MICROBIAL AND TRANSPORT MECHANISM IN THE SEDIMENTS: INTERPLAY AND RELATIVE IMPORTANCE FOR SIMULATED C- AND N-CYCLES

K. W. Wirtz

Introduction

Complex biogeochemical cycles in marine sediments only very partially allow for empirical investigations and are therefore often assessed by means of numerical models. Most of these approaches apply to continental shelf or deep-sea sites (SOETAERT et al., 2000). Their meaningful application to near-shore systems remains a challenging task so that for quantifying near-shore C- and N-fluxes on an ecosystem, regional or global scale, a new set of tools is strongly demanded for.

The dynamic and heterogeneous nature of coastal benthic systems broadens the spectrum of relevant processes to be considered in a model frame. Among these processes, microbiology plays the key role as it sensitively controls the temporal onset and extent of geochemical pathways. Hence, one of the challenges in marine biogeochemistry as well as aquatic microbial ecology is to link the vast array of microscale properties of bacteria to macroscale descriptions of biogeochemical cycles (AZAM, 1998).

Secondly, a broader set of transport mechanisms acting in the sediments as in part listed in the textbook of BOUDREAU (1997) has never been included into a single modelling frame. In addition to bio-irrigation, e. g., hydrodynamically induced pore-water advection creates steep two- or three-dimensional gradients in permeable systems (RUSCH et al., 2001), eventually leading to a more complex zonation of pathways than revealed by more simple one-dimensional models, and significantly alters exchange rates at the sediment-water interface (MEILE & VAN CAPPELLEN, 2003).

In order to combine process descriptions of microbial processes and physical transport here an Integrated Sediment Model (ISM) is presented. The ISM builds upon a synthesis of existing approaches, extended into various directions. Most effective improvements are made with respect to the set of geochemical reactions resolved, microbially controlled kinetics and an array of exchange processes resolved in two spatial dimensions.

Model construction, however, although re-evaluating existing knowledge, can itself not produce new insights for the problems under consideration. Instead, we stress three uses of the ISM where indeed a fresh understanding of biogeochemical cycles may arise:

- model and hypothesis validation,
- model and hypothesis falsification,
- systematic scenario analysis.

Negative outcomes of model validation can equally be termed falsification but are nonetheless set as an extra item in the above list. Even many modellers underestimate the positive value of model failures, although these in principle may provide as much useful information as model results in agreement with existing data.

Before the three items can be worked out, a short overview over the structure of the ISM is given in the first part of this paper.

In the second stage of the study, the ISM will be used for numerical experiments where the role of single microbial properties such as the adaptive regulation of bacterial metabolism for total carbon remineralisation is investigated.

A complex diagenesis model

Geochemical module

A first description of the Integrated Sediment Model (ISM) used in this study is given by WIRTZ (2003). Its geochemical submodel is based on state-of-the-art models reported in the literature (WANG & VAN CAPPELLEN, 1996; SOETAERT et al., 1996; HUNTER et al., 1998; BOUDREAU, 1992). The ISM includes four different types of reactions, degradation of particulate organic carbon (POC), fermentation and oxidation of high-molecular-weight dissolved organic carbon (HM-DOC) together with the oxidation of the low molecular-weight classes (LM-DOC), re-oxidation of reduced substances and mineral precipitation. An overview of all carbon-based degradation and redox reactions is given in Fig. 1.
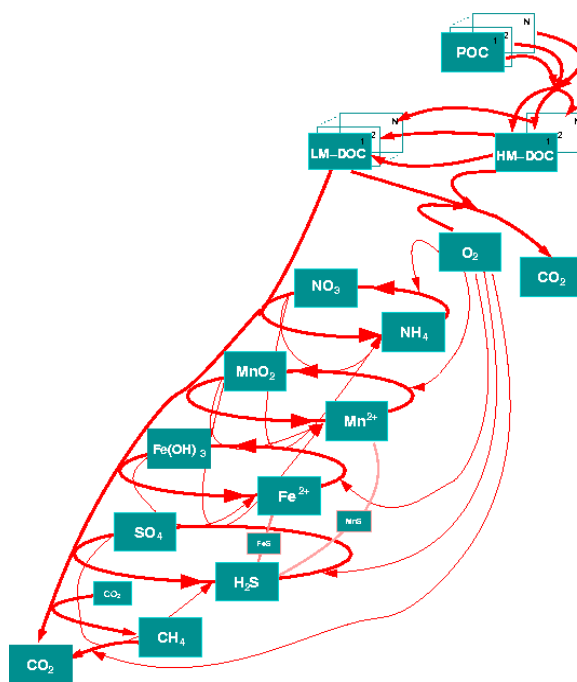

