Quantitative Chemical Mass Transfer in Coastal Sediments During Early Diagenesis: Effects of Biological Transport, Mineralogy, and Fabric

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LONG-TERM GOAL

The long-term goal of the study is to develop a better mechanistic and quantitative understanding of the effects of biologically-enhanced transport, mineralogy, sediment fabric, and particle surface chemistry on the biogeochemical dynamics of coastal marine sediments.

OBJECTIVES

Objectives of the study are to (1) develop robust mathematical representations for sediment mixing, irrigation and sediment fabric, (2) parameterize transport and fabric functions using tracer experiments, high-resolution deterministic and stochastic submodels, measured profiles of physical and chemical properties of sediments plus pore waters, and high-resolution imaging of sediment fabric and statistical analysis of burrow networks, (3) incorporate the transport and fabric functions in an existing computer code for multicomponent reactive transport in aquatic sediments, and (4) perform sensitivity analyses and simulations.

APPROACH

Due to the complexity of the chemical, biological, and physical dynamics of coastal marine sediments, the development of quantitative models for mass transfer and sediment biogeochemistry requires an integrated field, laboratory, and computational approach. To this end an interdisciplinary consortium was formed which includes investigators from Naval Research Laboratory (Dawn Lavoie & Yoko Furukawa), Scripps Institution of Oceanography (Barbara Ransom) and Georgia Institute of Technology (Philippe Van Cappellen). Georgia Tech is responsible for the numerical modeling work.

The theoretical and computational efforts focus on the development of multi-dimensional stochastic models for biologically-enhanced solute and particle transport. The stochastic realizations are used to define average vertical transfer functions for irrigation and bioturbation, and constrain the horizontal spatial scales over which the one-dimensional functions are valid. Data collection at coastal sites in Georgia and Mississippi provide field-verification and calibration of the models.

The vertical transfer functions are incorporated into the one-dimensional reactive transport model for early diagenesis, STEADYSED. This model fully accounts for the reaction couplings among the reactive species of C, H, O, N, S, Ca, Fe and Mn. It is used to simulate vertical distributions of chemical species and reaction rates in sediments, as well as to calculate benthic and burial fluxes under variable depositional conditions at the seafloor.

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WORK COMPLETED

A 3-dimensional stochastic model has been developed to study the effects of variations in the distributions of burrow shapes, sizes and densities on bioirrigation in sedimentary environments. The model allows the user to specify a mean burrow density and mean burrow sizes for ten end-member burrow shapes (e.g., V-, Y-, L- or U-shaped, straight or inclined). In addition, the probability of each type of burrow occurring at the site is user-specified. With this information, a Rayleigh cumulative distribution function is used to generate a burrow density, Gaussian distribution functions are used to calculate burrow sizes and the probabilities of each burrow occurring are used to calculate the distribution of burrow shapes. This simulation is repeated 5000 times and the average number of burrows encountered (a proxy for the intensity of irrigation) as a function of depth is calculated. In this way, a completely stochastic representation of the irrigation intensity can be simulated using parameters such as burrow density, shape and size. Distribution functions for the parameters are obtained from the benthic ecology literature, as well as the statistical data collected at the field sites in Georgia and Mississippi.

Using measured pore water sulfate profiles and sulfate reduction rate profiles together with calculated sulfate diffusion coefficients, a numerical reaction-transport model has been used to quantify bioirrigation intensity at three saltmarsh sites on Sapelo Island, a barrier island off the Georgia coast. Irrigation is treated using a non-local transport term with a bioirrigation coefficient that varies as function of depth. The model has been used to constrain bioirrigation intensity and depth as a function of site and season at the Sapelo Island saltmarsh sites.

RESULTS

The reaction-transport model of bioirrigation at Sapelo Island, GA indicates that bioirrigation is most intense in mid-summer and in winter, and is least intense in spring and fall. In addition, there is a distinct variation of bioirrigation intensity and depth at the three sites, with the most intense bioirrigation occurring at a heavily bioturbated creek bank site and the least intense bioirrigation occurring at a ponded marsh site. Calculated irrigation intensities for this marsh are very high compared to those that have been reported for other environments, such as near-shore sediments. Results of the modeling show that the activities of burrowing infauna are a major driving force of the biogeochemistry in the saltmarsh sediments.

Preliminary results of the 3-D stochastic model yield average numbers of burrows intersected as a function of depth that are in qualitative agreement with the distributions of bioirrigation coefficients obtained from the numerical reaction-transport model. Further work is planned to explore the effect of differing burrow densities, sizes and shapes on bioirrigation in a variety of sedimentary environments. In addition, the effects of seasonal changes in burrowing activity due to behavioral changes or changes in population densities are being investigated.

IMPACT/APPLICATIONS

A comprehensive reactive transport model for early diagenesis has many potential applications. By including realistic representations of biological transport (bioturbation and irrigation) and mineral-organic interactions, it is possible to examine the effects of these processes on the preservation of organic matter and the evolution of textural properties. A comprehensive model allows one to simulate the response of chemical mass transfer fluxes and reaction rates to a variety of natural and

anthropogenic perturbations of the normal depositional regime, for example, input of pollutants, attempts at reclamation, eutrophication, storm events, changes in land use, and engineering projects.

TRANSITIONS

STEADYSED version 1.0 is available as public domain software on the P.I.'s server.

RELATED PROJECTS

1. "Trace Metal Dynamics in Reducing Sediments: Determination of Adsorption and Coprecipitation on Undisturbed Sediment Core Sections Using a Plug Flow-Through Reactor" (P.I. Van Cappellen, EPA). The kinetic and thermodynamic parameters that are measured in this study are being incorporated into a trace metal subroutine which is coupled to STEADYSED.
2. "Biogeochemistry of Anaerobic Environments: An Integrated Geochemical and Microbiological Study of Dissimilatory Iron and Sulfate Reduction" (P.I.s Van Cappellen and DiChristina, NSF). This study investigates the geochemical and microbial controls on two major anaerobic pathways of organic matter degradation in coastal marine sediments.

REFERENCES

An overview of projects on biogeochemistry can be found at www.eas.gatech.edu/bae.html.