NUMERICAL SIMULATION AND QUANTITATIVE UNCERTAINTY ASSESSMENT OF ELECTROCHEMICAL MICROCHANNEL FLOW

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In this talk, we present a model for two-dimensional electrochemical microchannel flow including the propagation of uncertainty from model parameters and boundary conditions to the simulation results. For a detailed representation of electroosmotic and pressure-driven microchannel flow, the model considers the coupled momentum, species transport, and electrostatic field equations, including variable zeta potential. The chemistry model accounts for pH-dependent protein labeling reactions as well as detailed buffer electrochemistry in a mixed finite-rate/equilibrium formulation. The model also has the unique capability to account for uncertainty in input parameters, such as species mobilities, and for stochastic processes, such as random ζ-potential variability. These uncertain input parameters and stochastic processes are handled with a pseudo-spectral stochastic formulation, which uses polynomial chaos (PC) representations for uncertain/stochastic model parameters, boundary conditions, and field quantities. Using a Galerkin approach, the governing equations are reformulated into equations for the coefficients in the PC expansions. Integration of the resulting equations gives the evolution of all variables with quantitative information on their uncertainty and the parameters that contribute the most to this uncertainty.

This formulation is applied to the simulation of two-dimensional electrochemical microchannel flow with protein-labeling reactions in a potassium phosphate buffer. Various phenomena are studied including the uncertainty in model results caused by the input parameters as well as the dispersion of sample peaks due to buffer disturbances from moving sample plugs or due to random ζ-potential variability from surface roughness or heterogeneous wall material properties.

Overall, the goal of this work is to explain important flow phenomena in microchannel flows and to provide a tool for assessing and maximizing the performance and reliability of microfluidic designs.

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