

Kenneth H Nealon^{1,2,3}Koki Horikoshi¹

¹Subground Animalcule Retrieval (SUGAR) Project, Frontier Research System for Extremophiles, Japan Marine Science and Technology Center (JAM-STE/C), Natsumishima-cho 2-15, Yokosuka 237-0061, Japan

²Department of Earth Sciences, University of Southern California, Hall 223, Los Angeles, CA 90089-0740, United States

³NASA Jet Propulsion Laboratory, 4800 Oak Grove Drive, Pasadena, CA 91109, United States

Subseafloor environments has already been recognized as the largest biosphere on the planet Earth, however, the microbial diversity and activity has been still poorly understood, even in their impacts on biogeochemical processes, tectonic settings, and paleoenvironmental events. We demonstrate here the evaluation of microbial community structure and active habitats in deeply buried cold marine sediments collected from the Sea of Okhotsk by a combined use of molecular ecological surveys and culturing assays.

The piston core sediment (MD01-2412) was collected by IMAGES (International Marine Global Change Study) Project from the southeastern Okhotsk Sea, June 2001. The total recovered length was about 58m. The lithology of the core sediment was mainly constructed from pelagic clay (PC) and volcanic ash layers (Ash). We collected aseptically the most inside core parts from 16 sections at different depths for microbiological study. The direct count of DAPI-stained cells revealed that the cells in Ash samples were present 1.2 to 2.2 times higher than in PC samples. The quantitative-PCR of 16S rDNA between bacterial and archaeal rDNA suggested that the increased population density in Ash layers was caused by the bacterial components. We studied approximately 650 and 550 sequences from bacterial and archaeal rDNA clone libraries, respectively. The similarity and phylogenetic analyses revealed that the microbial community structures were apparently different between in Ash layers and PC samples. From bacterial rDNA clone libraries, the members within gamma-Proteobacteria such as genera Halomonas, Shewanella, Psychromonas and Methylosinus were predominantly detected in Ash layers whereas the Dehalococcoides group and delta-Proteobacteria were major bacterial components in PC samples. From archaeal libraries, the sequences from Ash and PC samples were affiliated into the clusters represented by the environmental sequences obtained from terrestrial and deep-sea environments, respectively. We evaluated the activity of microorganisms in subseafloor environments by the culturing assay. The colony forming unit (CFU) counts on three kinds of media and at four different incubation temperatures (5, 15, 25, 35 deg.C) revealed that the bacteria in Ash layers were in fact alive even at around in-situ temperature (<15 deg.C). In addition, the rDNA phylogenetic analysis of these isolates indicated the consistency results of environmental rDNA analyses.

In conclusion, the permeable ash layer buried in subseafloor environments is significant for discrete microbial habitat, and at least most of bacteria in ash layers within 60 m are indeed alive and may impact on the biogeochemical circulations in subseafloor environments.

B72B MCC: Hall C Sunday 1330h Biogeochemical Reaction Modeling in Sediment and Soil Environments Posters (joint with H, OS)

Presiding: E Roden, University of Alabama; W Burgos, Pennsylvania State University

B72B-0761 1330h POSTER

Reaction-based modeling of quinone-mediated bacterial iron(III) reduction

William D Burgos¹ (814-863-0578; bburgos@psu.edu)

Yilin Fang¹

Richard A Royer¹

Gour Tsyh Yeh²

Brian A Dempsey¹

¹Pennsylvania State University, Department of Civil and Environmental Engineering 212 Sackett Building, University Park, PA 16802-1408, United States

²University of Central Florida, Department of Civil and Environmental Engineering 4000 Central Florida Blvd., Orlando, FL 32816-2450, United States

