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An Eulerian joint velocity-concentration PDF method for reactive transport in highly heterogeneous porous media

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In risk analysis applications involving heterogeneous formations, the knowledge of the concentration probability density function (PDF) at different spatial locations and times is crucial. A new joint velocity-concentration PDF method is proposed that is applicable for highly heterogeneous porous media. It accounts for advective transport, pore-scale dispersion, molecular diffusion, and chemical reactions. The corresponding PDF transport equation is solved numerically using an efficient particle-based approach. Similar methods are successfully applied for the simulation of turbulent flows mainly because the reactive source term in the PDF transport equation appears in closed form. Mixing at the pore-scale, however, needs to be modeled. Standard mixing models applied in PDF methods for turbulent flows, like the interaction by exchange with the mean (IEM) model, however, perform poorly. An alternative model better suited for applications involving highly heterogeneous porous media is formulated. The resulting joint PDF method is validated successfully by comparison with reactive (fast bimolecular reaction) and non-reactive Monte Carlo simulations for σ_Y^2 up to 4 and Péclet numbers ranging from 100 to 10000. Reference data was provided by Cirpka, and Caroni and Fiorotto for the reactive and non-reactive cases, respectively.