Novel Laboratory Methods to Study Reactive Transport in Groundwater

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Scope of the Presentation

- In situ bioremediation by natural attenuation
- Field scale observations and modelling
- Bench scale studies of model plumes
- Studies of attached microbial growth
Monitored Natural Attenuation

- Application of passive biotechnology in situ
- Soils and aquifers are treated as natural bioreactors
- Avoids excavating or pumping out contamination
- *In situ* natural processes reduce environmental risk
  - Dilution to reduce concentration
  - Adsorption to slow down transport
  - Biodegradation to reduce mass
  - Precipitation to immobilise
Conceptual Plume Model
(from D.N. Lerner)

- Ground-water flow
- Slow non-equilibrium mixing
- E-donor or e-acceptor
- Contaminant flux across control plane
- Mixing and anaerobic degradation in the plume interior
- Mixing and aerobic degradation at the plume fringe
The In Situ Bioreactor

Source Term: Organics as Electron Donors

Vertical Dispersive Mixing: $O_2$, $NO_3^-$

Horizontal Dispersive Mixing: $O_2$, $NO_3^-$

Plume Residual: organics; Mineral Oxidants: FeOOH, MnOOH

Horizontal Dispersive Mixing: $O_2$, $NO_3^-$

Background Groundwater: $O_2$, $NO_3^-$

Vertical Dispersive Mixing: $O_2$, $NO_3^-$

Electron and Mass Flux Balance
Anaerobic Biodegradation


Diagram:
- Complex Organic Matter → Hydrolysis
- Sectors: Aromatics, Fermenters, H₂ Acetate Short Chain Fatty Acids, H₂ and SCFA oxidisers, LCFA Oxidisers
- CO₂

- Aromatics
- Sugars Amino Acids → Fermenters
- Long Chain Fatty Acids
- H₂ Acetate Short Chain Fatty Acids
- H₂ and SCFA oxidisers
- LCFA Oxidisers
Numerical Simulations

- Handling Complexity
  - Physical transport processes
  - Geochemical processes
  - Microbiological system dynamics
  - Spatial variability
  - Lots of variables (20-25 solutes, minerals, microbes)

- Apply advanced numerical methods
  - Parallel processors
  - Unstructured mesh generation
  - Automatic adaptive mesh
  - Multi-grid solution methods

The Corona
Plume-Aquifer Interface

Final Grid
• Numerical models now analogous to climate simulations with high speed computing
• Microbiological ecosystem dynamics embedded with geochemical reactive transport model
• Physical and chemical processes well understood
• Understanding microbial processes lags far behind
  – Unknown genotypes and physiologies
  – Unknown interactions with environment
  – Unknown kinetics and parameter values
  – Ripe for a step-change over next decade
Model Laboratory Systems

- 15cm x 30cm bed of quartz sand
- Introduce flow at a point
- Sample flow downstream
- Lab analogue to field plumes
- Controlled experiment
  - Good mass balance
  - Can “design” the reactions
  - Can monitor with fluorescent tracers
Image Analysis
Spatial Resolution of $[O_2(aq)]$
Mathematical Modelling

- Kinetic parameters from batch reactors
- Include cell death
- Simulate active cell numbers
- No change in community
- Map biodegradation rates spatially
Simulating Biomass and Biodegradation Rates
Biofilm on sand grains
RC92 attached to hydrophobic PS
Macromolecules in biofilms

Use confocal Raman micro-spectroscopy to investigate the macromolecular make-up of biofilms

- Demonstrate that planktonic and biofilm cells are phenotypically different
- Verify the role of lipids in *Rhodococcus* sp. biofilms
- Identify key molecules involved in Gram negative cell attachment and biofilm proliferation
Future work

• Investigate by confocal microscopy the putative role for proteins in *Sphingomonas* biofilm formation

• Establish rules for ecological selection of classes of organisms and function within natural biofilms
A Quick Glance to the Past

- Metal coordination chemistry and electrolyte theory
- Synthetic ligands and metal ion hydrolysis
- Mineral surface chemistry
- Aquatic chemistry with Garrels, Mackenzie
- .... What next?

Alfred Werner 1913 Nobel
- Schwarzenbach EDTA chemistry
  - Svante Arrhenius 1903 Nobel
  - Sillén Aqueous coordination chemistry
  - Stumm and Schindler Surface coordination chemistry

?
A Look to the Future

• The Cell-Mineral Interface
  – Fundamental research on chemistry of living surfaces
  – Combines molecular and cell biology with nanosciences
  – Big impacts on many environmental applications
  – Builds the biology component into phase interface reactions
  – Provides the conceptual basis for process models

• Biological Imaging
  – Biophotonics: interaction of near-vis light sources with organisms
  – Use of non-destructive, non-invasive imaging in real time
  – Provides chemical state information with spatial structure of living cells
  – Combines with molecular biology of living cells
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Civil & Structural Eng  Animal & Plant Sciences  Chemistry
Physics & Astronomy  Eng Materials  Chemical & Process Eng

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