Dynamics of Coupled Contaminant and Microbial Transport in Heterogeneous Media

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Statement of the Need

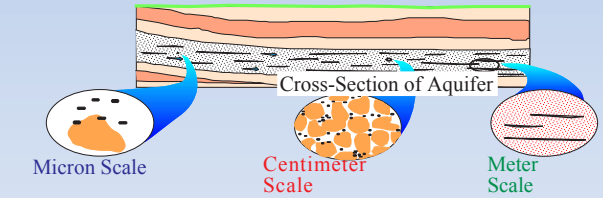
OEM subsurface remediation involves contaminant mixtures in physically, chemically, and microbiologically heterogeneous environments:

- Heterogeneities affect the contaminant and microorganism distribution and therefore influence subsurface manipulation strategies.
- Bioremediation design requires understanding basic processes controlling degradation and microbial transport with dynamic growth conditions in natural heterogeneous systems.
- We do not understand the transport behavior of anaerobes.

Bacteria move during biodegradation, yet biomass is generally treated as a fixed phase in models. If we understood transport behavior we could:

- develop more robust predictive tools
- enhance bioremediation to take advantage of the transport behavior of bacteria, especially those involved in consortium ecosystems.
- assess staged remediation strategies for dealing sequentially with mixed contaminants under transient conditions.

Research Approach Based on Scales of Observation



Batch Experiments

- Kinetics of solute degradation and bacterial growth
- Bacterial attachment/ detachment

Microflow chamber experiments

- kinetics of bacterial attachment/ detachment in controlled flow field

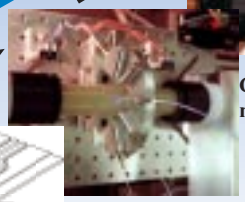
Column Experiments

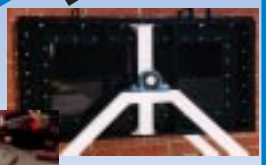
- Convective-dispersive solute and microbial transport in saturated porous media.
- Bulk phase kinetics of bacterial degradation and attachment/ detachment.

Intermediate-Scale Experiments

- Coupled fate and transport in meter-scale flow cell with analog hetero-geneities.

Field.





Particle-scale modeling (Purdue)

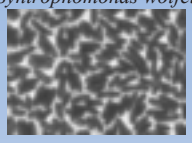
- transport
- attachment/detachment

Continuum-scale modeling (UC Davis)

- consortium biodegradation
- growth-coupled transport and attachment/ detachment

Anaerobic Consortia Used in Experiments

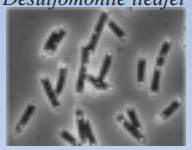
Syntrophomonas wolfei

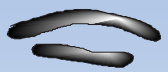


0.5-1 x 2-3 µm
slightly motile

butyrate $\xrightarrow{\text{fermentation}}$ formate, acetate, H_2

Desulfomonile tiedjei



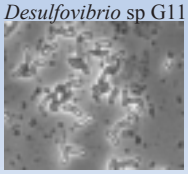


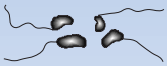
1 x 5-10 µm
non-motile

PCE or TCE → TCE + Cl^- or DCEs + Cl^-

formate $\xrightarrow{e^-}$ CO_2; SO_4^{2-} $\xrightarrow{e^-}$ S^{2-}

Desulfovibrio sp G11





0.5 x 1-2 µm
highly motile

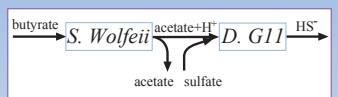
formate $\xrightarrow{e^-}$ CO_2; SO_4^{2-} $\xrightarrow{e^-}$ S^{2-}

Anaerobe	Function/Reason for Selection
Desulfomonile tiedjei	reductive dehalogenation of chlorinated hydrocarbons
Syntrophomonas wolfei	propionate-degrading, produces H_2, formate for *D. tiedjei*
Desulfovibrio G-11	competes with *D. tiedjei* for sulfate as e- acceptor & formate
Methanospirillum hungateii	competes with *D. tiedjei* for formate, naturally fluorescent

Degradation and growth kinetics

Anaerobe degradation and growth is modeled via an accounting of dynamic product inhibition, where G is the mass-action ratio for the degradation reaction...

