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Probability density functions of solute concentration in heterogeneous aquifers

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In recent years, statistical theory has been used to compute the ensemble mean and variance of concentration in formations with second-order stationary log-conductivity fields. These approaches have been extended to account for nonstationarity, and to achieve higher-order approximations. The value of accurately estimating the mean and variance of concentration, however, remains unclear without knowing the shape of the probability density function (*pdf*). In a set-up where a conservative solute is continuously injected into a domain, the concentration can never exceed the range between zero and the concentration value in the injected solution. At small travel distances close to the fringe of the plume, an observation point may fall into the plume or outside, so that the statistical concentration distribution clusters at the two limiting values. Obviously, this results in non-Gaussian *pdf*s of concentration. The latter is important when point-like measurements of concentration are used to infer the spatial distributions of concentration itself (interpolation) or hydraulic conductivity (inverse modeling).

We perform three-dimensional Monte Carlo simulations (10,000 realizations) of steady-state flow and transport to determine the empirical *pdf* of concentration at each location. The spatial domain measures $200\ m$ in the flow direction and $50 \times 25\ m$ in the two transverse directions. Groundwater flow and solute transport are solved via the finite element method (FEM) with a discretization resolution of $2\ m$ in the longitudinal and $1/3\ m$ in the transverse directions, leading to more than 10^6 elements.

We determine the statistical distribution of solute concentration at each location in the domain. The shape of the empirical *pdf* changes with distance to the contaminant source: Near the source, the distribution can best be fitted by a beta distribution, whereas it becomes Gaussian like far away from the contaminant source. This implies

that geostatistical techniques for interpolation and other statistical inferences based on Gaussian distributions, such as kriging and cokriging, are feasible only far away from the contaminant source. For calculations near the source, the beta-like distribution of concentration must not be neglected. Increasing the measurement volume decreases the distance over which non-Gaussianity is a predominant feature of the concentration *pdf*.