Irrigation in early diagenetic models: From one-dimensional mass transfer coefficients to multi-dimensional, ecologically-based models

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Construction and ventilation of macrofaunal burrows fundamentally alters the biogeochemical functioning of sediments. In one-dimensional (1D) early diagenetic models, the effect of bioirrigation on solute transport is typically included via a nonlocal mass transfer, or irrigation, coefficient α. Furthermore, all pore water species are usually assigned the same α value. The simple nonlocal exchange model successfully reproduces some of the effects of bioirrigation on the chemical structure of sediments and benthic exchange fluxes. The 1D nonlocal mass transfer formulation also owes its wide acceptance to the theoretical demonstration of its equivalence, under certain conditions, to the so-called Aller tube model, in which the burrow network is approximated as a system of perfectly flushed, equally-spaced, vertical cyclinders of uniform size. The equivalence implies that, at some basic level, the coefficient α captures some of the essential features of the burrowing and flushing activities of benthic macrofauna. It also points out that more realistic descriptions of burrow networks are likely to improve the representation of the effects of bioirrigation on sediment biogeochemistry. A major recent advance in early diagenetic modeling is therefore the introduction of bioirrigation models that allow for variable shapes, sizes and orientations of the burrows. In particular, stochastic burrow network models are well-suited for incorporating benthic ecological data in reactive transport calculations, and for constraining the expected heterogeneity in chemical distributions and reaction rates due to the inherently variable nature of macrofaunal burrowing. Another major recent advance is the development of multidimensional models that explicitly account for reactive transport in and around burrows. These models show that 1D irrigation coefficients, which were originally introduced strictly as transport parameters, actually strongly depend on the biogeochemical reactivity of the solute species.

Heterogeneity in aquatic sediments: 1D representations of a 3D environment

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The vast majority of datasets quantifying early diagenetic processes in aquatic sediments consists of benthic exchange fluxes and concentration profiles, documenting compositional changes in the vertical direction. As a consequence, most models of early diagenesis represent aquatic sediments with a one-dimensional description. In such reactive transport models (RTMs), horizontal heterogeneity can not be incorporated explicitly but requires proper model parameterization. For example, solute transport through macrofaunal burrow networks is typically formulated as non-local exchange, where an irrigation coefficient α serves as a measure for the mixing intensity of a given solute. α can be estimated from tracer experiments. Due to difficulties in separating effects of reactions, reactive solutes are generally assumed to be subject to the same bioirrigation coefficient.

In this study, the effect of representing the 3D process of bioirrigation in a 1D model is investigated by performing numerical simulations of a simplified reaction network including the main pore water solutes around a cylindrical burrow. From the resulting concentration fields, irrigation coefficients can be determined such that the 1D formulation matches the solute mass flux due to bioirrigation. Simulations mimicking the transient intrusion into the sediment of an inert tracer during an incubation experiment yield apparent mixing intensities that depend on the incubation time. For reactive solutes, the diffusive solute exchange across burrow walls can be strongly affected by reactions, and adjusting α-values for redox sensitive chemicals may be necessary. Furthermore, horizontal segregation of reactions poses a challenge for the proper choice of 1D reaction rate constants, as direct application of rate parameters determined in well-mixed laboratory experiments may over-predict in situ rates.

Our results illustrate that a fundamental understanding of transport and reaction processes at the level of individual burrows may help the parameterization of 1D RTMs. Within the foreseeable future, the latter are likely to remain the major quantitative tool for analyzing the predominantly vertical data sets. It is therefore crucial to identify the potential pitfalls of representing inherently three-dimensional processes in 1D models.