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Breakthrough curve prediction in heterogeneous aquifers: ADE is alive and kicking

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The modeling and prediction of the contaminant Breakthrough curve (BTC) in natural aquifers is still a challenging task, especially for strongly heterogeneous porous formations. Significant research has been carried out in the last two decades, in which the predictive capabilities, as well as the overall significance, of the Advection Dispersion Equation (ADE) have been often questioned. Other alternative approaches have been developed during the years in an attempt to move beyond the ADE-based formulation of contaminant transport. We further explore here the predictive capabilities of ADE, with the macrodispersivity α_L given by the First Order Approximation (FOA), by checking in a quantitative manner its applicability. The setup is the one of natural gradient steady flow of mean velocity U taking place in heterogeneous aquifers of random logconductivity $Y = \ln K$, characterized by the normal univariate PDF $f(Y)$ and autocorrelation ρ_Y, of variance σ_Y^2 and horizontal integral scale I. The study is based on extensive three-dimensional numerical simulations of flow and transport for different 3D conductivity structures. We find that the ADE-FOA solution is a sufficiently accurate predictor for applications, the many other sources of uncertainty prevailing in practice notwithstanding, provided that the correct injection and detection conditions are applied. We checked by least squares and by comparison of travel time of quantiles of the cumulative mass arrival at a control plane (correspondent to the BTC) that indeed the analytical Inverse Gaussian travel time distribution with $\alpha_L = \sigma_Y^2 I$ is able to fit well the bulk of the simulated BTCs. It tends to underestimate the late arrival time of the thin and persistent tail, which is better reproduced by the semi-analytical MIMSCA model. The results strengthen the confidence in the applicability of the ADE and the FOA to predicting longitudinal spreading in solute transport through heterogeneous aquifers of stationary random structure.