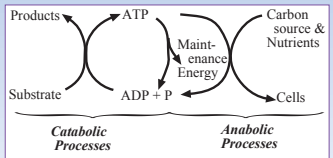
$$\mu = \mu_{max} \frac{S\left(1-\Gamma/K\right)}{K_s + S\left(1-\Gamma/K\right)}$$



Schematic diagram of an anaerobic syntropic butyrate-degrading coculture composed of S. Wolfeii and D. G11

...and maintenance energy limitations on anabolic growth when ATP required for maintenance requirements exceeds the ATP produced from the catabolic reaction.

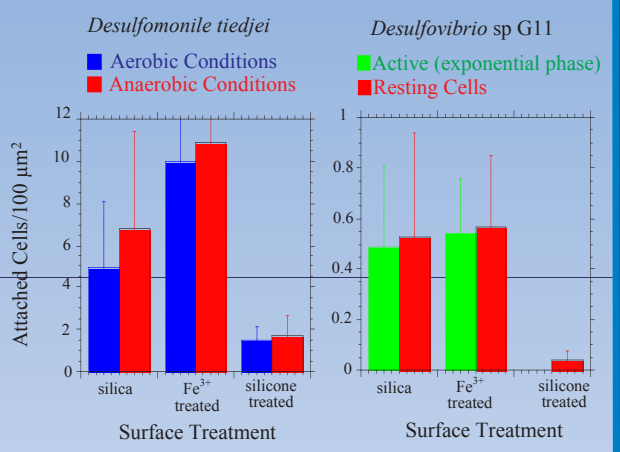
$$\frac{\partial X}{\partial t} = \begin{cases} 0 & \frac{\partial C_{ATP}^{X}}{\partial t} < 0 \\ Y \frac{\partial C_{ATP}^{X}}{\partial t} & \frac{\partial C_{ATP}^{X}}{\partial t} \geq 0 \end{cases}$$

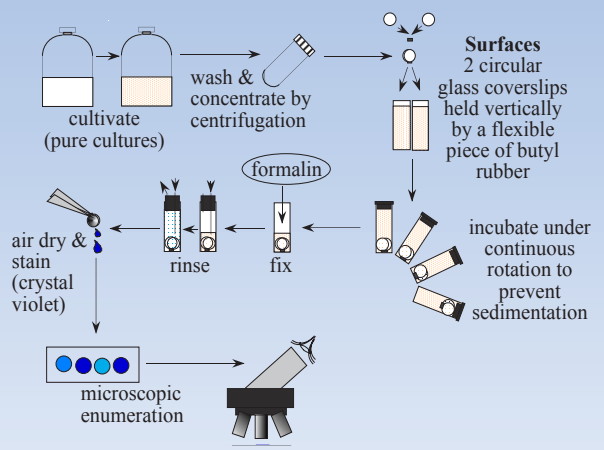


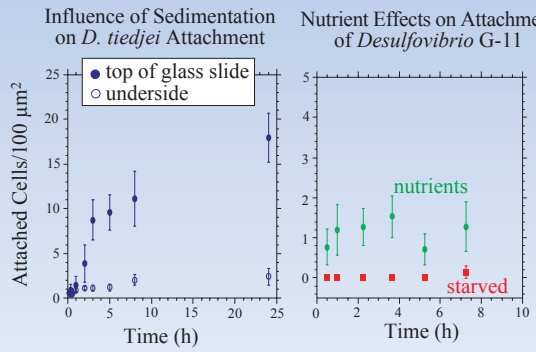
Schematic diagram of carbon and energy flow through a simplified microbial metabolic system. Our kinetics distinguish ATP availability for anabolic growth.

Micron-Scale Experiments of Bacterial Adhesion Processes

Batch studies of attachment to surfaces
- attachment to different surface treatments
- attachment by sedimentation
- attachment differences between actively growing and starved cells
- consortium member interactions on attachment

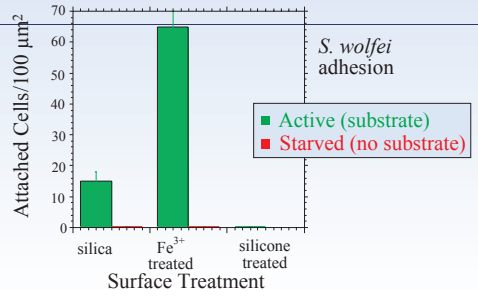






Results of Micron Scale Experiments:

- Mineral surface charge has variable effects on anaerobe adhesion within the consortia
- Sedimentation significantly affects the adhesion of *D. tiedjei* and *D. tiedjei* adhesion is irreversible
- Distinction between active phase (exponential growth) and active phase (presence of nutrients) on the attachment behavior of *Desulfovibrio*--- attachment greater in the presence of nutrients.
- *S. wolfei* showed strong adhesion to surfaces, but only in the presence of substrate (crotonate).