This paper presents and validates a new paradigm for modeling complex biogeochemical systems using a diagonalized reaction-based approach. The bioreduction kinetics of hematite by the dissimilatory metal-reducing bacterium (DMRB) *Shewanella putrefaciens* strain CN32 in the presence of the soluble electron shuttling compound anthraquinone-2,6-disulfonate (AQDS) is used for presentation/validation purposes. Experiments were conducted under nongrowth conditions with H₂ as the electron donor. In the presence of AQDS, both direct biological reduction and indirect chemical reduction of hematite by bioreduced anthrahydroquinone-2,6-disulfonate (AH2DS) can produce Fe(II). Separate experiments were performed to describe the bioreduction of hematite, bioreduction of AQDS, chemical reduction of hematite by AH2DS, Fe(II) sorption to hematite, and Fe(II) biosorption to DMRB. The independently determined rate parameters and equilibrium constants were then used to simulate the parallel kinetic reactions of Fe(II) production in the hematite-with-AQDS experiments. Previously determined rate formulations/parameters for the bioreduction of hematite and Fe(II) sorption to hematite were systematically tested by conducting experiments with different initial conditions. As a result, the rate formulation/parameter for hematite bioreduction was not modified, but the rate parameters for Fe(II) sorption to hematite were modified slightly. The hematite bioreduction rate formulation was first-order with respect to hematite free surface sites and zero-order with respect to DMRB based on experiments conducted with variable concentrations of hematite and DMRB. The AQDS bioreduction rate formulation was first-order with respect to AQDS and first-order with respect to DMRB based on experiments conducted with variable concentrations of AQDS and DMRB. The chemical reduction of hematite by AH2DS was fast and considered to be an equilibrium reaction. The simulations of hematite-with-AQDS experiments were very sensitive to the equilibrium constant for the hematite-AH2DS reaction. The model simulated the hematite-with-AQDS experiments well if it was assumed that the ferric oxide surface phase was a non-crystalline hydroxide rather than hematite. This is the first reported study where a diagonalized reaction-based model was used to simulate parallel kinetic reactions based on rate formulations/parameters independently obtained from segregated experiments.

B72B-0762 1330h POSTER

Kinetic Modeling of Biogeochemical Processes in Subsurface Environments: Coupling Transport, Microbial Metabolism and Geochemistry

Yifeng Wang (505-234-0030; ywang@sandia.gov)

Sandia National Laboratories, 4100 National Parks Highway, Carlsbad, NM 88220, United States

Microbial reactions play an important role in regulating pore water chemistry (e.g., pH and Eh) as well as secondary mineral distribution in many subsurface systems and therefore directly control trace metal migration and recycling in those systems. In this paper, we present a multicomponent kinetic model that explicitly accounts for the coupling of microbial metabolism, microbial population dynamics, advective/dispersive transport of chemical species, aqueous speciation, and mineral precipitation/dissolution in porous geologic media. A modification to the traditional microbial growth kinetic equation is proposed, to account for the likely achievement of quasi-steady state biomass accumulations in natural environments. A scale dependence of microbial reaction rates is derived based on both field observations and the scaling analysis of reactive transport equations. As an example, we use the model to simulate a subsurface contaminant migration scenario, in which a water flow containing both uranium and a complexing organic ligand is recharged into an oxic carbonate aquifer. The model simulation shows that Mn and Fe oxyhydroxides may vary significantly along a flow path. The simulation also shows that uranium (VI) can be reduced and therefore immobilized in the anoxic zone created by microbial degradation.

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B72B-0763 1330h POSTER

Moving from Batch to Field Using the RT3D Reactive Transport Modeling System

T. Prabhakar Clement¹ (1-334-844-6268; clement@eng.auburn.edu)

Tirtha Raj Gautam² (61-8-9380-3083; gautam@cwr.uwa.edu.au)

¹Department of Civil Engineering, 212 Harbert Engineering Center, Auburn University, Auburn, AL 36849-5337, United States

²Centre for Water Research, The University of Western Australia, Crawley, WA 6009, Australia

The public domain reactive transport code RT3D (Clement, 1997) is a general-purpose numerical code for solving coupled, multi-species reactive transport in saturated groundwater systems. The code uses MODFLOW to simulate flow and several modules of RT3D to simulate the advection and dispersion processes. RT3D employs the operator-split strategy which allows the code solve the coupled reactive transport problem in a modular fashion. The coupling between reaction and transport is defined through a separate module where the reaction equations are specified. The code supports a versatile user-defined reaction option that allows users to define their own reaction system through a Fortran-90 subroutine, known as the RT3D-reaction package. Further a utility code, known as BATCHRXN, allows the users to independently test and debug their reaction package. To analyze a new reaction system at a batch scale, users should first run BATCHRXN to test the ability of their reaction package to model the batch data. After testing, the reaction package can simply be ported to the RT3D environment to study the model response under 1-, 2-, or 3-dimensional transport conditions. This paper presents example problems that demonstrate the methods for moving from batch to field-scale simulations using BATCHRXN and RT3D codes. The first example describes a simple first-order reaction system for simulating the sequential degradation of Tetrachloroethene (PCE) and its daughter products. The second example uses a relatively complex reaction system for describing the multiple degradation pathways of Tetrachloroethane (PCA) and its daughter products.

