

# Environmental Management Science Program

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## **Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media**

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## Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Porous Media

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### Research Objective

Dynamic microbial attachment/detachment occurs in subsurface systems in response to changing environmental conditions caused by contaminant movement and degradation. Understanding the environmental conditions and mechanisms by which anaerobic bacteria partition between aqueous and solid phases is a critical requirement for designing and evaluating in-situ bioremediation efforts. This interdisciplinary research project will provide fundamental information on the attachment/detachment dynamics of anaerobic bacteria in heterogeneous porous media under growth and growth-limiting conditions. Experiments will provide information on passive and active attachment/detachment mechanisms used by growing anaerobes capable of reductive dechlorination. Theoretical representations of these attachment/detachment mechanisms will be incorporated into existing flow and transport models that incorporate heterogeneity effects and can be used to predict behavior at field scales. These mechanistic-based models will be tested against experimental data provided through controlled laboratory experiments in heterogeneous porous media in large (meter-scale) 2-D flow cells. In addition to a mechanistic-based predictive model, this research will lead to new theories for the transient spatial distribution of microbial populations and contaminant plumes in heterogeneous porous media, improving our capability for designing staged remediation strategies for dealing with mixed contaminants.

### Research Progress and Implications

The central challenge of in-situ remediation strategies is the control of the transient spatial distribution of contaminants and remediation reagents (e.g., nutrients or microorganisms) in the presence of natural physical and chemical heterogeneities. Currently available predictive tools rely almost exclusively on the representation of passive attachment/detachment processes (e.g., filtration, sedimentation) with the bacterium treated as an inert biocolloid. One of the most intractable aspects of bioactive transport, however, is active microbial partitioning (e.g., attachment/ detachment) under growth and transport in physically and chemically heterogeneous systems. Active attachment/detachment is associated with microbial physiologic response to changes in local aqueous concentrations of nutrients and electron-acceptors: this process is treated rarely in field-scale bacterial transport theories, and not at all in available predictive tools.

Understanding coupled contaminant and bacterial transport in real media is critical to the success of potential future bioremediation/biobarrier strategies at DOE sites. Disposal of chlorinated hydrocarbons has generated extensive contaminant plumes in sand/gravel aquifers at DOE's Savannah River Site (SRS) in South Carolina and Paducah Gaseous Diffusion Plant (PGDP) in Kentucky, and such organic solutes interact with natural environments in coupled complex ways that have serious ramifications for remediation. For example, during the SRS in-situ bioremediation demonstration, 90% of the increase in methanotroph biomass arising from degradation of trichloroethylene (TCE) partitioned into the aqueous phase. Initially, this methanotroph population was primarily attached to solid surfaces. If this partitioning behavior during bioremediation were understood and could be predicted, the knowledge could be exploited to effectively distribute the biomass across a contaminated area and to plan an injection network so as to minimize costly well construction and dampen or

eliminate microbially-induced reductions in hydraulic conductivity. This basic knowledge on the transport response of microorganisms is required for any subsurface remediation involving microbes, including staged approaches that sequentially degrade and immobilize multiple contaminants. Staged approaches (temporal or spatial) can exploit the different transport properties of distinct microbial populations and are especially well suited to DOE mixed contaminant problems.

### **Research Progress**

The work on this project is being coordinated among six different investigators at five different institutions, Madilyn Fletcher (University of South Carolina), John Cushman (Purdue University), Timothy Ginn (University of California, Davis), David Boone (Oregon Graduate Institute), and Ellyn Murphy and Donald Friedrich (Pacific Northwest National Laboratory). In addition, three post doctoral students have been supported by this project, Paula van Schie (USC), Robert Smits (Purdue), and Zheming Wang (PNNL).