Fig. 1. Structure of the geochemical module for carbon mineralisation in the ISM. Most reactions are controlled by microbial activity.

Nitrogen dynamics is coupled to the carbon cycle through nitrification, denitrification, nitrous oxide production and ammonification. Extensions to the redox reactions resolved by the models of WANG & VAN CAPPELLEN (1996) are made, e. g., with respect to the annamox reaction.

Nearly all (re)oxidation reaction rates are controlled by the variable and reaction-specific activity of bacteria. The model regulates the partitioning of chemical pathways through increasing and decreasing population densities of active microorganisms. In accordance with empirical evidence, the old picture of mutual inhibition is shifted to dominance and activity patterns of microbial populations.

Microbial module

The relative growth rate (RGR) of each microbial population is mainly determined by the gross rate of the reaction catalysed by the specific microbes. In this way, the model links cell energetics to reaction kinetics. By taking into account the finding that bacterial yield increases with higher free energy release (VALLINO et al., 1996), the sequence of oxidation pathways is translated into the competition of different functional groups. The latter is in turn regulated by the availability of the various electron acceptors. Removal of individuals, i. e. mortality and bacterivory, as well as

maintenance respiration is described by a temperature dependent loss term.

In the ISM, microorganisms can switch between an active and a dormant stage (see also BOUDREAU, 1999). It is assumed that dormant cells respire at a lower rate compared to active organisms. After the onset of famine or feast conditions, respectively, the fraction of dormant cells is adaptively altered according to a simple algorithm:

$$X_{dorm} = X_0 \cdot \begin{cases} \beta & : \text{if } RGR < 0 \\ 1 - \beta & : \text{else} \end{cases}$$

X_0 represents an average microbial biomass for a specific site and functional group. The coefficient β describes the flexibility of the switch between the active and dormant state. Considering a high flexibility ($\beta = 1$), the biomass of dormant cells X_{dorm} strongly increases as soon as RGR falls below zero so that respiratory losses are diminished. *Vice versa*, more cells turn to higher activity under favourable conditions, giving rise to a rapid recuperation of metabolising bacteria.

Transport mechanisms

Near-shore sediments are subjected to spatially and temporally highly variable external forces, mediated through a set of transport processes. Those resolved by the ISM comprise settlement or re-suspension of particulate material at the boundary layer, bio-irrigation, diffusion and hydrodynamically induced advection in sediments, acting differently on the three phases (1) dissolved chemical species, (2) free-floating particulate material in the pore-water and (3) particles attached to the sediment matrix (see also Fig. 2). The relative amount of suspended *versus* attached particulate material is calculated in a subroutine which uses the pore-water velocity field, a critical re-suspension velocity and a specific stickiness parameter.

Molecular diffusion only affects the pore-water phase, whereas pore-water advection transports suspended as well as dissolved material. All phases are exchanged with seawater pools by bio-irrigation. Bacteria may in addition regulate their transportation in the sediments by attaching to sand grains or trapped particles.

The sediment column is represented by an array of boxes, increasing in size going to deeper layers.

