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

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LONG-TERM GOALS

Multicomponent reaction transport models used to study early diagenesis in marine systems are typically limited by rudimentary descriptions of bioirrigation (enhanced solute transport). It was the goal of this project to develop better representations of bioirrigation, through independent ecologically-based stochastic and chemically-based inverse modeling approaches. These complementary approaches provide tools for independent, objective assessments of the depth-dependence of transport intensities in coastal sediments, and the influence of bioirrigation on biogeochemical cycling in these sediments.

OBJECTIVES

The overall objective of the study is to develop better representations of spatial and temporal variations in bioirrigation and bioturbation in early diagenetic models, such as STEADYSED (Van Cappellen and Wang, 1996). Specific tasks for FY02 included, (1) publication and dissemination of stochastic (ecological) model and (2) application of stochastic model to mesocosm and field data.

APPROACH

A stochastic model of burrow distributions was developed to function as a link between ecological data and nonlocal bioirrigation coefficients. This approach allows the extreme spatial and temporal heterogeneity of nearshore deposition environments to be considered explicitly in constraining solute transport via bioirrigation. The basic approach is to develop probabilistic descriptions of burrow morphologies and densities and to use these to simulate 3D macrofaunal burrow networks. Probabilistic densities are derived for individual organisms based on resin cast and X-radiography data (e.g., Furukawa et al., 2001). The volume occupied by the burrows is used to calculate the sediment porosity due to burrow networks as a function of depth, and the burrow surface area as a function of depth is used to derive nonlocal bioirrigation coefficient profiles according to:

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14. ABSTRACT

Multicomponent reaction transport models used to study early diagenesis in marine systems are typically limited by rudimentary descriptions of bioirrigation (enhanced solute transport). It was the goal of this project to develop better representations of bioirrigation, through independent ecologically-based stochastic and chemically-based inverse modeling approaches. These complementary approaches provide tools for independent, objective assessments of the depth-dependence of transport intensities in coastal sediments, and the influence of bioirrigation on biogeochemical cycling in these sediments.

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$$\alpha_i = \frac{SA_{slice}}{V_{slice}} \frac{D_i}{\bar{r}_i - r_1}$$

where α_i is the nonlocal exchange coefficient, SA_{slice} is the total burrow surface area over a discrete depth interval, V_{slice} is the corresponding volume of sediment, D_i is the effective molecular diffusion coefficient of solute i, r_1 is the radii of burrows assuming that they are cylindrical, and $\bar{r} - r_1$ is the reactive length scale (L), that is, the distance from the burrow at which solute i reaches the bulk sediment concentration ($C_{average}(x)$) (Aller, 1980; Boudreau, 1984). $\bar{r}$ is constrained using (1) direct measurements across burrow walls ($\bar{r} = r_1 + L$) (b) measurements across the sediment-water interface (SWI) corrected for the radial geometry of burrows ($\bar{r} = \sqrt{r_1^2(x) + 2r_1(x)L}$) or (c) by calculation using a depth-dependent measured or estimated reaction rate, R(x), for solute i, according to

$$L = \sqrt{\frac{D_i \cdot (C_o - C_{average}(x))}{R(x)}}\ .$$

where C_o is the concentration of solute i at the SWI. Our approach allows biologically induced solute mass transfer to be directly linked to information regarding the community of burrowing organisms. This approach is quite different than, but complementary to, existing models in which mixing intensities are inferred from observed chemical profiles.