**Adhesion Behavior of Anaerobes:** Thus far, the adhesion characteristics of two anaerobes (*D. tiedjei* and *Desulfovibrio*) have been tested, with greatest emphasis on *D. tiedjei*. Results have demonstrated interesting contrasts among these strains, which will be useful when designing experiments for consortium transport. First, the three organisms demonstrate very different attachment properties: *D. tiedjei* adheres in highest numbers, whereas *Desulfovibrio* G11 adheres only when it is actively. Second, the adhesion of *D. tiedjei* remains the same whether the cells are actively growing or starved, whereas that of *Desulfovibrio* is reduced when the cells are starved.

Additional features of the attachment of these organisms will increase the complexity of modeling their transport. Both *D. tiedjei* and *Desulfovibrio* G11 demonstrate significant detachment rates, after initial attachment has occurred. Also, sedimentation of cells has been found to influence attachment numbers on the top-side of surfaces. Thus, cell mass and sedimentation must be accounted for in model development, particularly for the relatively large *D. tiedjei*.

**Stochastic Representations of Bacterial Transport in Porous Media:** A microflow chamber is being constructed at PNNL for use with the confocal microscope to determine the residence time of anaerobic bacteria on porous media. To quantitatively evaluate these experiments, a model of microbial dynamics in the porous media has been developed. This multi-dimensional mathematical model depicts sticky Brownian motion with drift, as a general representation of microbial transport with attachment/detachment. A sticky Brownian motion with drift allows a particle (e.g., microbe) to diffuse by classical Brownian motion in a pressure-induced convective field, except when it hits a wall. When it hits the wall it sticks for a random period of time, which is dictated by a probabilistic stickiness condition. Therefore, this model predicts the location in space of a microorganism as a function of the random force, the drift, and the boundary force. The random force is the diffusive, Brownian-like motion (e.g., motility) and kinematic dispersion in porous media; drift is the convection due to water flow; and the boundary force is the sticking probability dependent on space. This pore-scale model has been successfully upscaled to that of a homogeneous porous medium via a central limit argument for continuous ergodic Markov processes.

**In Situ Spectroscopy:** A laser and fiber optic system has been constructed to observe real-time biomass distribution in porous media. This system takes advantage of the natural fluorescent properties of methanogens (e.g., cofactor F420) or genetically-engineered microorganisms containing a green fluorescent protein. The prototype system has been tested with microspheres which fluoresce in the blue region like the methanogens and with *Pseudomonas cepacia* containing the green fluorescent protein. As the pulse of microspheres move along the length of the column some tailing is observed and an increase in effective macrodispersion with increasing distance along the column, is also observed. The characteristics of the interior breakthrough curves are consistent with the breakthrough curve at the end of the column suggesting that the laser fiber optic system is observing a “representative” interior cross-section of the column. This system will next be implemented in the flow cell.

**Design of Flow Cell Experiments:** A numerical representation of a heterogeneous flow field found at the Oyster Site was used to conduct a theoretical experiment to demonstrate the relative effect of dynamic attachment/detachment of bacteria on the degradation of a contaminant plume. We define kinetic attachment/detachment as a partitioning process which arises from cell division and growth

and can be described by determining a forward (attachment) and reverse (detachment) rate kinetic within a growth model. Dynamic attachment/detachment occurs when the forward and reverse rate kinetic varies with metabolic activity. In the mechanistic description, the forward attachment kinetic varies inversely with the specific growth rate, or as growth activity increases, aqueous partitioning of the bacteria increases. Two anaerobic bacteria were used in the consortium, *Syntrophobacter* which degrades propionate to formate and hydrogen, and *D. tiedjei* which uses formate as an electron donor and dechlorinates hydrocarbons as an electron acceptor. In one experiment, both *Syntrophobacter* and *D. tiedjei* were controlled by kinetic attachment/detachment rates and in the second experiment *Syntrophobacter* attachment was dynamic (varies with metabolic activity) and *D. tiedjei* attachment remained kinetic.