Model calibration under uncertainty

The problem of parameter uncertainty is addresses by a newly developed technique. After an initial sensitivity study based on the methodology described by KÖHLER & WIRTZ (2002), 19 most sensitive parameters were selected for an automatic calibration. Due to this still relatively high number one has to employ a Monte Carlo technique in which parameter values were set to independent random numbers within meaningful limits. For each of the random parameters set, the error of the resulting model dynamics with respect to the data was calculated. We referred to an existing data-base of the preceding Wadden Sea ecosystem project ELAWAT (DITTMANN, 1999) since coherent measurements in our present study area are still in progress.

Time series of pelagic POC, NH_4^+, NO_3^- and O_2 for the period of 1995 to 1996 were used as driving forces. As reference values for the Monte Carlo calibration, sediment profiles of TOC, DOC, SO_4^{2-}, H_2S, total pools of extractable sulfur (TS) and iron (TFe), colony forming units of anaerobes as well as aerobes and the total cell count were used (RUSCH et al., 1998; STOECK & ALBERS, 2000; and unpublished data).

From a large number of 10^5 random sets the ensemble of 40 parameterisations were selected which led to the best fits.
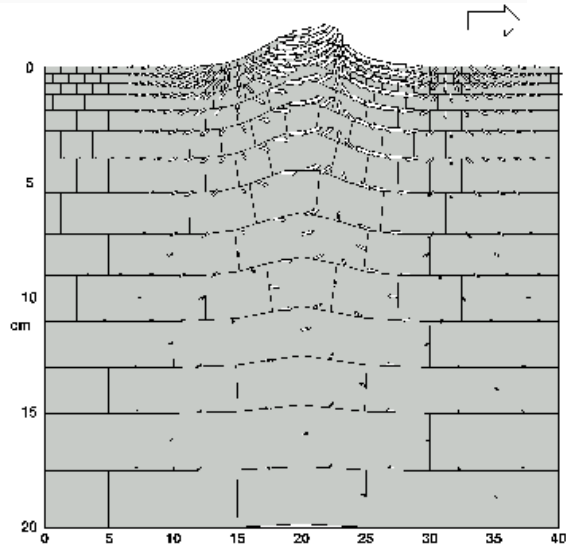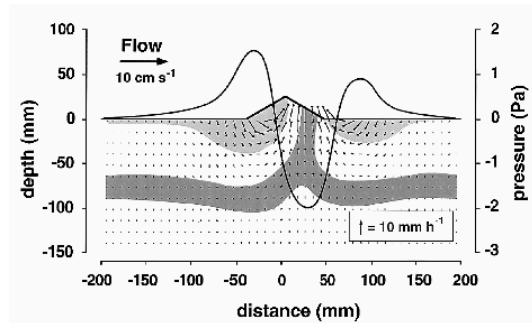

Fig. 2. Pore-water flow beneath a sand ripple, reconstructed based on tracer measurements (top; from HUETTEL et al., 1998, with kond permission of the publisher) and calculated by the ISM transport module (bottom).

Verification of the 2D setup

In addition to the parameter calibration, the overall consistency of the two-dimensional transport module is studied with reference to the channel experiment conducted by HUETTEL et al. (1998). There, 2D transects of various geochemical parameters within a permeable sediment were extracted beneath a surface structure above which a constant water stream was established. The induced advection field as projected by the authors is simulated by the model using Darcy's law together with a phenomenological approach for horizontal pressure gradients above a structured topography (Fig. 2). Also other boundary conditions reported for the experiment were successfully implemented in the ISM.

Variation experiments

While the model is repeatedly run over a period of 8 days with typical external forcing including a singular storm event, the dormancy flexibility β is varied from zero to one. Considering exclusively the ensemble of best-fitting parameter sets, the variations are computed 40 times each. Resulting relative growth rates (RGR) of functional groups and CO_2 production are averaged while standard deviations are calculated on the base of the 40 ensemble values.