References

1) Clement, T.P., RT3D - A modular computer code for simulating reactive multi-species transport in 3-Dimensional groundwater aquifers, Battelle Pacific Northwest National Laboratory Research Report, PNNL-SA-28967, September, 1997. Available at: <http://bioprocess.pnl.gov/rt3d.htm>.

B72B-0764 1330h POSTER

Reactive Iron deposition and ground water inflow control neutralization processes in acidic mine lakes

Christian Blodau (0049-921-552223; christian.blodau@uni-bayreuth.de)

Limmological Research Station and Department of Hydrology, University of Bayreuth, Universitaetsstrasse 30, Bayreuth 95444, Germany

The controls on the internal neutralization of highly acidified waters by iron sulphide accumulation are yet poorly understood. To elucidate the influence of ground water inflow on neutralization processes, inventories of solid phase iron and sulphur, pore water profiles and rates of ferrous iron and sulphate production and consumption were analyzed in different areas of an acidic mine lake. Ground water inflow had previously been determined by ground water modelling and chamber measurements (Knoll et al., 1999). The investigated sediments adjacent to mine tailings, which were subject to the inflow of groundwater (10-30 L d⁻¹ m⁻²), were richer in dissolved ferrous iron (30 vs. 5 mmol L⁻¹) and sulphate (30 vs. 10 mmol L⁻¹) and showed higher pH values (6 vs. 4) than the sediments in areas of the lake not being influenced by groundwater inflow. Sediments adjacent to the mine tailings also showed higher rates of sulphate reduction and iron sulphide accumulation (Fig. 1). From these data it is suggested that neutralization processes in iron rich, acidic mine lakes neutralization processes primarily occur in areas influenced by the inflow of acid mine groundwater. These waters usually have considerably higher pH values than the surface waters in the lakes due to buffering processes in the tailings. The seepage of this water through the sediment might thus lead to higher pH values and thus to a higher thermodynamic competitiveness of sulfate reduction vs. iron reduction (Blodau and Peiffer 2002). This causes increased neutralization rates. These findings have consequences for remediation measures in highly acidic lakes. In areas influenced by the inflow of mine drainage increases in carbon availability, for example by the deposition of particulate organic matter, should enhance iron sulphide formation rates, whereas in other areas increases in carbon availability would only result in enhanced rates of iron reduction without a lasting gain in alkalinity.

Blodau, C. and Peiffer, S. (2002): Thermodynamics and organic matter: Constraints on the internal neutralization of highly acidic waters. Applied Geochemistry, in print. Knoll, D. Weber, L., and Schfer, W. (1999): Grundwasseranbindung von alten Tagebaurestseen im Niederlausitzer Braunkohletagebauebiet. Grundwasser 2/99: 55-61

B72B-0765 1330h POSTER

Reactive Transport Modeling of Microbially-Mediated Chromate Reduction in 1-D Soil Columns

Hanxue Qiu¹ (509-335-7205; qiuh@mail.wsu.edu);Sridhar Viamaajala¹ (509-335-7417;vsridhar@mail.wsu.edu); Mahbub MD. Alam¹

(509-335-2576; mahbub@mail.wsu.edu); Brent M.

Peyton¹ (509-335-4002; bmp@wsu.edu); James N.Petersen¹ (509-335-9141; jnp@wsu.edu); David R.Yonge¹ (509-335-2147; yonge@wsu.edu)¹Center for Multiphase Environmental Research Washington State University, PO Box 642719, Pullman, WA 99164-2719, United States

