



Geological entropy and solute transport: when good descriptors of aquifer heterogeneity go right

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Accurate predictions of fluid flow and solute transport in the subsurface require effective approaches to describe and represent the spatial variability of physical properties. In a recent work, we introduced the geological entropy approach (Bianchi and Pedretti, 2017, *Water Resour. Res.*, doi: 10.1002/2016WR020195) based on information theory concepts to quantify spatial disorder (or order) in the structure of the hydraulic conductivity (K) field, which it was shown to be correlated to certain characteristics of the observed transport behaviour. In this work, we complement and expand the geological entropy approach by introducing a novel tool for spatial analysis called entrogram to assess spatial order at different scales. Based on the entrogram calculation, we also define a new metric called entropic scale to measure the persistency of patterns of spatial association in the K field structure. We show that the entropic scale is a global measure of spatial order that allows robust comparisons between different structures. The entrogram and entropic scale analysis are applied to investigate the link between spatial order and the solute transport in K fields modelled as the distribution of three hydrofacies in alluvial aquifers. Reliable relationships are found between the entropic scale and the temporal moments of the breakthrough curves (BTCs), as well as key statistics defining early- and late-time solute particle arrivals. These relationships confirm the clear correlation between transport behaviour and the degree of spatial order in the K field. Entrograms and entropic scales are also calculated for 2-D and 3-D fields having univariate identical log-normal K distribution and different spatial structures in terms of connectivity of the values at the tails of the distribution. Results of detailed numerical transport simulations confirm the conclusions of previous studies showing that transport behaviour in 3-D fields is not as sensitive to the structure as in 2-D fields. Comparisons of the entrograms and entropic scales for the different K and corresponding Eulerian velocity fields provide sensible explanations for this difference. Results from this study show that the entrogram and the entropic scale are fundamental properties of the K field that need to be evaluated for predicting solute transport behaviour simply from knowledge of the field heterogeneity.