed increments to represent dispersion. Many recent particle methods seek to loosen this assumption. Hence, it is important to get a better understanding of the processes at pore scale.

For our analysis we track the positions of 10.000 particles migrating through the pore space over time. The data we use come from micro CT scans of a homogeneous sandstone and encompass about 10 grain sizes. Based on those images we discretize the pore structure and simulate flow at the pore scale based on the Navier-Stokes equation. This flow field realistically describes flow inside the pore space and we do not need to add artificial dispersion during the transport simulation. Next, we use particle tracking random walk and simulate pore-scale transport. Finally, we use the obtained particle trajectories to do a multivariate statistical analysis of the particle motion at the pore scale.

Our analysis is based on copulas. Every multivariate joint distribution is a combination of its univariate marginal distributions. The copula represents the dependence structure of those univariate marginals and is therefore useful to observe correlation and non-Gaussian interactions (i.e. non-Fickian transport).

The first goal of this analysis is to better understand the validity regions of commonly made assumptions. We are investigating three different transport distances:

1) The distance where the statistical dependence between particle increments can be modelled as an order-one Markov process. This would be the Markovian distance for the process, where the validity of yet-unexplored non-Gaussian-but-Markovian random walks start.

2) The distance where bivariate statistical dependence simplifies to a multi-Gaussian dependence based on simple linear correlation (validity of correlated PTRW/CTRW).

3) The distance of complete statistical independence (validity of classical PTRW/CTRW).

The second objective is to reveal characteristic dependencies influencing transport the most. Those dependencies can be very complex. Copulas are highly capable of representing linear dependence as well as non-linear dependence. With that tool we are able to detect persistent characteristics dominating transport even across different scales.

The results derived from our experimental data set suggest that there are many more non-Fickian aspects of pore-scale transport than the univariate statistics of longitudinal displacements. Non-Fickianity can also be found in transverse displacements, and in the relations between increments at different time steps. Also, the found dependence is non-linear (i.e. beyond simple correlation) and persists over long distances. Thus, our results strongly support the further refinement of techniques like correlated PTRW or correlated CTRW towards non-linear statistical relations.