Cr(VI) reduction tests were performed with the well known metal reducing bacterium *Shewanella oneidensis* MR-1 in liquid phase batch reactors and continuous flow soil columns under anaerobic conditions. In the batch tests, the cultures were grown with fumarate as the terminal electron acceptor and lactate as the electron donor in a simulated groundwater medium to determine yield coefficients and specific growth rates. The bench-scale soil column experiments were carried out with MR-1 to test the hypothesis that the kinetic parameters obtained in batch studies, combined with microbial attachment/detachment processes, will accurately predict reactive transport of Cr(VI) during bacterial Cr(VI) reduction in a soil matrix. Cr(VI)-free simulated groundwater media containing fumarate as the limiting substrate and lactate was supplied to a 2.1cm (ID) x 45 cm soil column inoculated with MR-1 for a duration of 9 residence times to allow for biomass to build-up in the column. Thereafter the column was supplied with both Cr(VI) and substrate. The concentrations of effluent substrate, biomass and Cr(VI) were monitored on a periodic basis and attached biomass in the column was measured in the termination of each column test. A reactive transport model was developed in which 6 governing equations deal with Cr(VI) bioreaction, fumarate (as electron donor) consumption, aqueous biomass growth and transport, solid biomass detachment and attachment kinetics, aqueous and solid phase enzyme reaction and transport, respectively. The model incorporating the enzyme reaction kinetics for Cr(VI) reduction, Monod kinetic expressions for substrate depletion, nonlinear attachment and detachment kinetics for aqueous and solid phase microorganism concentration, was solved by a fully implicit, finite-difference procedure using RT3D (A Modular Computer Code for Reactive Multi-species Transport in 3-Dimensional Groundwater Systems) platform in one dimension. Cr(VI)-free column data was used to calibrate the biomass attachment and detachment terms used in the model. Column data collected with Cr(VI) in the influent was used to calibrate the model. The modeling results indicate that the Cr(VI) and substrate predictions match closely with the column data. The calibrated model was also able to match attached biomass profiles within the column as well as aqueous biomass in the effluent.

B72B-0766 1330h POSTER

Reactive Transport Modelling of pH Dynamics in Aquatic Sediments

Parisa Jourabchi¹ (p.jourabchi@geo.uu.nl)Philippe Van Cappellen¹ (pvc@geo.uu.nl)Pierre Regnier¹ (p.regnier@geo.uu.nl)¹Geochemistry Department Faculty of Earth Sciences Utrecht University, P.O. Box 80021, Utrecht 3508 TA, Netherlands

Reactive transport models can account for the complex set of transport and reaction processes that control the geochemical conditions in aquatic sediments. A diagnostic indicator of reaction processes is pore water pH. Thus, the combination of high resolution pH profiles and reactive transport models has the potential to unravel the interplay of the major biogeochemical processes occurring in sediments.

Existing models do not satisfactorily reproduce measured pH profiles, however. This points to an incomplete understanding, or inadequate representation of the processes that affect the proton balance in sediments. In order to quantify the factors controlling pore water pH distributions, we adopt a systematic approach to modelling the relevant processes. In this contribution, the role of particulate deposition fluxes and calcite dissolution are evaluated.

We used the Biogeochemical Reaction Network Simulator (BRNS), which provides an efficient and flexible modelling environment in that modifications of model formulations are easily implemented and tested. The kinetic formulations of primary and secondary redox reactions, aqueous carbonate and sulfide equilibrium reactions, and calcite dissolution kinetics constitute the reaction network. These reactions are coupled to the transport processes: sedimentation, diffusion, and bioturbation in one dimension.

The buffering effect of calcite dissolution on the pH profiles is evaluated quantitatively under contrasting conditions of inorganic carbon fluxes reaching the sediment-water interface. Two simulation environments are considered, namely deep-sea sediments above and below the lysocline, for which published data exist. These environments display similar redox conditions, yet distinctly different pH profiles. The calculated pH profiles are found to be a highly non-linear function of the solid (organic and inorganic) deposition fluxes. By varying the organic carbon flux, a close correlation between the oxygen penetration depths and the depths of pH minima is observed. This correlation is independent of the pH buffering by calcite dissolution.

B72B-0767 1330h POSTER

Modeling Soil Aquifer Treatment for Artificial Recharge for Sustainable Wastewater Reuse

Jeongkon Kim¹ (614-292-2033;

jkkim@geology.ohio-state.edu)

Jung-Woo Kim² (jwookim@kjist.ac.kr)Heechul Choi² (hchoi@kjist.ac.kr)Franklin Schwartz¹ (frank@geology.ohio-state.edu)¹The Ohio State University, 275 Mendenhall Laboratory 125 South Oval Mall, Columbus, OH 43210, United States²Kwangju Institute of Science and Technology, 1 Oryong Buk-gu, Kwangju 500-712, Korea, Republic of

