Mechanistically-Based Field-Scale Models of Uranium Biogeochemistry from Upscaling Pore-Scale Experiments and Models

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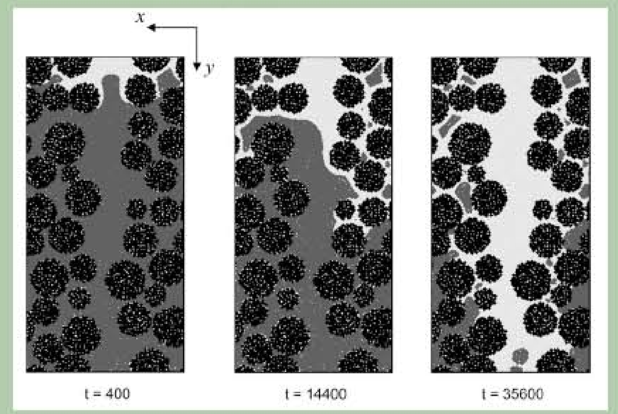
Tim Scheibe, Alexandre Tartakovsky (Pacific Northwest National Laboratory)
Brian Wood (Oregon State University) Joe Seymour (Montana State University)

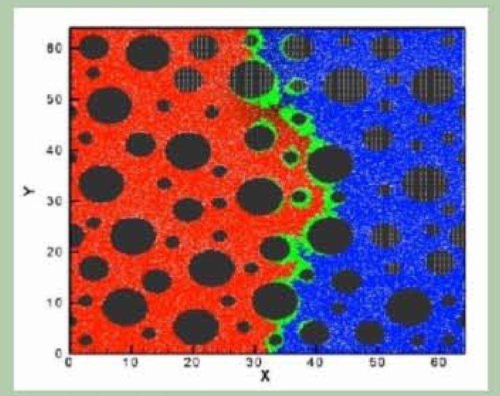
PORE-SCALE LMODELING

Smoothed Particle Hydrodynamics

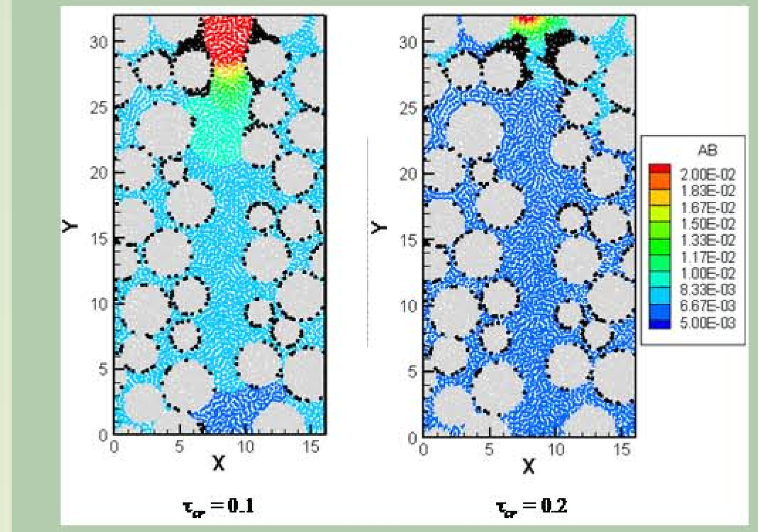
Smoothed Particle Hydrodynamics (SPH) is a particle-based simulation method developed initially for astrophysical applications. Our research group has applied this technique to simulation of multiphase flow and solute transport in porous media (top image to the right; Tartakovsky and Meakin, Vadose Zone Journal, 2006) and pore-scale mineral precipitation (bottom image to the right; Tartakovsky et al., Journal of Computational Physics, 2007).

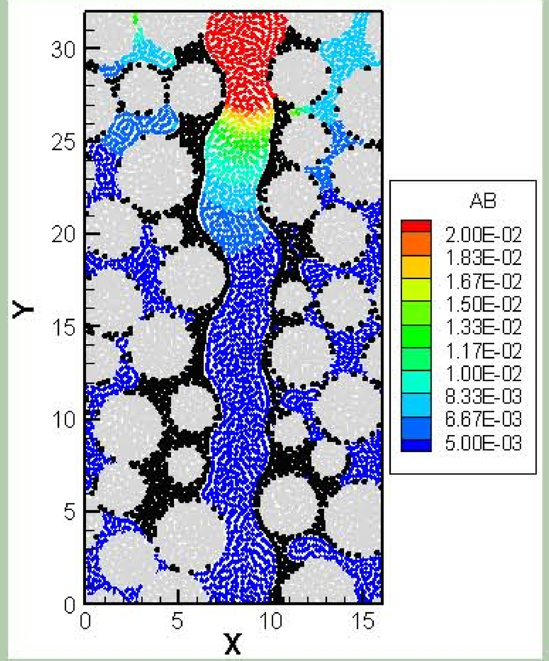


Under this project we have initiated the application of SPH to simulation of biofilm development in porous media at the pore scale (see images below from Tartakovsky et al, submitted).



