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On the formation of localized peaks and non-monotonic tailing of breakthrough curves

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While breakthrough curve (BTC) analysis is a traditional tool in hydrogeology to obtain hydraulic parameters, in recent years emphasis has been placed on analyzing the shape of the receding portion of the curve. A number of field and laboratory observations have found a constant BTC slope in log-log space, and thus it has been hypothesized that a power law behavior is representative of real aquifers. Usually, monotonicity of the late-time BTC slope is just assumed, meaning that local peaks in the BTC are not considered, and that a local (in time) increase or decrease of BTC slope is also not considered. We contend that local peaks may exist but are sometimes not reported for a number of reasons. For example, when BTCs are obtained from actual measurements, sub-sampling may mask non-monotonicity, or small peaks may be reported as measurement errors and thus smoothed out or removed. When numerical analyses of synthetic aquifers are performed, the simulation method may yield artificially monotonous curves as a consequence of the methods used. For example, Eulerian methods may suffer from numerical dispersion, where curves tend to become over-smoothed while Lagrangian methods may suffer from artificial BTC oscillations stemming from the reconstruction of concentrations from a limited number of particles.

A paradigm shift in terms of the BTC shape must also accompany two major advancements within the hydrogeology field: 1) the increase of high frequency data and progression of data collection techniques that diminish the problems of under-sampling BTCs and 2) advancements in supercomputing and numerical simulation allowing for higher resolution of flow and transport problems. As more information is incorporated into BTCs and/or they are obtained in more spatial locations, it is likely that classical definitions of BTC shapes will no longer be adequate descriptors for future treatment of contaminant transport problems. For example, the presence of localized peaks in BTCs (when, at what magnitude and duration) is imperative in accurately assessing environmental and human health risk, as discrepancies in the environmental concentration at a given time could potentially affect risk management decisions.

In this work, the presence of multiple peaks in BTCs is assessed from high-resolution numerical simulations with particle tracking techniques and a kernel density estimator. Individual realizations of three-dimensional heterogeneous hydraulic conductivity fields with varying combinations of statistical anisotropy, geostatistical models, and local dispersivity are utilized to test for mechanisms of physical mass transfer. BTCs of non-reactive solutes are analyzed for the presence of local maxima, and for the corresponding slope of the receding limb of the curve as a function of travel distance and number of integral scales traveled, a question which has received little to no attention in the literature. This uniquely designed numerical experiment allows the discussion of BTC evolution in terms of not only the number of local peaks in the BTC, but also how knowledge of the number of local peaks in a BTC relates to pre-Fickian transport. We show that the number of local peaks and corresponding slopes strongly depend on statistical anisotropy and travel distance, but are less sensitive to the number of integral scales traveled. We also illustrate the sensitivity of BTC shapes resulting from the geostatistical model used, how local peaks may potentially change the apparent overall slope of the curves, and the implications of these results in water quality management decisions.