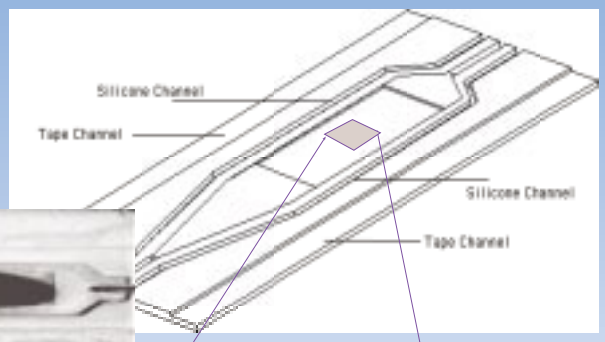


Microflow chamber experiments
- advective transport through planar flow field
- nonuniform microscale velocity field
- serial imaging for bacterium trajectory observation

Steady flow through narrow rectangular section with coverslip top allows confocal imaging of tracers and bacteria in real time.

Molecular tracer transport is by convection with Taylor diffusion.

Modeling cytoscale transport with cytoscale observations allows formation and **upscaling** of quantitative descriptions of transport and attachment processes.



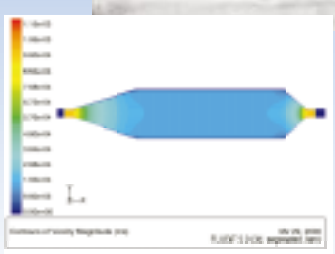
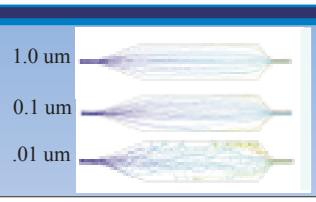


Image of Desulfomonile tiedjei during transport in microflowchamber

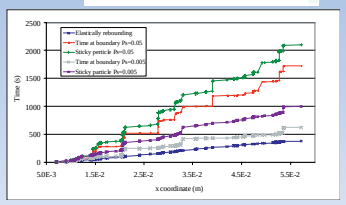
Mechanisms of Dymanic Attachment/Detachment and Upscaling

Modeling bacterial transport and attachment/detachment in the microflow chamber

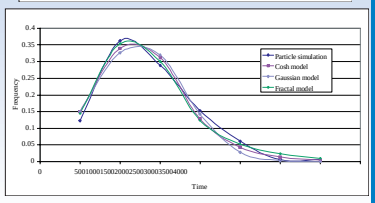
Force-Balance Particle Tracking using numerical solution to velocity field: Here are pathlines shown for three particle diameters:



Single particle x position vs. time: elastically rebounding particle, with time spent at boundary for sticky particle trajectories. Two different slow time probabilities modeled: Ps=0.005 and Ps=0.05 seconds.



Breakthrough curves for Brownian particles of diameter 1 um, bimodal attachment (two sticking intervals). Simulated and Gaussian, hyperbolic cosine, and exponential-fractal models with best fit statistical parameters.

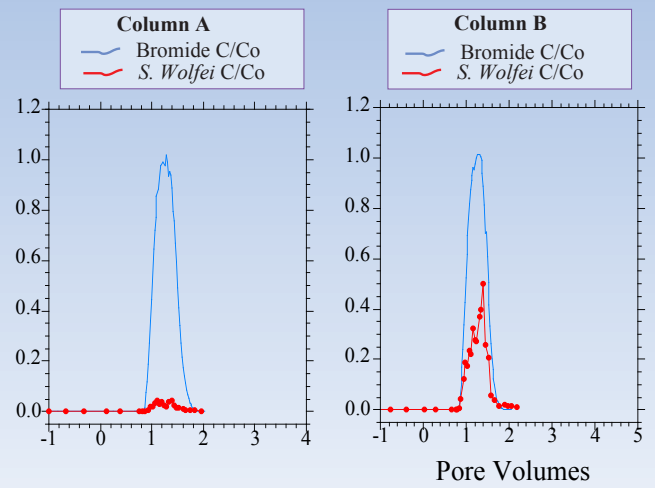


Column Experiments to observe effects of substrate degradation activity on the transport of *S. Wolfei* in porous media

***D. tidjeii* and *S. wolfei* Combined Column Experiment**

Objective:to determine the effect of metabolic activity on the attachment/ detachment kinetics of *S. wolfei* and *D. tiedjeii*. 60/40 Accusand is presaturated with *D. tiedjeii* (shown to irreversibly attach in the batch experiments) in both columns A and B. . .

