Geophysical Research Abstracts
Vol. 16, EGU2014-13195, 2014
EGU General Assembly 2014

Higher order concentration moments collapse in the expected mass fraction (EMF) based risk assessment

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In this work Langrangian framework is used for conservative tracer transport simulations through 2-D extremely heterogeneous porous media. Conducted numerical simulations enable large sets of concentration values in both spatial and temporal domains. In addition to the advection, which acts on all scales, an additional mechanism considered is local scale dispersion (LSD), accounting for both mechanical dispersion and molecular diffusion. The ratio between these two mechanisms is quantified by the Peclet (Pe) number.
In its base, the work gives answers to concentration scalar features when influenced by: i) different log-conductivity variance; ii) log-conductivity structures defined by the same global variogram but with different log conductivity patterns correlated; and iii) for a wide range of Peclet values.
Results conducted by Monte Carlo analysis show a complex interplay between the aforementioned parameters, indicating the influence of aquifer properties to temporal LSD evolution. A remarkable collapse of higher order to second-order concentration moments [Yee, 2009] leads to the conclusion that only two concentration moments are required for an accurate description of concentration fluctuations. This explicitly holds for the pure advection case, while in the case of LSD presence the moment deriving function(MDF) is involved to ensure the moment collapse validity.
An inspection of the Beta distribution leads to the conclusion that the two-parametric distribution can be used for concentration fluctuation characterization even in cases of high aquifer heterogeneity and/or for different log-conductivity structures, independent of the sampling volume used.
Furthermore, the expected mass fraction (EMF) [Heagy & Sullivan, 1996] concept is applied in groundwater transport. In its origin, EMF is function of the concentration but with lower number of realizations needed for its determination, compared to the one point PDF. From practical point of view, EMF excludes meandering effect and incorporates information about exposure time for each non-zero concentration value present. Also, it is shown that EMF is able to clearly reflect the effects of aquifer heterogeneity and structure as well as the Pe value. The latter is demonstrated through the non-carcinogenic risk assessment framework. To demonstrate the uniqueness of the moment collapse feature and ability of the Beta distribution to account for the concentration frequencies even in real cases, Macrodispersion Experiment (MADE1) [Boggs et al, 1992] data sets are used for validation.