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

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LONG-TERM GOALS

Current multicomponent reactive transport models developed to study early diagenesis in nearshore environments are limited by their rudimentary mathematical descriptions of biologically-enhanced solute transport (bioirrigation) and biologically-enhanced particle transport (bioturbation). The long-term goal of this study is to develop models employing stochastic and inverse methods to quantify the spatial and temporal variation of bioirrigation and bioturbation in nearshore sediments and to incorporate information derived from these models into the multicomponent reaction transport model STEADYSED (Van Cappellen and Wang, 1996). This will greatly improve our ability to quantitatively describe early diagenesis in shallow-marine environments.

OBJECTIVES

The overall objective of this study was to quantify the effects of bioirrigation and biologically-induced mixing of particles on the early diagenesis of shallow-marine sediments. Specific objectives for FY99 included (1) the development of a stochastic model to describe bioirrigation intensity as a function of sediment depth in spatially and temporally heterogeneous environments using macrofaunal burrow densities and morphologies, (2) the development of an inverse nonlocal-transport model to describe bioirrigation intensity as a function of sediment depth based on vertical profiles of chemical species, and (3) the extraction of depth profiles of bioirrigation intensity for a field site using both the inverse and stochastic models.

APPROACH

An inverse, steady-state, 1-D reaction-transport model was developed with terms accounting for diffusion, advection, reaction and bioirrigation (e.g., Emerson et al., 1984; Boudreau, 1996),

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$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial z}\left(D\frac{\partial C}{\partial z}\right) - R - v\frac{\partial C}{\partial z} + \alpha\left(C_0 - C\right) = 0$$

where C is concentration of a given chemical species of interest, t is time, z is depth with respect to the sediment-water interface, D is the diffusion coefficient of the chemical species of interest, R is the depth-dependent rate of production or consumption of that species, v is the advective velocity, α is the depth-dependent bioirrigation coefficient and C_o is the concentration of the species at the sediment-water interface. Depth-dependent bioirrigation coefficients were constrained with the model using sulfate concentration profiles measured in our laboratory and sulfate reduction rate profiles measured by J. Kostka (Skidaway Institute of Oceanography) for a series of sites at a saltmarsh on Sapelo Island, GA. Permeability measurements made by Y. Furukawa and D. Lavoie (Naval Research Laboratory) were used to constrain advective velocities in the sediments. A downhill simplex algorithm (Press et al., 1989) was used to minimize deviations between measured and calculated data and Monte Carlo simulations were used to avoid local minima. In addition, various vertical discretizations of the data were tested, so that the best regressed irrigation coefficient profile with the least number of fitting parameters could be extracted from the measured data.

A stochastic model of burrow distributions was developed to function as a link between ecological data and bioirrigation coefficients. This approach allows the extreme spatial and temporal heterogeneity of nearshore depositional environments to be considered explicitly in constraining solute transport via bioirrigation. The basic approach of the stochastic modeling is to create probabilistic descriptions of burrow densities and morphologies and to use those descriptions to simulate burrow networks under different ecological scenarios (i.e., for sediments with only one type of burrow or for sediments with a mixture of burrow types). The burrow networks are then used to calculated the number of burrows encountered as a function of depth (a proxy for the surface area of exchange) which is directly related to the bioirrigation coefficients.

WORK COMPLETED

An inverse model to minimize deviations between measured and calculated data was developed and used to extract seasonal irrigation coefficient profiles at three sites in a saltmarsh at Sapelo Island, GA.

A stochastic model was developed to relate the distribution and morphology of burrows to bioirrigation intensity (Koretsky et al., 1999). Burrow networks were simulated using probability functions derived from literature data (Basan and Frey, 1977; Teal, 1958) and from X-ray data collected by Y. Furukawa and D. Lavoie (NRL) for saltmarsh sites at Sapelo Island, GA. Simulated networks were used to calculate the depth-dependent surface area of exchange between burrow walls and the porous sediment matrix (a proxy for the bioirrigation coefficient).

RESULTS

The inverse model has been used to regress irrigation coefficient profiles for three sites (a creek bank, the adjacent levee and a ponded marsh site) in a saltmarsh at Sapelo Island, GA using sulfate concentration and reduction rate profiles measured in summer, spring and fall. Irrigation was always found to be the *dominant solute transport process* at all three sites. Total calculated irrigation fluxes of dissolved sulfate are shown in Figure 1.

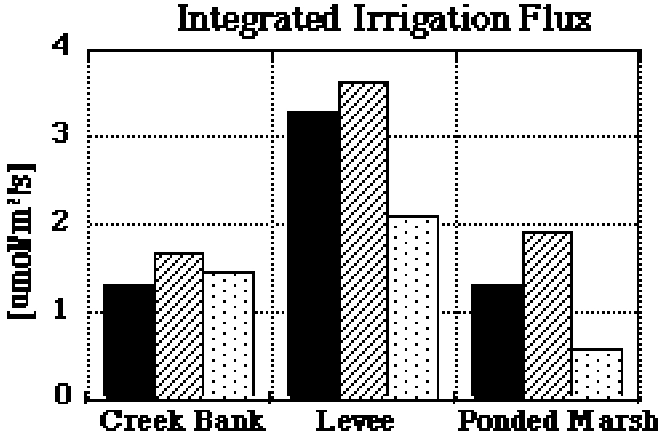

Figure 1. Integrated irrigation fluxes of sulfate for creek bank, levee and ponded marsh sites at Sapelo Island, GA for spring (solid), summer (hatched) and fall (stipled).