Both of the 30.5 cm long columns receive anaerobic MSNS (0.01M/L PIPES/ MSNS), but column A also has a constant amount of 20 mM crotonate present in solution, as substrate for the *S. Wolfeii*, a 1PV pulse of which at10^8 cells/mL is injected into each column at t = 0 hrs. The tracer solution of *S. wolfeii* also contains a 50 ppm Cl tracer.



- **Column experiments in medium sand exhibit *S. Wolfei/D. Tiedjei* behaviour that is consistent with that discovered in the batch studies.**
- ***S. Wolfei* transport is strongly dependent on its growth state.**
- **This consortium exhibits differential (among members) and dynamic (with activity) bacterial transport, which can have dramatic impacts and dramatic opportunities for in situ bioremediation.**

Example of How Dynamic Partitioning of Bacteria can Effect the Degradation of a Contaminant Plume

Kinetic Attachment/Detachment: A forward (attachment) and reverse (detachment) rate kinetic determines the relative concentrations of bacteria in the aqueous and solid phases.

$$\phi \frac{\partial C_{Lm}}{\partial t} + \nabla \cdot (C_{Lm} V) = \nabla \cdot [D \nabla C_{Lm}] + \mu_L C_{Lm} \left[\frac{C_p}{K_p + C_p} \right] - K_{Lf} C_{Lm} + K_{Lr} C_{Li}$$

$$\frac{\partial C_{Li}}{\partial t} = \mu_L C_{Li} \left[\frac{C_p}{K_p + C_p} \right] + K_{Lf} C_{Lm} - K_{Lr} C_{Li}$$

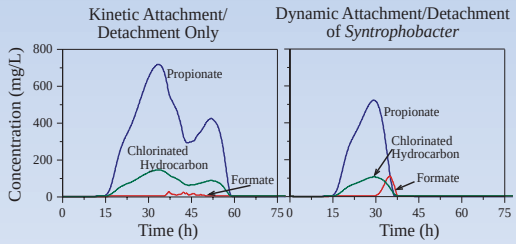
Dynamic Attachment/Detachment: the forward and reverse rate kinetic varies dynamically with growth.

$$\phi \frac{\partial C_{Lm}}{\partial t} + \nabla \cdot (C_{Lm} V) = \nabla \cdot [D \nabla C_{Lm}] + \mu_L C_{Lm} \left[\frac{C_p}{K_p + C_p} \right] - K_{Lf} C_{Lm} \left(1 - \left[\frac{C_p}{K_p + C_p} \right] \right)^n + K_{Lr} C_{Li}$$

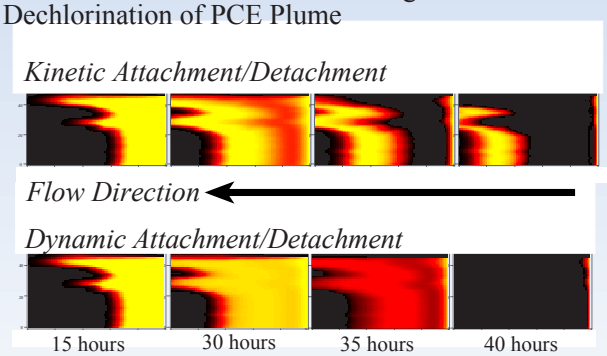
$$\frac{\partial C_{Li}}{\partial t} = \mu_L C_{Li} \left[\frac{C_p}{K_p + C_p} \right] + K_{Lf} C_{Lm} \left(1 - \left[\frac{C_p}{K_p + C_p} \right] \right)^n - K_{Lr} C_{Li}$$

In this simulation we compare the dechlorination of PCE when *D. tiedjei* and *Syntrophobacter* attachment/detachment is:

- kinetic only
- *D. tiedjei* kinetic while *Syntrophobacter* dynamic



Cross Section of Flow Cell Showing Transient Dechlorination of PCE Plume



Simulation Results

58% more of the contaminant is degraded when *Syntrophobacter* undergoes dynamic attachment/detachment. This is due to enhanced aqueous partitioning of *Syntrophobacter* which results in an increasing population of this propionate-degrading organism as the contaminant moves along the groundwater flow path.

For further information, see Timothy Ginn, UC Davis Civil and Environmental Engineering, trginn@ucdavis.edu