We have developed and are currently testing a fully three-dimensional parallel SPH code for performing high-resolution pore-scale modeling in arbitrary 3D pore geometries.



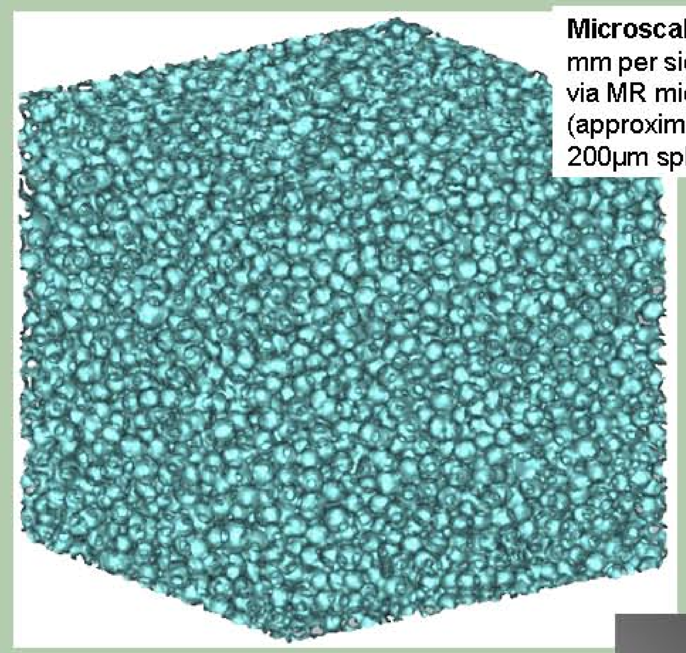


Simulation of biofilm (black) development and propagation through a micro-fractured porous medium using two different models of biofilm growth. Color scale indicates the product of the concentrations of electron donor and acceptor. In Model 1 (above), the deformation and attachment/detachment of biomass was modeled through combination of pair-wise short range repulsive and medium range attractive forces and hydrodynamics forces resulting from the fluid flow. Model 2 (right) is a cellular automata model that explicitly assumes that biomass can grow only in directions with shear stresses smaller than a prescribed critical value.

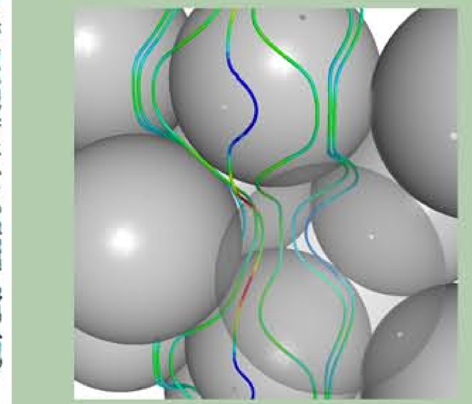
Finite Volume CFD Methods

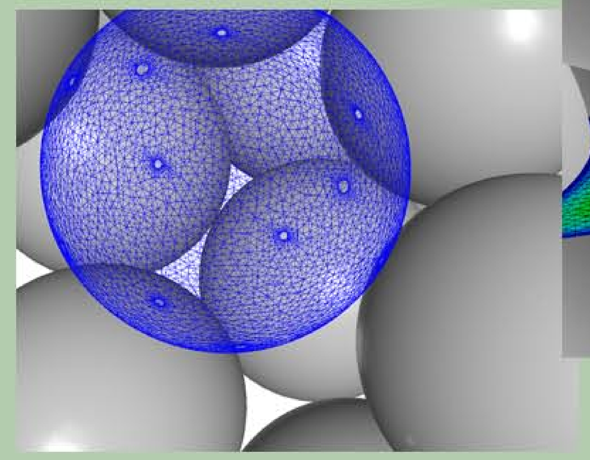
We are also applying grid-based finite volume methods drawn from the field of Computational Fluid Dynamics (CFD) to pore-scale simulation of flow and reactive transport. Grid generation issues for arbitrary and highly complex pore geometry have been addressed and we have conducted 3D pore-scale flow simulations using both STAR-CD and a PNNL-developed code (TETHYS) using a mutli-processor Linux cluster

