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 Capelle, 1996; Soetaert et al., 1996; Hunter et al., 1998; Boudeau, 1992). The ISM includes four different types of reactions, degradation of particulate organic carbon (POC), fermentation 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 Capelle (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 (Valino 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:

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

\( X_0 \) represents an average microbial biomass for a specific site and functional group. The coefficient \( \beta \) describes the flexibility of the switch between the active and dormant state. Considering a high flexibility (\( \beta = 1 \)), the biomass of dormant cells \( X_{\text{dorm}} \) 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 sedimentation 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 addressed 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, NH4+, NO3 and O2 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, SO2-, H2S, 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; STÖECK & 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.

**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 \( \beta \) 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 CO2 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
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 HÜTTEL 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 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**

We observe a counter-intuitive, non-linear response in the CO$_2$ production after shifting the specific dormancy flexibility ($\beta$) 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 $\beta$.

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 CO₂ 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.

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