Growing populations, increasing water demands, and worsening environmental conditions have led to the need for new water supplies in addition to existing surface and groundwater. Recycled water is being considered as one of new water supplies, and a wide variety of options to reuse water has been developed. Where soil and groundwater conditions are favorable, artificial recharge of water through infiltration basins results in a significant improvement in water quality. The unsaturated (vadose) zone acts as a natural filter where physico-chemical and biological processes operate to remove pollutants of concern such as suspended solids, organic and inorganic materials, bacteria, and viruses. The saturated subsurface provide seasonal and longer storage, as well as additional treatment. We developed a 3-dimensional numerical model to simulate the physico-chemical and biological behavior of key constituents, including nitrate, organic carbon, oxygen, ammonia, in recycled water as a consequence of transport in soil/groundwater systems. The model developed in this study was found to effectively describe the dynamics of the key constituents and microorganisms in both unsaturated and saturated subsurface environments. Then, the model was employed to estimate optimum operational conditions of the soil aquifer treatment process. Operation conditions relating to dissolved oxygen levels were found to be a key to obtaining desired water quality improvements. Our ultimate goal is to estimate long-term sustainability of systems and evaluate the efficacy of this approach.

B72B-0768 1330h POSTER

Numerical Modeling of NAPL Source Zone Treatment

Glenn E Hammond¹ (217-333-4162;

ghammond@uiuc.edu)

Albert J Valocchi¹ (217-333-3176;

valocchi@uiuc.edu)

Peter C Lichtner² (505-667-3420; lichtner@lanl.gov)¹Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, 2527 HydroSystems Laboratory, MC-250, 205 N. Mathews, Urbana, IL 61801, United States²EES-6, Los Alamos National Laboratory, MS D469, SM-30 Bikini Atoll Rd., Los Alamos, NM 87545, United States

Experience has demonstrated the poor performance of conventional approaches to remediating NAPL contaminated sites (e.g. pump-and-treat, air sparging, soil vapor extraction, etc.). More recently, researchers have been investigating novel approaches to NAPL source zone treatment such as the HERTZ (Halorespiration Enhancing Redox Transition Zone) technology for bioremediation where carbon sources are injected into the subsurface enhancing in situ reductive dechlorination of halogenated NAPLS (i.e. PCE, TCE). Although this innovative approach has proven effective in controlled small-scale laboratory experiments, this technology still remains relatively unverified at the field scale in a natural subsurface environment. One tool for evaluating the performance of HERTZ in the more complex subsurface is detailed numerical simulation through sophisticated biogeochemical transport modeling.

Recent advances in computational science including superior computational hardware, more efficient numerical algorithms and increased understanding of the

governing equations describing biogeochemical transport have enabled the use of numerical models to more accurately predict/validate the performance of different remediation strategies. In this presentation we investigate the use of numerical models to describe NAPL source zone treatment using HERTZ. The multiphase reactive transport model PARTRAN is used in the simulations. This model is capable of tightly coupling three-dimensional transport and geochemical reaction on large, high-resolution grids through the use of parallel high-performance supercomputers. Simulations are carried out to investigate the influence of small-scale heterogeneities on retention of NAPL contamination during remediation.

URL: <http://www.cce.uiuc.edu/transport/publications/hammond/agu2002/>

B72B-0769 1330h POSTER

Soil Surface CO₂ Flux in a Wheat Field: Measurements and ModelingGeoff L. Doyle¹ (405 262-5291 x261;

gdoyle@gr11.grl.ars.usda.gov)

Peter J. Vaughan² (909 369-4875;

pvaughan@ussl.ars.usda.gov)

¹Grazinglands Research Lab USDA-ARS, 7207 West Cheyenne St, El Reno, OK 73036, United States²George E. Brown, Jr. Salinity Lab USDA-ARS, 450 W Big Springs Road, Riverside, CA 92507, United States

Soil surface CO₂ flux (F_s) is generated primarily by microbial and root respiration. Evaluation of which ecosystem parameters dominate production and transport of CO₂ in soil is necessary to determine those land management techniques that cause an agroecosystem to be a source or sink of carbon. The objective of this study was comparison of numerical model (UNSATCHEM) results to field measurements of F_s by a chamber flux measurement system. Soil temperature, moisture, microbial biomass C, microbial activity, leaf area index (LAI) and F_s were monitored at a winter wheat (*Triticum aestivum* L.) site in Oklahoma from 1998-2001. F_s rates were highest during December-May (8 μmoles m⁻² s⁻¹). Microbial respiration was 82% of the total annual flux (1100 g C m⁻²) for this system. A Q₁₀ of 2.9 (r²=0.998) was determined from 48 h laboratory soil incubations at temperatures between 5 and 45°C. Initial UNSATCHEM modeling of CO₂ production and transport in the uppermost 1.5 m for 958 days starting August 21, 1997 was conducted using standard CO₂ production parameter values for microbial and root respiration. Model prediction generally conformed to measured soil surface CO₂ flux but during each springtime, the period of rapid growth of the wheat, the measured fluxes exceeded model predictions by a factor of approximately 2.5.

