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Statistical distributions of concentration in heterogeneous domains: why the mean and variance are not enough

O.A. Cirpka (1), R.L. Schwede (1)

(1) Swiss Federal Institute of Aquatic Science and Technology (Eawag), Überlandstr. 133, CH-8600 Dübendorf, Switzerland (olaf.cirpka@eawag.ch)

Uncertainty in the distribution of hydraulic parameters leads to uncertainty in flow and reactive transport. Traditional stochastic analysis of solute transport in heterogeneous media has focused on the ensemble mean of conservative-tracer concentration. Studies in the past years have shown that the mean concentration often is associated with a high variance. Because the range of possible concentration values is bounded, a high variance implies high probability weights on the extreme values. We present a simple method of estimating the full cumulative distribution function of concentration in heterogeneous random media. The approach makes use of first-order analytical results regarding spatial moments of solute plumes. The resulting distributions resemble the shape of bimodal beta distributions, at least at small travel distance..

In certain cases of mixing-controlled reactive transport, concentrations of conservative tracers, denoted mixing ratios, can be mapped to those of compounds that react with each other upon mixing. This facilitates mapping entire statistical distributions from mixing ratios to reactive-species concentrations. In perturbative approximations, only the mean and variance of the mixing-ratio distribution are used. We demonstrate that the second-order perturbative approximation leads to erroneous or even physically impossible estimates of mean reactive-species concentrations when the variance of the mixing ratio is high and the relationship between the mixing ratio and the reactive-species concentrations strongly deviates from a quadratic function. The latter might be the case in biokinetic reactions or in equilibrium reactions with small equilibrium

constant in comparison to the range of reactive-species concentrations.