Insights into characterizing anomalous diffusion with bimolecular reactions, and the origins of anomalous transport in heterogeneous porous media

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Particle tracking (PT) techniques are proving useful in the context of modelling anomalous diffusion and transport, particularly in the context of the continuous time random walk (CTRW) framework. We employ CTRW-PT models to provide two insights into the occurrence and origin of anomalous behavior in porous media.

In the first case, we examine mixing zone dynamics of a reaction product C during diffusion of two species A and B, using a 2-D CTRW-PT model for the reaction $A + B \rightarrow C$, allowing for both Fickian and non-Fickian (anomalous) transitions. We find that the basic patterns of the C dynamics – the temporal evolution of the spatial profile and the temporal C production – are similar for both modes of diffusion. However, the distinctive time scale for the non-Fickian case is very much larger even when the median transition steps are matched to the Fickian case. For immobile C, the spatial profile pattern is a broadening (Gaussian) reaction front evolving to a concentration-fluctuation dominated (Lorentzian) shape. The temporal C production is fit well by a stretched exponential for both diffusion types. In analyzing experiments, the appearance of a Gaussian C profile does not prove that the diffusion process is Fickian.

In the second case, we quantitatively identify the origin of anomalous transport in a representative heterogeneous porous medium, under uniform (in the mean) flow conditions. The heterogeneity is based on lognormally distributed hydraulic conductivity (K) fields, with several decades of K values. Transport in the domains is determined by a particle tracking technique and characterized by breakthrough curves (BTCs). The BTC averaged over multiple realizations demonstrates anomalous transport in all cases, which is accounted for entirely by a power-law distribution $\sim t^{-1-\beta}$ of local transition times, contained in the probability density function $\psi(t)$ of transition times, using the framework of a CTRW. A unique feature of our analysis is the derivation of $\psi(t)$ as a function of parameters quantifying the heterogeneity of the domain. In this context, we first establish the dominance of preferential pathways across each domain, and characterize the statistics of these pathways by forming a particle-visitation weighted histogram $H_w(K)$. By converting the $\ln(K)$ dependence of $H_w(K)$ into time, we demonstrate the equivalence of $H_w(K)$ and $\psi(t)$, and delineate the region of $H_w(K)$ that forms the power law of $\psi(t)$. This thus defines the origin of anomalous transport. Analysis of the preferential pathways clearly demonstrates the limitations of critical path analysis and percolation theory as a basis for determining the origin of anomalous transport.

[1] Y. Berkowitz, Y. Edery, H. Scher and B. Berkowitz, Phys. Rev. E, 87, 032812 (2013).
[2] Y. Edery, A. Guadagnini, H. Scher and B. Berkowitz, Water Resour. Res., 50, 1490-1505 (2014).