PDF Methods for Uncertainty Quantification in Diffusion-Reaction Systems

Stochastic Analysis of Advection-Diffusion-Reactive Systems with Applications to Reactive Transport in Porous Media

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Abstract

The complexity of scientific and technical issues facing the Department of Energy (DOE) requires the development of new predictive capabilities for physical, chemical, and biological processes, many of which are fundamentally uncertain. We present a new mathematical and numerical framework for tracking parametric uncertainty in simulations of nonlinear advection-diffusion-reaction (ADR) phenomena in highly heterogeneous environments with uncertain physical and (bio)chemical properties.

Uncertainty about spatio-temporal variability of system parameters (e.g., reaction rate constants and flow velocity) makes deterministic predictions of macroscopic system states (e.g., species' concentration) elusive. To quantify the impact of this parametric uncertainty on predictive uncertainty of ADR models, we treat the system parameters as random fields whose ensemble statistics (e.g., means, variances, and correlation functions) are inferred from available measurements. This renders corresponding ADR equations stochastic. Distributions of system states generally exhibit highly non-Gaussian behavior, which cannot be captured solely by the corresponding mean and variance. Instead, these features of transport are described by the probability density function (PDF) of a system state, e.g., the PDF of concentration at a certain point in space and time. We present a hierarchy of models and their PDF solutions.

First, we consider advective-reactive transport in heterogeneous environments with uncertain advective velocity and reaction rate constants. We derive a deterministic equation for the PDF of the concentration of a species that undergoes heterogeneous reactions, e.g., precipitation or dissolution. The derivation treats exactly (without linearization) a reactive term in the transport equation accounts for uncertainty (randomness) in both flow velocity and kinetic rate constants but requires a closure, such as a Large-Eddy-Diffusivity approximation used in the present analysis. No closure is required when reaction rates are the only source of uncertainty. We use exact concentration PDFs obtained for this setting to analyze the accuracy of our general, LED-based PDF equations.

Second, we study the PDF of a passive scalar that disperses in a random velocity field. We derive an explicit map between the velocity distribution and the scalar PDF, and obtain approximate solutions for the PDF of the normalized scalar. These solutions enable one to quantify explicitly the impact of dispersion on the evolution of the passive scalar PDF without recurrence to classical closure approximations used in mixing models.