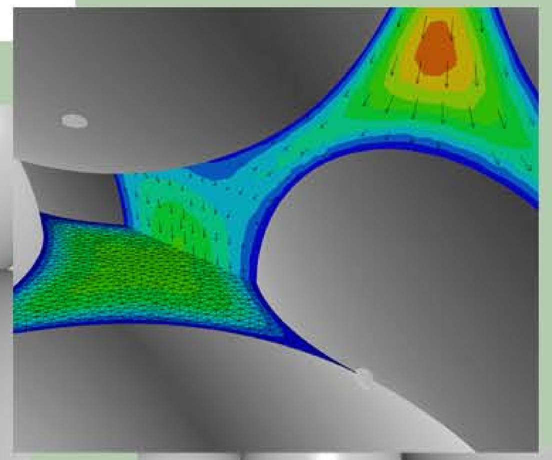
These simulations are used both for direct simulation of pore-scale processes, and for solution of the upscaling closure equations for arbitrarily complex pore structures. The latter allows the relaxation of restrictive assumptions (such as unit cell periodicity) required for previous upscaling analyses.

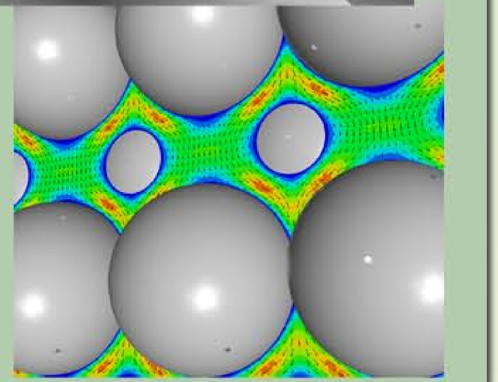


Microscale Geometry. 4.8 mm per side cube, measured via MR microscopy (approximately 8000 individual 200μm spheres)





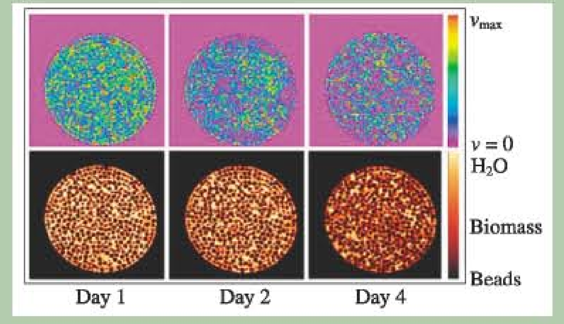




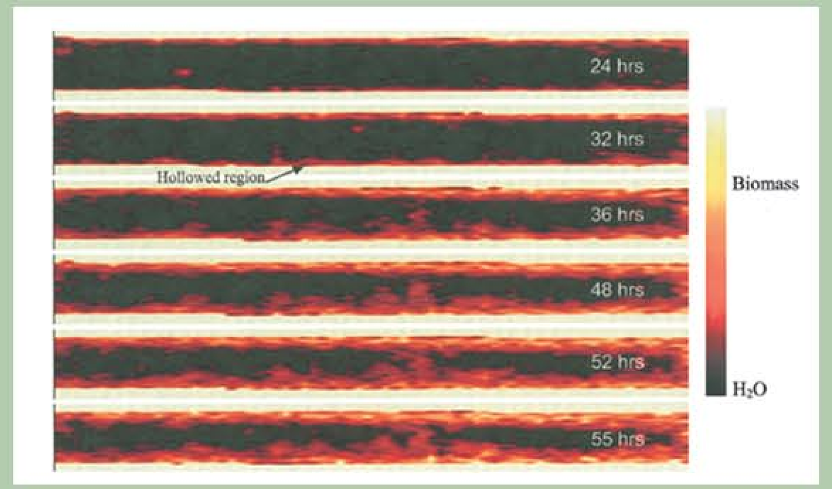
Above: Visualization of the grid on the surface of one spherical grain in a periodic media. Upper right: Simulated streamlines in the solved flow field. Lower right: Colors represent velocity magnitude in the visualized plane (red - high velocity; blue - low velocity). Middle right: A closeup of the velocity distribution in a selected pore.

PORE-SCALE EXPERIMENTS

Magnetic resonance microscopy (MRM) maps of velocity (top row) and T2 magnetic relaxation (bottom row) as a function of biofilm growth time (left to right). From Seymour et al., Physical Review Letters, 93(19), 2004.

