

# **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) and bioturbation (enhanced particle transport). It is the goal of this project to develop better representations of bioirrigation and bioturbation, through both stochastic and inverse modeling approaches. These approaches will be tools for independent, objective assessments of the depth-dependence of transport intensities in coastal sediments that will allow us to capture the dynamic nature of biogeochemical cycling in aquatic 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 FY01 included, (1) development of quantitative link between stochastic (ecological) and inverse nonlocal (chemical) models of bioirrigation, (2) application of stochastic model to mesocosm data, (3) application of stochastic model to field data (Dry Tortugas, FL and Sapelo Island, GA) and (4) development of inverse and stochastic particle mixing models.

## **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

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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:

$$\alpha_i = \frac{SA_{slice}}{V_{slice}} \frac{D_i}{r_i - r_1}$$

where  $\alpha_i$  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  $r - r_1$  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).  $r$  is constrained using (1) direct measurements across burrow walls ( $r = r_1 + L$ ) (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

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

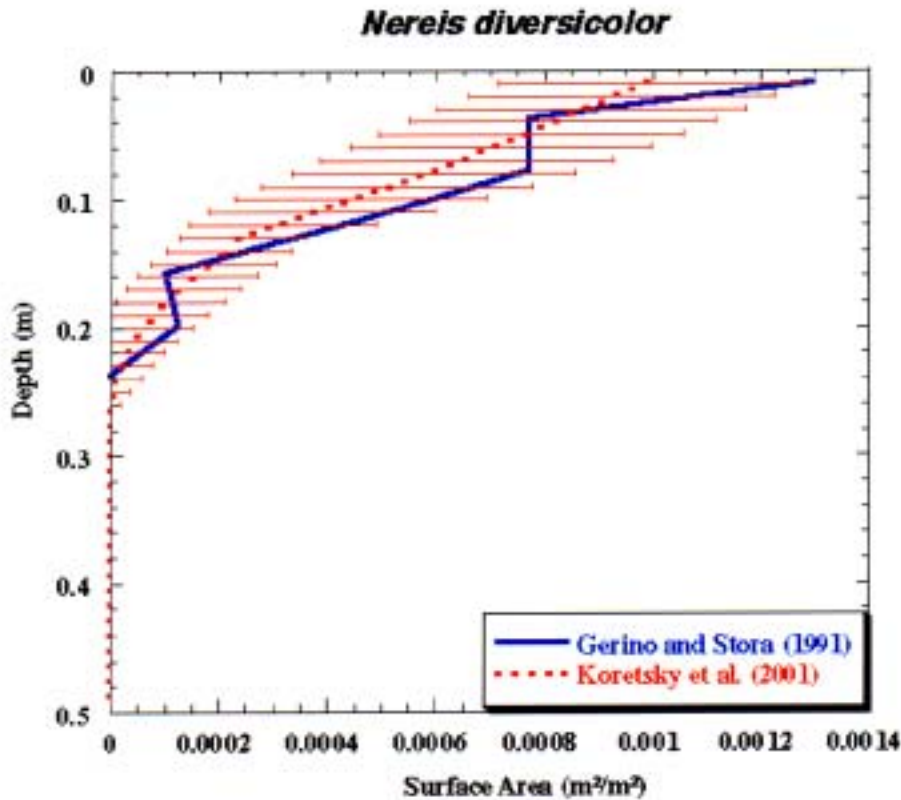
where  $C_o$  is the concentration of solute  $i$  at the SWI. Our approach allows biologically induced solute mass transfer to be directly linked to information regarding the community of burrowing organisms. This approach is quite different than, but complementary to, existing models in which mixing 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 *Callinassa 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 two intertidal saltmarsh sites (vegetated ponded marsh 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

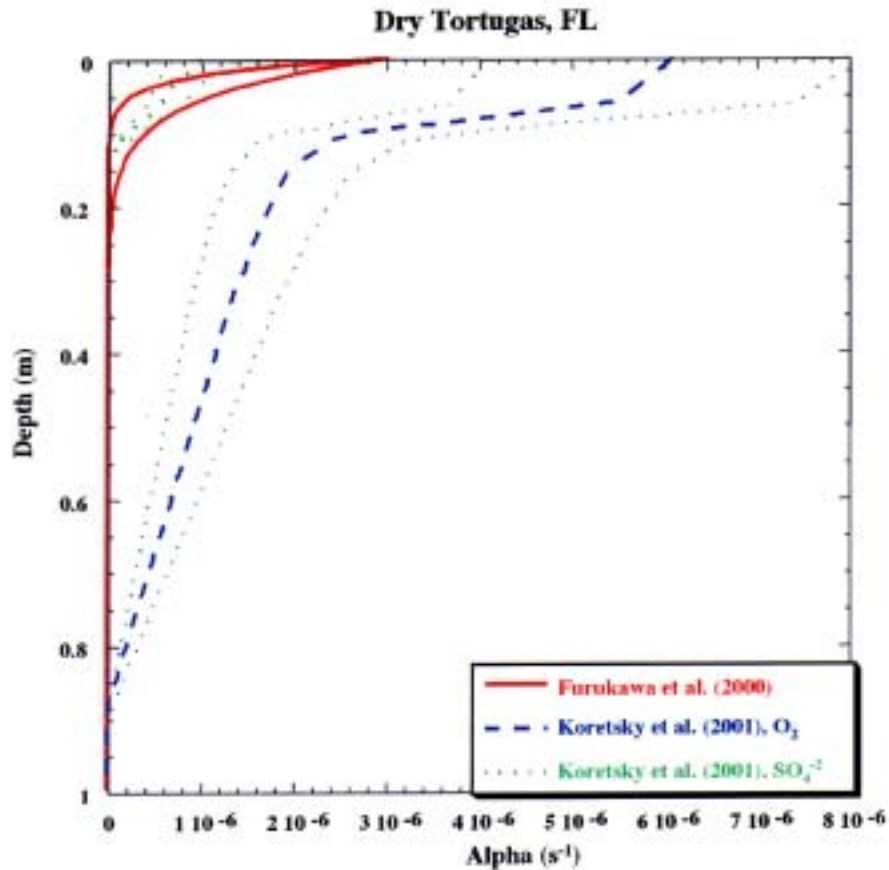
The stochastic burrow network model has been used to calculate burrow surface areas for a wide-range of model organisms. These surface areas are in excellent agreement with independent surface area estimates from mesocosm studies (Figure 1).