Results and discussion

Lessons from successes and failures

The parameter training yields an ambiguous picture of the model ability to reproduce the data. The seasonality of the
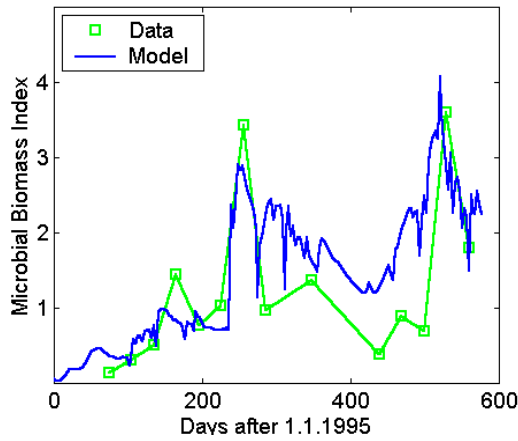
Fig. 3. Simulated and measured microbial biomass index. Data derived from STOECK & ALBERS (2000) and unpublished studies. The model simulation was carried out with a trained parameter set.
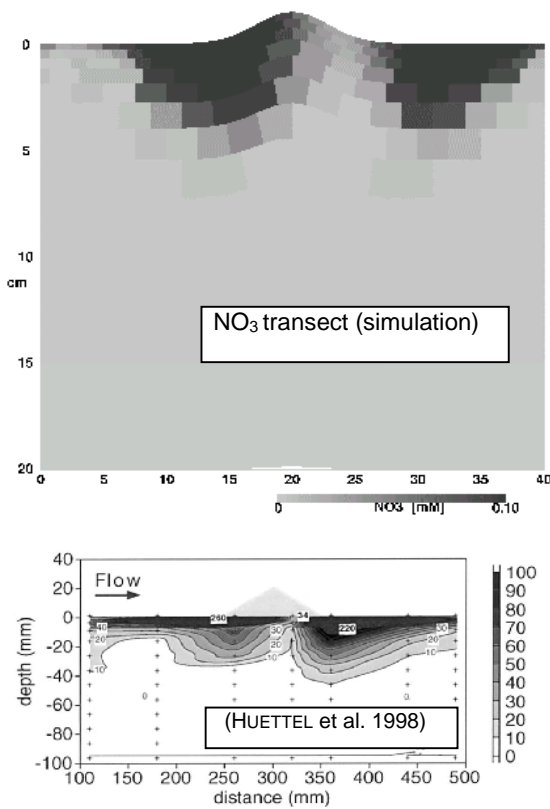

Fig. 4. 2D maps of the nitrate concentration beneath a structured topography simulated by the ISM (top) and measured by HÜTTEL *et al.* (1998; reprinted with kind permission of the publisher). The flow of above channel water is held constant.

microbial biomass index (MBI, a function of different measures for bacterial abundance) in the upper 1 cm of the sediment is accurately redrawn by the ISM (Fig. 3). Excellent agreement is also found if 2D transects of NH_4^+ and NO_3^- are compared with the figures given by HUETTEL *et al.* (Figs. 4 and 5). According to these outcomes it can be supposed that major elements of the N-cycle as well as of the microbial dynamics are realistically resolved by the model. In detail, one can derive from this result, e. g., a minor role of bacterivory on the seasonal biomass patterns.

