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What is geological entropy and why measure it? A parsimonious approach for predicting transport behaviour in heterogeneous aquifers

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We present an approach to predict non-Fickian transport behaviour in alluvial aquifers from knowledge of physical heterogeneity. This parsimonious approach is based on only two measurable parameters describing the global variability and the structure of the hydraulic conductivity (K) field: the variance of the ln(K) values (σ_Y^2), and a newly developed index of geological entropy (H_R), based on the concept of Shannon information entropy. Both σ_Y^2 and H_R can be obtained from data collected during conventional hydrogeological investigations and from the analysis of a representative model of the spatial distribution of K classes (e.g. hydrofacies) over the domain of interest. The new index H_R integrates multiple characteristics of the K field, including the presence of well-connected features, into a unique metric that quantifies the degrees of spatial disorder in the K field structure. Stochastic simulations of tracer tests in synthetic K fields based on realistic distributions of hydrofacies in alluvial aquifers are conducted to identify empirical relations between H_R, σ_Y^2, and the first three central temporal moments of the resulting breakthrough curves (BTCs). Results indicate that the first and second moments tend to increase with spatial disorder (i.e, H_R increasing). Conversely, high values of the third moment (i.e. skewness), which indicate significant post-peak tailing in the BTCs and non-Fickian transport behaviour, are observed in more orderly structures (i.e, H_R decreasing), or for very high σ_Y^2 values. We show that simple closed-form empirical expressions can be derived to describe the bivariate dependency between the skewness of the BTC and corresponding pairs of H_R and σ_Y^2. This dependency shows clear correlation for a broad range of structures and Kvariability levels. Therefore, it provides an effective and broadly applicable approach to explain and predict non-Fickian transport in real aquifers, such as those at the well-known MADE site and at the Lawrence Livermore National Laboratory.