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Multiscale sensitivity analysis of nanoporous materials

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Ubiquitous uncertainty about pore geometry inevitably undermines the veracity of pore- and multi-scale simulations of transport phenomena in porous media. It raises two fundamental issues: sensitivity of effective material properties to pore-scale parameters and statistical parameterization of Darcy-scale models that accounts for pore-scale uncertainty. Homogenization-based maps of pore-scale parameters onto their Darcy-scale counterparts facilitate both sensitivity analysis (SA) and uncertainty quantification. We treat uncertain geometric characteristics of a hierarchical porous medium as random variables to conduct global SA and to derive probabilistic descriptors of effective diffusion coefficients and effective sorption rate. Our analysis is formulated in terms of solute transport diffusing through a fluid-filled pore space, while sorbing to the solid matrix. Yet it is sufficiently general to be applied to other multiscale porous media phenomena that are amenable to homogenization.

References

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Primary authors: Mr UM, Kimoon (University of California, San Diego); Prof. KATSOULAKIS, Markos (University of Massachusetts, Amherst); Prof. TARTAKOVSKY, Daniel M. (Stanford University); HALL, Eric (University of Massachusetts Amherst)

Presenter: HALL, Eric (University of Massachusetts Amherst)

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