However, the temporal course or the spatial distribution of iron species was only poorly described by the model (results not shown). We suggest that the simple model formulation of FeS genesis does not reflect major sensitivities of the dissolution and precipitation process on changing conditions
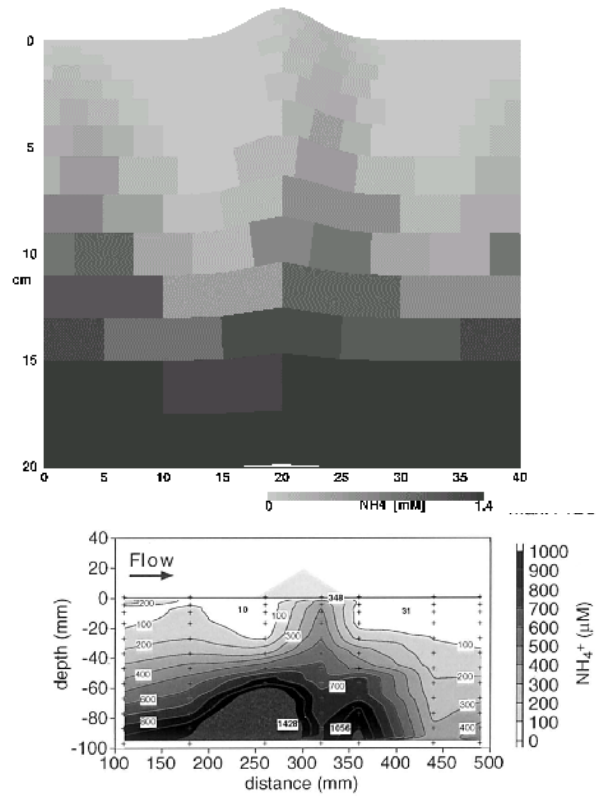

Fig. 5: Simulated and observed ammonium transects (see Fig. 4).

like temperature or pH, for example. Here, the geochemical model has to be refined what in turn requires more empirical studies on this behalf as literature data are difficult to retrieve.
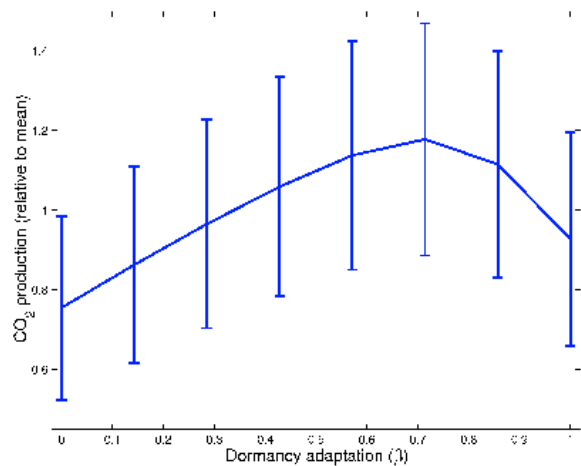
Significance of dormancy

Fig. 6. Model-based CO_2 production in relation to the specific dormancy flexibility. Means over the ensemble calculations are plotted together with standard deviations.

We observe a counter-intuitive, non-linear response in the CO_2 production after shifting the specific dormancy flexibility (β) from zero to one (Fig. 6). One could expect that with faster switches to lower activity and respiration under starvation, the net performance of microorganism and, thus, the total turnover rate of the system should grow. However, this effect only works up to an intermediate value of β.

For model populations living at the edge of their habitat, temporal fluctuations gain high importance. If RGR tends to be around zero and changes are very likely to arrive in near

future, it may be more profitable to maintain a suboptimal level of activity. Thus, responding after some lag time or, equivalently, keeping a larger fraction active under starvation may improve the fitness in variable habitats like the suboxic zone. This effect then attributes to the anomaly of reduced CO_2 production at high values of β as displayed in Fig. 7.

Conclusions

We outlined only few examples of possible ways in which a complex biogeochemical model of near-shore sediments can test existing hypotheses or produce new quantitative informations. A major prerequisite for such potential is the complexity of the ISM which on the other hand creates the fundamental problem of a high model and parameter uncertainty. Although the use of automatic calibration and trained ensembles of parameter sets reduces uncertainty, we aim at a more aggregated model representation. These may be more suited for more specific applications like the calculation of total benthic P- and N-remineralisation to be included into a pelagic ecosystem model.

A paper of BERNHARDT *et al.* (this volume) provides further and more sophisticated model analysis results which lay the ground for an efficient up-scaling.

But still in its complex form, the ISM serves as a frame for designing interdisciplinary field campaigns. Unresolved process areas which are found to be sensitive to the model are, e. g., iron and manganese cycles together with the transportation of oxidised metal species into the upper sediment layers.

