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Pore-scale Mixing and the Evolution of Hydrodynamic Dispersion

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Transport of dissolved substances through natural and engineered porous media is determined by the inherent complexity of the pore space, and diffusive mass transfer within and between pores. The interplay of pore-scale mixing and network-scale flow variability are key for the understanding of transport and contact processes in porous media with diverse applications ranging from groundwater contamination and geological carbon dioxide storage, to the design of batteries, and transport in brain microcirculation. Therefore, hydrodynamic transport has been the focus of research over decades in different disciplines. Nevertheless, questions of fundamental nature remain concerning both the evolution of hydrodynamic dispersion, and the dependence of asymptotic hydrodynamic dispersion coefficients on the Péclet number. We use a Lagrangian framework to identify and quantify three fundamental mechanisms of pore-scale mixing that determine the stochastic dynamics of pore- and network-scale particle motion: (i) The smoothing of intra-pore velocity contrasts, (ii) the increase of the tortuosity of particle paths, and (iii) the setting of a maximum time for particle transitions. Based on these mechanisms, we derive an upscaled approach that predicts anomalous and normal hydrodynamic dispersion in terms of the characteristic pore length, Eulerian velocity distribution and P\'eclet number. The theoretical developments are supported and validated by direct numerical flow and transport simulations in three-dimensional digitized porous medium samples. Solute breakthrough curves are characterized by intermediate power-law behaviors and exponential cut-off, which reflect pore-scale velocity variability and intra-pore solute mixing. Similarly, dispersion coefficients evolve from molecular diffusion at early times to asymptotic hydrodynamics dispersion via an intermediate superdiffusive regime. The theory captures the full evolution form anomalous to normal transport behavior at different Péclet numbers as well as the Pécletdependence of asymptotic dispersion.

It is not constrained by transport measurements. The fundamental nature of the considered flow and transport processes allows application of the key elements of the derived theory to transport of dissolved chemicals, bacteria and colloids in a wide range of porous media also under different flow conditions.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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