**Figure 1. Surface area of *Nereis diversicolor* burrows as a function of depth. Solid line indicates measured surface areas from mesocosm studies (Gerino and Stora, 1991). Dotted line indicates predicted surface areas from stochastic models, with error bars showing one standard deviation. [Surface areas from both studies decay gradually from .0014 m<sup>2</sup>/m<sup>2</sup> at the SWI to 0 at ~25 cm depth.]**

The stochastic model has also been used to calculate nonlocal irrigation coefficient profiles for a shallow carbonate sediment site at Dry Tortugas, FL (Figure 2) and for two sites (an unvegetated creek bank and a vegetated ponded marsh area) in an intertidal saltmarsh at Sapelo Island, GA. Near the sediment-water interface (SWI) bioirrigation coefficients from the stochastic model agree within a factor of two with those obtained using chemical data by Furukawa et al. (2000). Bioirrigation coefficient profiles calculated for the Dry Tortugas site using the stochastic network with reactive length scales estimated using sulfate concentration and reduction rate profiles are in excellent agreement with Furukawa et al. (2000). Results obtained using reactive length scales for O<sub>2</sub> suggest higher bioirrigation at depth than those derived from early diagenetic modeling. This is likely due to the implicit assumption when relating the stochastic results to nonlocal bioirrigation coefficients that burrows are efficiently flushed, such that concentrations of solutes within burrows are always equal to those at the sediment water interface. For highly reactive solutes like O<sub>2</sub>, the time-averaged concentrations in deeper parts of the burrow are probably considerably lower than the overlying water concentration. Thus, the contribution of deep burrows to bioirrigation is likely overestimated. Similarly, nonlocal bioirrigation coefficient profiles calculated using the stochastic model for an unvegetated creek bank at Sapelo Island indicate very rapid biologically enhanced solute transport. This is in good agreement with independently derived nonlocal bioirrigation coefficient profiles from

Meile et al. (2001), however, the stochastic simulation results do not decrease with depth as quickly as the chemically-derived irrigation coefficients.



*Figure 2. Nonlocal irrigation coefficient ( $\alpha$ ) as a function of depth for dissolved  $\text{SO}_4^{2-}$  and  $\text{O}_2$  in a carbonate sediment at Dry Tortugas, FL. Dashed lines were derived using  $\text{O}_2$  profiles (Furukawa et al., 2000). Solid lines were calculated using the stochastic mode with the  $\text{O}_2$  reactive length scale and dotted lines were calculated using the stochastic model with the  $\text{SO}_4^{2-}$  reactive length scale; light dotted lines indicate irrigation coefficient profiles using the mean surface area  $\pm$  one standard deviation. [Profiles from Furukawa et al., 2000 decay from approximately  $3 \cdot 10^{-6} \text{ s}^{-1}$  at the sediment-water interface to 0 at a depth of approximately 20cm. Profiles from the stochastic model for  $\text{O}_2$  decay from approximately  $6 \cdot 10^{-6} \text{ s}^{-1}$  at the sediment-water interface to 0 at a depth of approximately 90 cm, whereas profiles calculated for  $\text{SO}_4^{2-}$  decay from  $\sim 1 \cdot 10^{-6} \text{ s}^{-1}$  at the SWI to 0 at  $\sim 15\text{cm}$ .]*

## **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.

## **RELATED PROJECTS**

Seasonal pore water profiles of dissolved species (e.g., Fe(II)/Fe(III), SO<sub>4</sub>(-II), H<sub>2</sub>S, PO<sub>4</sub><sup>-3</sup>, NH<sub>3</sub> 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 biogeochemistry 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. In addition, preliminary studies of the influence of vegetation on redox zonation suggest that plants may trap particles that are subsequently redistributed by bioturbation. This may lead to an enhancement of microbial activity in newly colonized sediments, and to more compressed redox zonation. Models developed in this study may also be of use in understanding the influence of bioturbation on sediment biogeochemistry. The stochastic model may also be useful in constraining irrigation intensities or rates of organic carbon degradation in ancient ocean sediments.

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## **PATENTS**

none