B72B-0770 1330h POSTER

Stability Constants for Sulfate Complexation of Yttrium and the Rare Earth Elements

Johan Schijf¹ (1-727-553-3936;

jschijf@seas.marine.usf.edu)

Robert H Byrne¹ (1-727-553-1508;

byrne@seas.marine.usf.edu)

¹College of Marine Science - University of South Florida, 140 7th Avenue S, St. Petersburg, FL 33701-5016, United States

In natural waters, yttrium and the rare earth elements (YREE) are mostly complexed with inorganic anions such as carbonate and chloride. YREE complexation with sulfate is minor (<5%) in seawater and generally negligible in fresh waters, yet it can be quite important in situations where oxidation of pyrite leads to high dissolved sulfate concentrations. The development of a consensus pattern of stability constants for YREE monosulfato-complexes has a quite convoluted history. It is based on a 1974 'compilation' that was derived from a much older, somewhat questionable, dataset, by adding interpolations and omitting a few elements. During subsequent transcriptions, some errors were introduced and the omitted data were interpolated rather than replaced with the original values. All this has resulted in a consensus pattern that is essentially flat, without any structure or fractionation between light and heavy REE. It is widely quoted and has been used to argue that sulfate complexation does not cause YREE fractionation. Conversely, flat YREE patterns in natural waters have been taken as evidence for substantial complexation of the YREE with sulfate. We have taken a new approach to measuring the stability constants of all YREE monosulfato-complexes with the greatest possible precision. Stability constants were determined by comparing the solubility of barium sulfate in YREE chloride solutions and in an ammonium chloride reference solution, all at the ionic strength of seawater. The reference solution and solutions of individual YREE chlorides were equilibrated with a small amount of high purity barium sulfate at t = 25°C for

at least one week. The equilibrated solutions were then filtered and analyzed for concentrations of YREE and Ba (ICP-MS), chloride and sulfate (ion chromatography), and pH (glass electrode). A simple model was used to determine the stability constants from these measurements.

Averaged results from four experiments, two with and two without added sulfate, have standard deviations of 0.03 log units or less. Within this precision, the pattern of stability constants is not flat, as has been assumed, but has a very distinct shape. The pattern is nearly flat from La to Gd, possibly with a slight maximum at Eu. From Gd to Lu it shows a gradual and almost linear decrease, with the stability constant of Lu being more than 0.2 log units below that of La. The stability constant of Y is close to that of Er. Our pattern is in broad agreement with several careful earlier studies that have been largely ignored in the recent literature. Comparison with the substantial body of existing work also indicates that our stability constants are well within the published range for individual YREE. This revised pattern may have significant consequences for the interpretation of YREE patterns in high-sulfate environments such as runoff from mine tailings and certain groundwaters.

B72B-0771 1330h POSTER

Surface Complexation Modelling in Metal-Mineral-Bacteria Systems

Kelly J Johnson¹ ((574) 276-7638; kjohnson@nd.edu)

Jeremy B. Fein¹ ((574) 631-6101; fein.1@nd.edu)

¹University of Notre Dame, Civil Engineering and Geological Sciences, 156 Fitzpatrick, Notre Dame, IN 46556, United States

The reactive surfaces of bacteria and minerals can determine the fate, transport, and bioavailability of aqueous heavy metal cations. Geochemical models are instrumental in accurately accounting for the partitioning of the metals between mineral surfaces and bacteria cell walls. Previous research has shown that surface complexation modelling (SCM) is accurate in two-component systems (metal:mineral and metal:bacteria); however, the ability of SCMs to account for metal distribution in mixed metal-mineral-bacteria systems has not been tested. In this study, we measure aqueous Cd distributions in water-bacteria-mineral systems, and compare these observations with predicted distributions based on a surface complexation modelling approach.