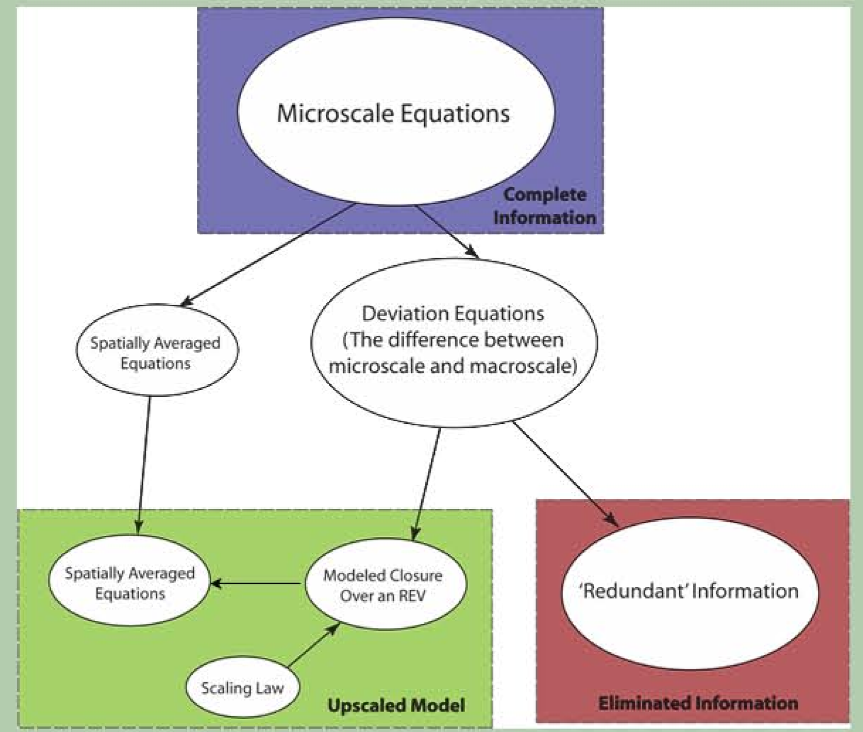


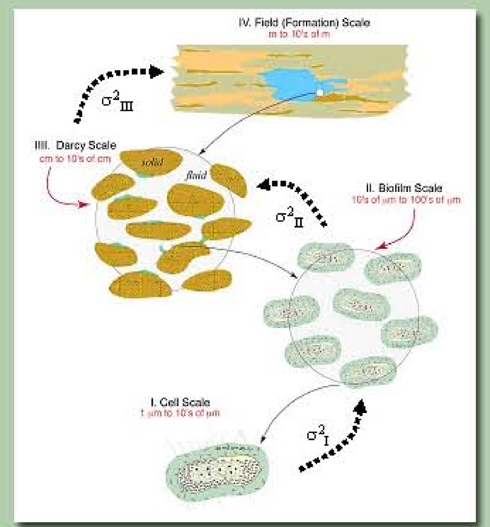
From Gjersing et al., Biotechnology and Bioengineering 89(7):822-834, 2005.

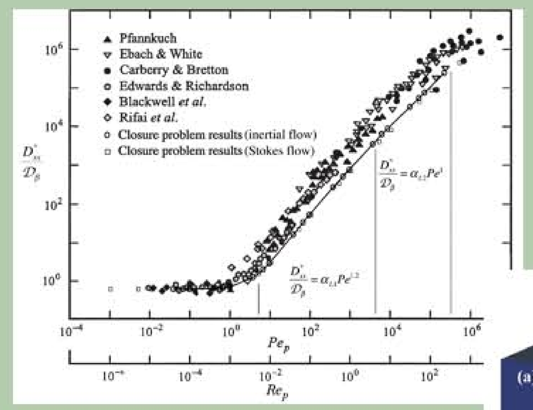


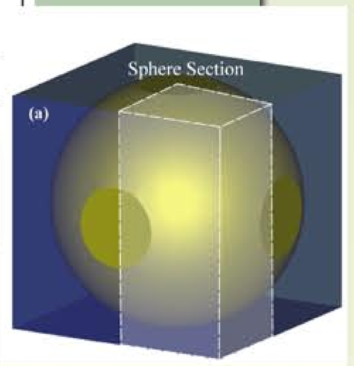
Time lapse maps of biofilm structure as a function of growth. The maps are collected at different stages in the growth of a biofilm at the time shown after initial inoculation. Orange tones indicate water restricted within a biofilm and black is the bulk unrestricted water. Images are acquired in the absence of flow, however, the flow direction for growth periods between images is left to right.