It can be seen in Figure 1 that irrigation varies strongly as a function of both site and season, with the greatest integrated irrigation flux occurring in summer at the levee site. Irrigation coefficient profiles showed that irrigation always decreases rapidly with depth at all sites.

Burrow networks were generated for these same three saltmarsh sites using the stochastic model. The resulting number of burrows intersected as a function of depth (a proxy for the bioirrigation intensity) and the associated standard deviation at the ponded marsh site are shown in Figures 2 and 3. These calculations suggest that the irrigation is most intense in the top ten to twenty centimeters of sediment, and that irrigation is deepest at the creek bank and levee sites and shallowest at the ponded marsh site. The model also suggests that irrigation is least intense at the ponded marsh site.

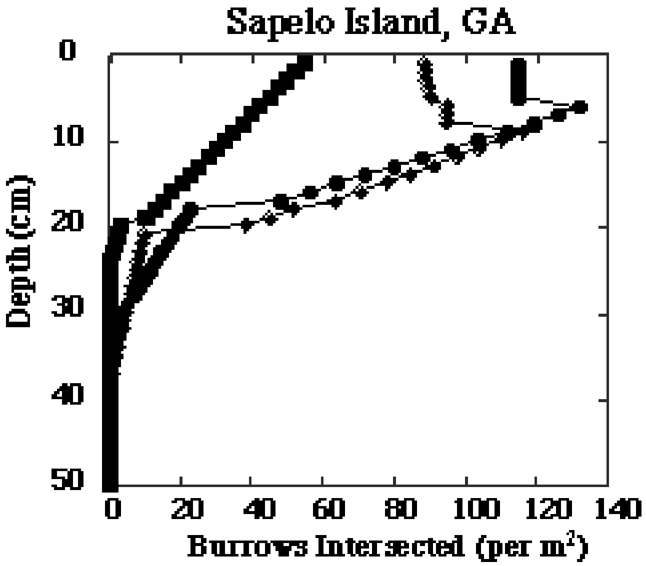

Figure 2. Number of burrows encountered as a function of depth for ponded marsh (squares), creek bank (diamonds) and levee (circles) sites calculated from stochastic model.

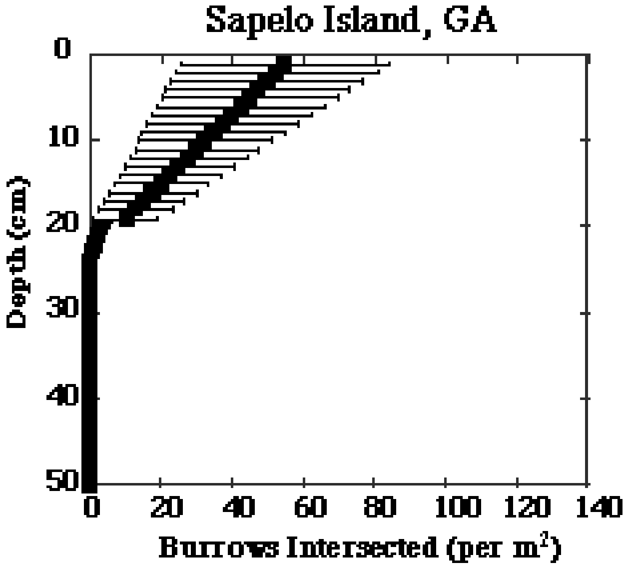

Figure 3. Number of burrows encountered as a function of depth for ponded marsh; error bars represent one standard deviation (based on 10,000 simulations).

IMPACT/APPLICATIONS

The inverse model developed in this study represents a significant improvement over previous nonlocal transport models (e.g., Emerson et al., 1984; Boudreau, 1984) because unbiased bioirrigation coefficient profiles may be extracted from chemical data, with explicit account taken of uncertainties in the measured data, and without imposing an a priori choice of the functional dependence of the irrigation exchange coefficient with depth. In addition, the model may be used to extract production/consumption rate profiles from measured concentration data for chemical species other than sulfate, once the irrigation coefficient profiles have been derived.

Calculated surface areas of exchange from the stochastic model were found to be qualitatively consistent with irrigation profiles obtained independently using the inverse model. However, differences in profiles obtained from the two models suggest that the treatment of burrow water chemistry and fluid dynamics (flushing intensity and frequency) must be improved if the two models are to be linked. For example, the intensity of irrigation at the creek bank site predicted from the inverse model is considerably less than predicted by the burrow network simulations. This may be due to decreased flushing frequency at this site, associated with lower sulfide pore water concentrations, a result which could not be predicted by burrow network size alone.

TRANSITIONS

The inverse and stochastic models developed in this study will be used by Y. Furukawa (NRL) to constrain bioirrigation at field sites (Bay St. Louis; Horn Island, MS) and in experimental mesocosms (in collaboration with S. Bentley, Louisiana State University).

RELATED PROJECTS

Seasonal pore water profiles of dissolved species (e.g., Fe(II)/Fe(III), SO_4(-II), H_2S, and Mn) have been measured along a transect in a saltmarsh at Sapelo Island, GA (Koretsky et al., in prep). The seasonal oscillation of microbial community structure at these same sites was studied in collaboration with Dr. T. DiChristina (Georgia Institute of Technology). The bioirrigation data obtained using the inverse and stochastic models in this study will aid in interpreting the observed temporal and spatial relationships between pore water and sediment geochemical conditions and microbial community structure in the saltmarsh. In addition, a global relationship has been found between irrigation intensities and rates of organic carbon degradation that may be useful in constraining irrigation intensities in modern and ancient ocean sediments.

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PATENTS

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