We measured Cd adsorption in 2- and 3-component batch adsorption experiments. In the 2-component experiments, we measured the extent of adsorption of 10 ppm aqueous Cd onto either a bacterial or hydrous ferric oxide sorbent. The metal:bacteria experiments contained 1 g/L (wet wt.) of *B. subtilis*, and were conducted as a function of pH; the metal:mineral experiments were conducted as a function of both pH and HFO content. Two types of 3-component Cd adsorption experiments were also conducted in which both mineral powder and bacteria were present as sorbents: 1) one in which the HFO was physically but not chemically isolated from the system using sealed dialysis tubing, and 2) others where the HFO, Cd and *B. subtilis* were all in physical contact. The dialysis tubing approach enabled the direct determination of the concentration of Cd on each sorbing surface, after separation and acidification of each sorbent.

The experiments indicate that both bacteria and mineral surfaces can dominate adsorption in the system, depending on pH and bacteria:mineral ratio. The stability constants, determined using the data from the 2-component systems, along with those for other surface and aqueous species in the systems, were used with FITEQL to independently predict the amount of adsorption and the partitioning of the Cd in the bacteria-metal-mineral systems. Results from these comparisons suggest that surface complexation modelling is a viable resource for predicting metal partitioning in multi-sorbent geologic systems.

B72B-0772 1330h POSTER

Reaction Kinetics of Alanine Solutions at Elevated Temperatures

Jenny S. Cox¹ (cox@erdw.ethz.ch)

Terry M. Seward¹ (tseward@erdw.ethz.ch)

¹Institut für Mineralogie und Petrographie, ETH-Zentrum, Zürich CH-8092, Switzerland

The reaction kinetics of α -alanine under non-enzymatic, aqueous hydrothermal conditions has been the subject of few experimental studies. Varying conclusions on the alanine system have been reached, with some observing breakdown by pathways such as decarboxylation, and others observing polymerization and cyclization reactions (e.g. Abelson et al.(1957), Berhardt et al.(1984), Kawamura et al.(2001), Li et al.(2002), Vallentyne et al.(1964)). We have been able to observe the reaction kinetics of alanine in situ

at temperature and pressure with a special gold-lined spectrophotometric cell which is also itself the reaction vessel. The identities of the reaction products were further confirmed using ion chromatography (Dionex AminoPAC). A postulated reaction scheme involving reversible polymerization and irreversible breakdown pathways will be presented and its dependence on temperature and other factors will be discussed, with an aim to reconciling conflicting data in the literature. Rate constants for this scheme, derived mathematically from the experimental data using a factor analysis-based method, will be presented up to 185 °C and 20 bar.

URL: <http://www.geochem.ethz.ch>

B72B-0773 1330h POSTER

Laboratory, Field, and Modeling Studies of Aerobic Cometabolism of CAHs by Butane-Utilizing Microorganisms

Maureen Mathias¹ (541-737-6895)

Lewis Semprini¹ (541-737-3099; lewis.semprini@orst.edu)

Mark E Dolan¹ (541-737-3862; mark.dolan@orst.edu)

Perry L McCarty² (650-723-4131)

Gary D Hopkins² (650-723-4131)

¹Department of Civil, Construction, and Environmental Engineering, Oregon State University, Corvallis, OR 97331, United States

²Department of Civil and Environmental Engineering, Stanford University, Stanford, CA 94035, United States

