

## INVESTIGATING THE ACCURACY OF A DARCY SCALE MODEL OF COMPETITIVE ADSORPTION IN A POROUS MEDIUM THROUGH SPH PORE SCALE MODELING

Emily M. Ryan<sup>\*,†</sup>, Alexandre M. Tartakovsky<sup>\*</sup> and Cristina Amon<sup>†,‡</sup>

<sup>\*</sup> Pacific Northwest National Laboratory (PNNL)  
P.O. Box 999, Richland, WA 99352, USA  
e-mail: [emily.ryan@pnl.gov](mailto:emily.ryan@pnl.gov), [alexandre.tartakovsky@pnl.gov](mailto:alexandre.tartakovsky@pnl.gov)

<sup>†</sup> Carnegie Mellon University, Mechanical Engineering Department  
5000 Forbes Ave, Scaife Hall, Pittsburgh, PA 15213, USA

<sup>‡</sup> University of Toronto, Faculty of Applied Science & Engineering  
Galbraith Building, 35 St. George Street, Toronto, Ontario, CANADA M5S 1A4  
e-mail: [dean@ecf.utoronto.ca](mailto:dean@ecf.utoronto.ca)

**Summary.** In this paper we investigate the accuracy of a Darcy-scale model for competitive adsorption in a porous medium through comparison with a smoothed particle hydrodynamics (SPH) pore-scale model. SPH is a Lagrangian, particle based modeling method which uses the particles as interpolation points to directly discretize the governing equations of the system. The models consider a binary system of competitively adsorbing species traveling through a porous medium due to advection and diffusion. The effects of Damköhler number and porous microstructure on the accuracy of the Darcy-scale model when compared to the pore-scale model are investigated. The comparison of the Darcy-scale model and the pore-scale model shows that the Darcy model overestimates the mass of a plume moving through the domain for all Damköhler numbers investigated and is not able to accurately predict the masses of both surface species in a reactive system.