UPSCALING









Right: Comparison of theoretical upscaling results (line) for dispersion in a periodic unit cell (lower right) with experimental observations of dispersion in porous media (symbols). Based on volume averaging techniques. From Wood, B. D. "Inertial influence on pore-scale dispersion in porous media," presented at the 2007 SIAM Conference on Mathematical and Computaional Issues in the Geosciences, March 18-22, 2007, Santa Fe, New Mexico.

ABSTRACT

Effective environmental management of DOE sites requires reliable prediction of reactive transport phenomena. A central issue in prediction of subsurface reactive transport is the impact of multiscale physical, chemical, and biological heterogeneity. Heterogeneity manifests itself through incomplete mixing of reactants at scales below those at which concentrations are explicitly defined (i.e., the numerical grid scale). This results in a mismatch between simulated reaction processes (formulated in terms of average concentrations) and actual processes (controlled by local concentrations). At the field scale, this results in apparent scale-dependence of model parameters and inability to utilize laboratory parameters in field models. Accordingly, most field modeling efforts are restricted to empirical estimation of model parameters by fitting to field observations, which renders extrapolation of model predictions beyond fitted conditions unreliable.

The objective of this project is to develop a theoretical and computational framework for 1) connecting models of coupled reactive transport from pore-scale processes to field-scale bioremediation through a hierarchy of models that maintain crucial information from the smaller scales at the larger scales; and 2) quantifying the uncertainty that is introduced by both the upscaling process and uncertainty in physical parameters.

One of the challenges of addressing scale-dependent effects of coupled processes in heterogeneous porous media is the problem-specificity of solutions. Much effort has been aimed at developing generalized scaling laws or theories, but these require restrictive assumptions that render them ineffective in many real problems. We propose instead an approach that applies physical and numerical experiments at small scales (specifically the pore scale) to a selected model system in order to identify the scaling approach appropriate to that type of problem. Although the results of such studies will generally not be applicable to other broad classes of problems, we believe that this approach (if applied over time to many types of problems) offers greater potential for long-term progress than attempts to discover a universal solution or theory. We are developing and testing this approach using porous media and model reaction systems that can be both experimentally measured and quantitatively simulated at the pore scale, specifically biofilm development and metal reduction in granular porous media.

The general approach we are using in this research follows the following steps:

1. Perform pore-scale characterization of pore geometry and biofilm development in selected porous media systems.
2. Simulate selected reactive transport processes at the pore scale in experimentally measured pore geometries.
3. Validate pore-scale models against laboratory-scale experiments.
4. Perform upscaling to derive continuum-scale (local darcy scale) process descriptions and effective parameters.
5. Use upscaled models and parameters to simulate reactive transport at the continuum scale in a macroscopically heterogeneous medium.

Collaborations:

This project is closely linked with two other projects, also initiated this year, that focus on scale issues in modeling reactive transport processes:

Hybrid Numerical Methods for Multiscale Simulations of Subsurface Biogeochemical Processes.

Funded by BER through the SciDAC program (joint with ASCR). This project is developing and evaluating methods for directly integrating models at different scales (e.g., pore- and continuum-scales) for cases in which upscaling is not effective. PIs: T. Scheibe, A. Tartakovsky, B. Palmer, K. Schuchardt (PNNL); D. Tartakovsky (UC San Diego); P. Meakin, G. Redden (INL); S. Brooks (ORNL). See http://subsurface.pnl.gov for more information.

Coupling In Silico Microbial Models with Reactive Transport Models to Predict the Fate of Contaminants in the Subsurface.

Funded by ERSP. This project will integrate cellular-scale in silico models of microbial function with continuum-scale reactive transport models. PIs: D. Lovley (UMass); T. Scheibe and P. Long (PNNL); R. Mahadevan (U. of Toronto).

PAPERS and PRESENTATIONS:

Tartakovsky, A. M., T. D. Scheibe, and P. Meakin. "Smoothed particle hydrodynamics model for reactive transport and biomass growth," submitted to Proceedings of the 2nd International Conference on Porous Media and its Applications in Science and Engineering (June 17-21, 2007, Kauai, Hawaii).

Niewiadomski, M. M. C. L. Rakowski, M. C. Richmond and W. P. Johnson. "Colloid Retention in Porous Media: CFD Flow Field Modelling in Colloid Trajectory Simulations in Porous Media with Particular Consideration of Grain to Grain Contact," Abstract submitted to the 81st ACS Colloid & Surface Science Symposium (June 24-27, 2007, Newark, Delaware).

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