The ability of butane-utilizing microorganisms to aerobically cometabolize a mixture of chlorinated aliphatic hydrocarbons (CAHs) in laboratory microcosms and in an in-situ field demonstration was modeled using parameter values measured in laboratory experiments. The butane grown culture was inoculated into soil and groundwater microcosms and exposed to butane with several repeated additions of 1,1,1-trichloroethane (TCA), 1,1-dichloroethylene (1,1-DCE), and 1,1-dichloroethane (1,1-DCA) at aqueous concentrations of 200 $\mu\text{g/L}$, 100 $\mu\text{g/L}$, and 200 $\mu\text{g/L}$, respectively. The utilization of butane and the transformation of the CAH mixture in the batch microcosms were simulated using differential equations accounting for Michaelis-Menten kinetics with cell growth and decay, substrate utilization, transformation product toxicity, and substrate inhibition of CAH transformation. Both competitive inhibition kinetics and mixed inhibition kinetics, determined in prior laboratory studies, were included in the model construct. The equations were solved simultaneously using fourth-order Runge-Kutta numerical integration. The batch microcosm experimental results were simulated well with parameter values determined independently in culture kinetic studies, with some minor adjustments. Having adequately defined the parameter values from laboratory studies, the biotransformation model was combined with 1-D advective-dispersive transport to simulate the results of in-situ bioremediation tests conducted at the Moffett Field Test Facility in CA. The butane-utilizing culture was injected into a 7 m subsurface test site and exposed to alternating pulses of oxygen and butane, along with TCA (150 $\mu\text{g/L}$), 1,1-DCE (50 $\mu\text{g/L}$) and 1,1-DCA (150 $\mu\text{g/L}$). The model simulated well the transient transformation of the CAHs in response to different butane and oxygen pulse cycles and injection concentrations. Model simulations correlated well with field results and indicated that better remediation performance was achieved when more butane and oxygen were injected in the field test plot with short pulse cycles. 1,1-DCE was the most effectively transformed, followed by 1,1-DCA, and TCA, consistent with model predictions. The model simulations also indicated that as time proceeded, indigenous microorganisms were likely responsible for the effective transformation of 1,1-DCE and limited transformation of 1,1-DCA and TCA. This was consistent with PCR based molecular analysis of the microbial population that was stimulated.

B72C MCC: 132 Sunday 1330h

Water, Energy, and Carbon Exchange in Forest Systems II (joint with A, H, GC)

Presiding: B Law, Oregon State University; P Thornton, National Center for Atmospheric Research; D Baldocchi, University of California, Berkeley

B72C-01 1330h INVITED

Controls on the seasonal cycle of NEE: Inferring temperature dependence of photosynthesis in evergreen needleleaf forests using eddy covariance data

Peter E Thornton¹ (thornton@ucar.edu)

Beverly E Law²

¹National Center for Atmospheric Research Climate and Global Dynamics Division, 1850 Table Mesa Dr., Boulder, CO 80305, United States

²Oregon State University, 328 Richardson Hall, Corvallis, OR 97331-5752, United States

An earlier study showed that simulations of coupled energy, water, carbon, and nitrogen cycles across a broad climate gradient in evergreen needleleaf forests were able to capture between-site variability in leaf area and annual and seasonal variability in evapotranspiration within and across sites, but that the simulated seasonal cycle of net ecosystem exchange of carbon (NEE) compared poorly to observations. In this study we show that this model bias is associated with the choice of Rubisco enzyme kinetic parameters. Optimization to minimize the model bias in seasonal cycle of NEE at each site results in a range of kinetic parameters across the climate gradient. We present results relating the optimized parameters to site climate. We also demonstrate the influence of model bias in the seasonal cycle of NEE on model estimates of NEE at annual and longer time scales.

B72C-02 1345h

A New Model for Scaling from Leaf Lifespan to Conifer Forest Structure and Function

Colin P Osborne¹ (+44 114 222 0146; c.p.osborne@sheffield.ac.uk)

David J Beerling¹ (+44 114 222 4359; d.j.beerling@sheffield.ac.uk)

¹University of Sheffield, Dept. of Animal and Plant Sciences, Sheffield S10 2TN, United Kingdom

Generic relationships between the lifespan, physiology and biochemistry of leaves have recently been quantified for the first time in contrasting biomes and functional groups. These relationships have important consequences for ecosystem biogeochemical cycles, and therefore offer the potential for simulating large-scale forest properties on the basis of leaf lifespan. We have used the scaling mechanisms involved to develop the University of Sheffield Conifer Model (USCM), a tool for simulating conifer carbon, nitrogen, and water fluxes using data on leaf lifespan, climate and soils as inputs. Simulations of net primary production and partitioning, leaf area index, evapotranspiration, nitrogen uptake and land surface energy partitioning show close agreement with observations from sites across a wide climatic gradient. This indicates the generic utility of our model for modern forests, and adequate representation of the key processes involved in forest function. The new development of a technique for estimating leaf lifespan from the anatomical properties of fossil woods provides a secure basis for extrapolating model simulations to conifer forests of the geological past. Future simulations with our model will therefore examine conifer forest feedbacks on paleoclimate during warm intervals in the Mesozoic and early Tertiary.

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Large Eddy Simulation of Coupled Water and Carbon Exchange and Transport Through and Above Forest Canopies

Darren T Drewry¹ (919-660-5463; darren.drewry@duke.edu)