WORK COMPLETED

A stochastic 3D burrow network model has been used to extract mean burrow densities and burrow wall surface areas and their variability as a function of sediment depth for model organisms including the polychaete worms *Nereis diversicolor* and *Schizocardium sp.*, the shrimp *Callianassa subterranea*, the echiuran worm *Maxmuelleria lankesteri*, the fiddler crabs *Uca minax*, *U. pugnax*, and *U. pugilator* and the mud crabs *Sesarma reticulatum* and *Eurytium limosum*. Consortia of model organisms were used to simulate burrow networks in shallow water carbonate sediments at Dry Tortugas, FL and in three intertidal saltmash sites (vegetated ponded marsh, vegetated levee and unvegetated creek bank) at Sapelo Island, GA. Depth-dependent surface areas from the consortia burrow network simulations have been used to derive nonlocal bioirrigation coefficient profiles two dissolved solutes, O_2 and SO_4^{-2}. The depth-dependent volumes of burrows have been used to calculate the sediment porosity due to burrows, and the probabilistic descriptions of burrow densities have also been used to derive representative sampling areas required for each of the field locales.

RESULTS

The stochastic model has been used to calculate nonlocal irrigation coefficient profiles for a shallow carbonate sediment site at Dry Tortugas, FL (Figure 1) and for two sites (an unvegetated creek bank and a vegetated ponded marsh area) in an intertidal saltmarsh at Sapelo Island, GA (Figure 2). Bioirrigation coefficients at Dry Tortugas calculated using sulfate concentration and reduction rate profiles are in excellent agreement with independent estimates from Furukawa et al. (2000). However, irrigation coefficients calculated using oxygen penetration depths at the sediment-water interface lead to considerably higher irrigation coefficients near the sediment surface. Furthermore, these irrigation coefficients exhibit a less pronounced decrease with depth than those of Furukawa et al. (2000). This probably reflects imperfect flushing of burrows, and also suggests that oxygen gradients measured at the SWI may not yield accurate estimates of radial diffusion scales at the burrow sediment interface in deeper, anoxic sediments. Correction of the irrigation profiles for imperfect flushing does result in much better agreement between the stochastic model results and results from the early diagenetic model of Furukawa et al. (2000). Application of the ecological model to saltmarsh sites at Sapelo Island, GA indicates that the presence of dense populations of macrofauna greatly enhances solute transport in the upper 50 cm of sediment. Sulfate irrigation coefficient profiles calculated using the stochastic model with macrofaunal data from an unvegetated creek bank at Sapelo Island, GA are in excellent agreement with independently derived irrigation coefficient profiles derived using the chemicall-based inverse model of Meile et al., 2001 (Figure 2).

IMPACT/APPLICATIONS

The stochastic model allows both the average and the expected variability of burrow surface areas to be assessed as a function of sediment depth. These surface areas provide an independent method for assessment of the depth-dependence of irrigation coefficients used in 1D nonlocal models of bioirrigation. The stochastic approach also provides a measure of the expected variability of irrigation in a given environment, which is difficult to assess using single profiles of chemical constituents or reaction rates. It also allows the expected (probabilistic) horizontal distribution of redox-interfaces to be quantified. This provides a framework for assessing the observed apparent overlap of distinct microbial organic matter degradation pathways in nearshore sedimentary environments. Finally, the burrow network model should allow irrigation coefficients to be estimated in environments, such as ancient sedimentary systems, for which little or no chemical data is available.

TRANSITIONS

The stochastic expression of depth-dependent burrow distributions will replace the deterministic treatment of burrow geometry in the reaction-transport model developed by Furukawa et al. (2001). This will allow the model to account explicitly for the spatial and temporal heterogeneity of bioturbation. The stochastic model is currently being used to evaluate bioirrigation in sediments located at Skidaway Island, GA (Y. Furukawa and J. Kostka, personal communication). The inverse model developed during this study has been used to assess benthic oxygen fluxes across the sediment water interface in a wide range of sedimentary environments (Meile and Van Cappellen, 2002).