A second major question derived from ISM simulations points to different evolutionary stable strategies of microbial functional groups. Here, the focus was laid on dormancy adaptations, but the list should also contain attachment behaviour of cells (WIRTZ, 2003) or differential temperature dependencies of activity rates.

References

AZAM, F. (1998) Microbial control of oceanic carbon flux: the plot thickens. Science, **280**, 694-696.

BOUDREAU, B. (1992) A kinetic model for microbic organic-matter decomposition in marine sediments. FEMS Microbiol. Ecol., **102**, 1-14.

BOUDREAU, B. P. (1997) Diagenetic models and their implementation. Springer, Berlin, 414 pp.

BOUDREAU, B. P. (1999) A theoretical investigation of the organic carbon-microbial biomass relation in muddy sediments. Aquat. Microb. Ecol., **17**, 181-189.

DITTMANN, S. (1999) The Wadden Sea ecosystem - Stability properties and mechanisms. Springer, Berlin, 307 pp.

HUETTEL, M., ZIEBIS, W., FORSTER, S. & LUTHER III., G. (1998) Advective transport reflecting metal and nutrient distribution and interfacial fluxes in permeable sediments. Geochim. Cosmochim. Acta, **62**, 613-631.

HUNTER, K. S., WANG, Y. & VAN CAPPELLEN, P. (1998) Kinetic modeling of microbially-driven redox chemistry of subsurface environments: coupling transport, microbial metabolism and geochemistry. J. Hydrol., **209**, 53-80.

KÖHLER, P. & WIRTZ, K. (2002) Linear understanding of a huge aquatic ecosystem model using a group-collecting sensitivity study. Environ. Model. Softw., **17**, 613-635.

MEILE, C. & VAN CAPPELLEN, P. (2003) Global estimates of enhanced solute transport in marine sediments. Limnol. Oceanogr., **48**, 777–786.

RUSCH, A., TÖPKEN, H., BÖTTCHER, M. E. & HÖPNER, T. (1998) Recovery from black spots: results of a loading experiment in the Wadden Sea. J. Sea Res., **40**, 205-219.

RUSCH, A., FORSTER, S. & HUETTEL, M. (2001) Bacteria, diatoms and detritus in an intertidal sand subject to advective transport across the water-sediment interface. Biogeochemistry, **55**, 1-27.

SOETAERT, K., HERMAN, P. & MIDDELBURG, J. (1996) Dynamic response of deep-sea sediments to seasonal variation: a model. Limnol. Oceanogr., **41**, 1651-1668.

SOETAERT, K., MIDDELBURG, J. J., HERMAN, P. M. & BUIS, K. (2000) On the coupling of benthic and pelagic biogeochemical models. Earth-Sci. Rev., **51**, 173-201.

STOECK, T. & ALBERS, B. P. (2000). Microbial biomass and activity in the vicinity of a mussel bed built up by the blue mussel *Mytilus edulis*. Helgoland Mar. Res., **54**, 39-46.

VALLINO, J. J., HOPKINSON, C. S. & HOBBIE, J. E. (1996) Modeling bacterial utilization of dissolved organic matter: Optimization replaces Monod kinetics. Limnol. Oceanogr., **41**, 1591-1609.

WANG, Y. & VAN CAPPELLEN, P. (1996) A multicomponent reactive transport model of early diagenesis: Application to redox cycling in coastal marine sediments. Geochim. Cosmochim. Acta, **60**, 2993-3014.

WIRTZ, K. W. (2003) Control of biogechemical cycling by mobility and metabolic strategies of microbes in the sediments: an integrated model study. FEMS Microbiol. Ecol., accepted.

K. W. Wirtz, Institute of Chemistry and Biology of the Marine Environment, Carl-von-Ossietzky-Str. 9-11, P.O. Box 25 03, D-26111 Oldenburg, Germany; e-mail: k.wirtz@icbm.de.