A pulse (or plume) of chlorinated hydrocarbon was injected into a heterogeneous flow field and the break-through curves of the contaminants were evaluated. When *Syntrophobacter* undergoes dynamic attachment/detachment, 58% more of the contaminant is degraded than when the attachment/detachment is kinetic. The enhanced degradation under dynamic conditions is due to the aqueous partitioning of *Syntrophobacter* which results in an increasing population of this propionate-degrading organism as the contaminant plume moves along the flow path. In this example, the rate of propionate degradation was limiting the metabolic activity of *D. tiedjei* which promotes the dechlorination reaction. This example clearly illustrates the importance of dynamic attachment/detachment in intrinsic bioremediation.

## Planned Activities

The different components of this multidisciplinary research are working towards an integrated intermediate scale flow cell experiment that will take place in FY99. This experiment will be conducted in heterogeneous porous media using a consortia of anaerobic bacteria that collectively dechlorinate hydrocarbons. The information that is currently being collected will be used in the design of this experiment and includes: 1) attachment/detachment kinetics of the different bacterial strains under conditions of growth and starvation; 2) mineralogical controls on the attachment/detachment kinetics of the different strains; 3) mechanistic relationships which describe transport under varying nutrient conditions; 4) in-situ, fiber optic detection of biomass in porous media; 5) growth kinetics of the individual species within the consortia; and 6) upscaling of biogeochemical reactions in heterogeneous porous media.

## Other Access To Information

- Cushman, J.H., and B.X. Hu. 1997. Solutions to the stochastic transport problem of  $O(\epsilon)$  for conservative solutes. *Stochastic Hydrology and Hydraulics* 11:297-302.
- Cushman, J.H., and T.R. Ginn. 1998. Reactive contaminant transport in the saturated zone. In "Groundwater Hydrology Handbook", J. W. Delleur (ed), CRC Press (in press).
- Smits, R.G., and J.H. Cushman. 1998a. Application of sticky Brownian motion to microbial dynamics in porous media. 1: Random walks (submitted).
- Smits, R.G., and J.H. Cushman. 1998b. Application of sticky Brownian motion to microbial dynamics in porous media 2: Upscaling via a central limit theorem (submitted)
- Hu, B.X., A. Hassan, and J.H. Cushman. 1998. Solutions to the conservative transport problem of  $O(\epsilon)$  coupled with the flow problem of  $O(\epsilon^4)$ . *Water Resources Research* (submitted).
- Irwin, N.C., S.A. Altobelli, J.H. Cushman, and R.A. Greenkorn. 1998a. Examination of stochastic perturbation theory by magnetic resonance imaging in aperiodic heterogeneous media. *Water Resources Research* (submitted).
- Irwin, N.C., S.A. Altobelli, J.H. Cushman, and R.A. Greenkorn. 1998b. Magnetic resonance imaging experiments for examination of solutions to the stochastic transport problem of order  $\epsilon^N$ . *Water Resources Research* (submitted).
- Ginn, T.R.. 1998. Comment on "Stochastic analysis of oxygen-limited biodegradation in three-dimensionally heterogeneous aquifers," by F. Miralles-Wilhelm et al., in press, *Water Resources Research*.
- Ginn, T.R. and E.M. Murphy. 1998. The influence of subsurface heterogeneity on biodegradation. *Invited Review for Soil Science Society of America Journal*.
- Murphy, E.M., T.R. Ginn, F.J. Brockman, and D.R. Boone. 1997. Growth effects on the partitioning and transport of bacteria, *American Geophysical Union Fall Meeting, EOS Transactions*, 78(46), pp F231.
- Murphy, E.M., and T.R. Ginn. 1996. The role of passive and active partitioning in microbial transport in natural and contaminated systems, *American Geophysical Union Fall Meeting, EOS Transactions*.
- van Schie, P.M., D.R. Boone, and M. Fletcher. 1998. Adhesion of biodegradative anaerobic bacteria to solid surfaces. 98th general meeting of the American Society for Microbiology, Atlanta, GA, May 17-21, 1998.