RELATED PROJECTS

Seasonal pore water profiles of dissolved species (e.g., Fe(II)/Fe(III), SO_4(-II), H_2S, PO_4^{-3}, NH_3 and Mn) have been measured in saltmarshes at Sapelo Island, GA and at the Scheldt Estuary (Netherlands and Belgium). The seasonal oscillation of microbial community structure at these same sites is being studied in collaboration with T. DiChristina and C. Moore (Georgia Institute of Technology). Interpretation of spatial and temporal oscillations in the saltmarsh geochemistry and microbiology has been greatly aided by results of inverse and stochastic models developed in this study. The relative compression of redox zones in these sediments has been shown to strongly depend on the depth and intensity of bioirrigation. Because ecological parameters for the stochastic model can be derived using trace fossil evidence, the models developed in this study may also be useful in constraining irrigation intensities or rates of

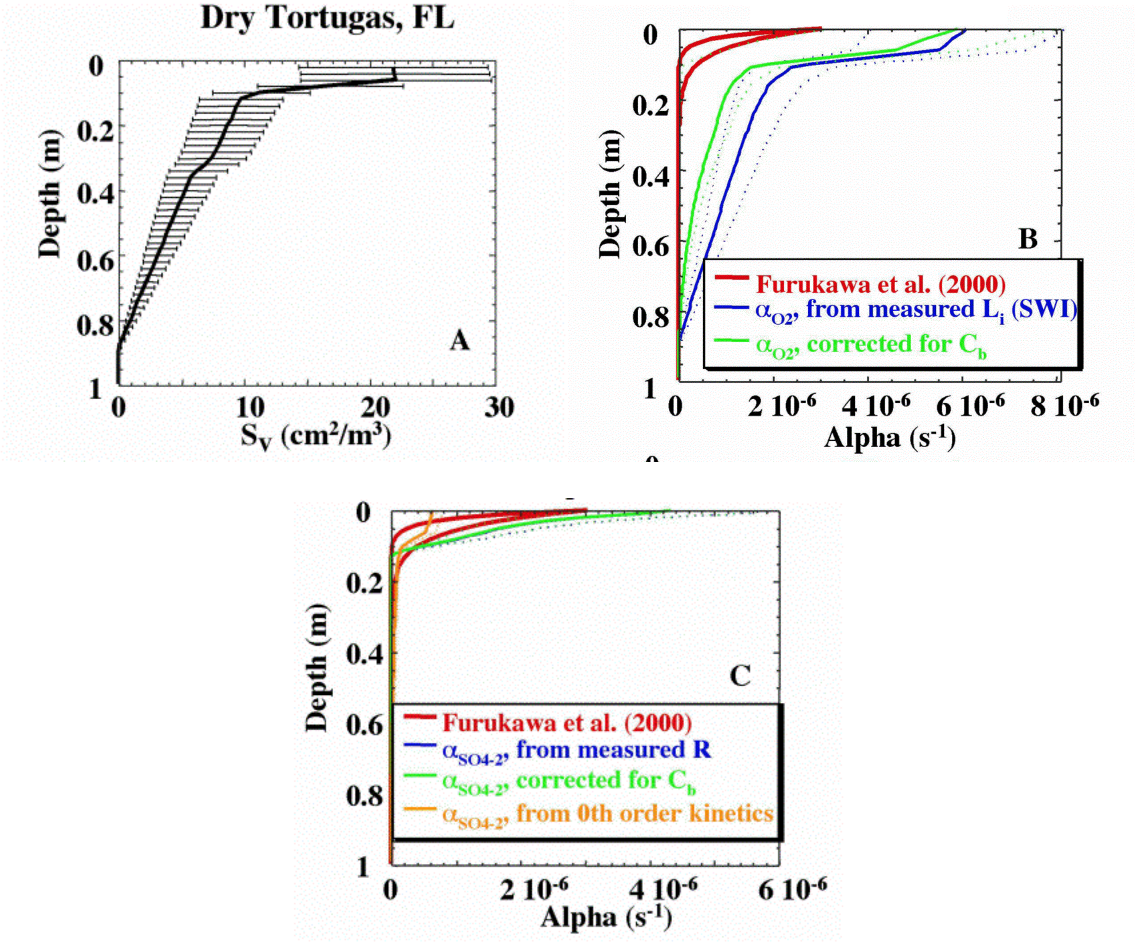

Figure 1. (A) Total burrow surface area per sediment volume (S_V) as a function of depth from stochastic burrow network simulations using Notomastus sp. and Callianassa sp. Error bars represent ±1 standard deviation in burrow density. [S_V decreases from 20 cm^2/m^3 at SWI to 0 cm^2/m^3 at approximately 0.9m depth] (B) Oxygen bioirrigation coefficients (•̈) as a function of depth derived using an early diagnetic model with measured pore water profiles (Furukawa et al., 2000; red lines), and estimated from the stochastic burrow network model. Blue line indicates estimates for oxygen without correction for imperfect burrow flushing; green line represents estimates for oxygen with correction (for more details see Koretsky et al., 2002). [Stochastic model estimates overestimate bioirrigation coefficient profiles by approximately a factor of 2 at the sediment water interface, and decrease more rapidly than the results of Furukawa et al. 2000. Correction for imperfect flushing improves the agreement between the stochastic model results and Furukawa et al. 2000] (C) Bioirrigation coefficients (s^{-1}) as a function of depth from Furukawa et al. (2000) (red lines) and estimated for sulfate using the stochastic model. Blue line is indicates results uncorrected for impefect flushing; green line shows estimates with correction. The orange solid line indicates results assuming zero order kinetics for sulfate reduction. [Orange line underestimates bioirrigation coefficients relative to other models. Both the stochastic model and Furukawa et al. indicate alpha values of approximately $4 \cdot 10^{-6} s^{-1}$ near the SWI, decreasing to 0 by approximately 2cm depth.]

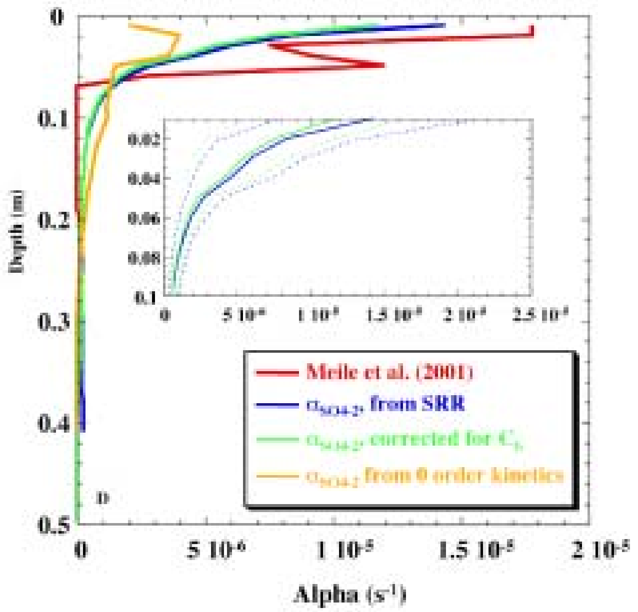

Figure 2. Bioirrigation coefficients (•̈) as a function of depth derived using an early diagnetic model with measured pore water profiles from Furukawa et al. (2000) (red lines), and estimated for sulfate from the stochastic burrow network model. Blue line indicates estimates without correction for imperfect burrow flushing; green line represents estimates with correction (for more details see Koretsky et al., 2002). The orange solid line indicates results assuming zero order kinetics for sulfate reduction. [Blue and green lines show good agreement with Furukawa et al. 2000. Both models indicate bioirrigation coefficients of approximately 1.5·10^{-5} s^{-1} at the SWI, decreasing to 0 by 0.1m .]

organic carbon degradation in ancient ocean sediments. This hypothesis is being pursued in collaboration with S. Walker (paleontologist, University of Georgia). Finally, the stochastic burrow network model is being used in the development of a 3D chemical model of bioirrigation (Meile et al., 2002).

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PATENTS

none