

# SED (1.0): A new, numerically efficient sediment module for the coupling to Earth System Models

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**Abstract.** TEXT

## 1 Introduction

Role of marine sediments for climate and global biogeochemical cycles

Diagenetic Models

5 How are sediment resolved in Earth System models

Problem with that

Alternative Model approaches, e.g. from coastal reserach

Solution presented here

See Van Cappellen and Wang (1996): “Metal cycling in surface sediments: Modeling the interplay

10 or transport and reaction” for some good basic info!

## 2 Model Description

This section describes the formulation and solution of the model (see Table 1 for the implemented processes). A glossary of parameters along with their respective units is provided in Tables ?? and ??.

## 15 2.1 General Model Approach

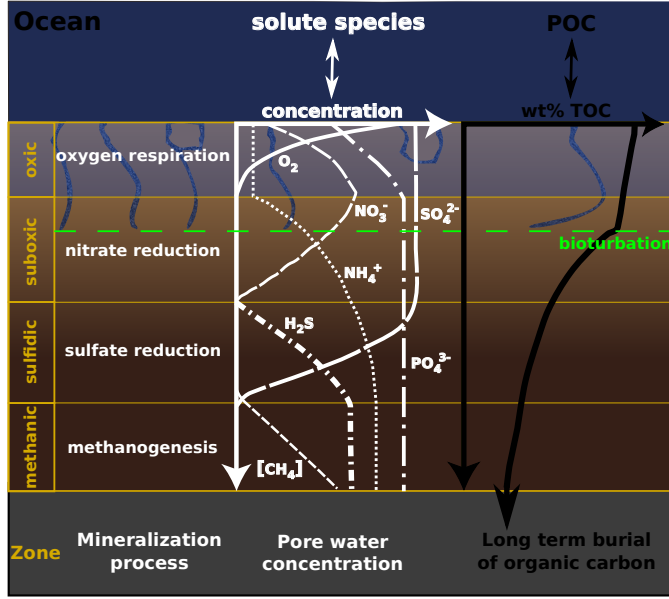
The calculation of benthic return/uptake and burial fluxes is based on the vertically resolved conservation equation for solid and dissolved species in porous media is given by (e.g. ??):

$$\frac{\partial \xi C_i}{\partial t} = -\frac{\partial F}{\partial z} + \xi \sum_j R_i^j \quad (1)$$

20 where  $C_i$  is the concentration of the biogeochemical species  $i$ ,  $\xi$  equals the porosity  $\phi$  for solute species and  $(1 - \phi)$  for solid species, hence represents the partitioning of species  $i$  into the solute and dissolved phase. The term  $z$  is the sediment depth,  $t$  denotes the time,  $F$  summarises the transport fluxes and  $\sum_j R_i^j$  represents the sum of production/consumption rates  $j$  that affect species  $i$ . The reaction network has to account for the most important primary and secondary redox reactions, 25 equilibrium reactions, mineral dissolution and precipitation, as well as adsorption and desorption processes.

State-of-the-art reaction-transport models generally solve the ordinary differential equation (ODE) (1) numerically and thus allow to account for transient conditions, depth-varying parameters or a high degree of coupling between different chemical species. Yet, numerical models are computa- 30 tional expensive, thus rendering their application in an Earth System Model framework prohibitive. An analytical solution of Eq. (1) provides an alternative and computational more efficient approach. Analytical models enjoyed great popularity in the early days of diagenetic modelling due to the low computing power. However, early analytical models were often very problem-specific and only considered one or two coupled species (e.g. Lehrman, Berner) ?? which pubs?. A number of more 35 complex analytical models describing the coupled dynamics of ....were developed (e.g. ???).

Finding an analytical solution to Eq. (1), especially when complex reaction networks are to be considered is not straightforward and generally requires the assumption of steady state. Because the Earth system model relevant variability in boundary conditions and fluxes is generally longer than the characteristic timescales of the reaction-transport processes, the sediment can be described by a 40 series of pseudo steady-states. In addition, the complexity of the reaction network can be reduced by dividing the sediment into distinct zones and accounting for the most pertinent biogeochemical processes within each zone, thus increasing the likelihood of finding an analytical solution to Eq. (1). The model divides the sediment into a bioturbated and a non-bioturbated zone defined by the constant bioturbation depth  $z_{\text{bio}}$ . In addition, it accounts for the dynamic redox zonation of marine sediments 45 by dividing the sediment into: 2) an oxic zone situated between the SWI and a dynamically calculated penetration depth of oxygen  $z_{\text{ox}}$ , 3) a denitrification zone situated between  $z_{\text{ox}}$  and a dynamically calculated penetration depth of nitrate  $z_{\text{NO}_3}$ , 4) a sulfate reduction zone situated between  $z_{\text{NO}_3}$  and a dynamically calculated penetration depth of sulfate  $z_{\text{SO}_4}$  and 5) a methanic zone situated below  $z_{\text{SO}_4}$  (Figure 1). Each zone is characterised by a set of diagenetic equations that encapsulate the most



**Figure 1.** Schematic of the different modelled species and layers in our sediment model. Here showing the case  $z_{ox} < z_{bio} < z_{NO_3} < z_{SO_4}$ .

50 pertinent reaction and transport processes in the respective zone (see section 2.2 and 2.3 for more details).

## 2.2 Transport

The model accounts for both advection and diffusion of dissolved and solid species, assuming that sediment compaction is negligible ( $\frac{\partial \phi}{\partial z} = 0$ ). The diffusion of dissolved species is described via an  
 55 apparent diffusion coefficient,  $D_{i0}$ . In addition, the activity of infaunal organisms in the bioturbated zone of the sediment ( $z < z_{bio}$ ) causes random displacements of sediments and porewaters and is simulated using a diffusive term (e.g. Boudreau, 1986), with a constant bioturbation coefficient  $D_{bio}$  in the bioturbated zone. The pumping activity by burrow-dwelling animals and the resulting ventilation of tubes, the so-called bioirrigation, is encapsulated in a factor,  $f_{ir}$  that enhances the molecular  
 60 diffusion coefficient,  $D_{mol,i}$  (hence,  $D_{i,0} = D_{mol,i} \cdot f_{ir}$ , ?). The divergence of the flux is thus given by:

$$\frac{\partial F}{\partial z} = -\frac{\partial}{\partial z} \left( -\xi D_i \frac{\partial C_i}{\partial z} + \xi w C_i \right) \quad (2)$$

where  $D_i$  is the diffusion coefficient of species  $i$  ( $D_i = D_{i,0} + D_{bio} = D_{mol,i} \cdot f_{ir} + D_{bio}$  for dissolved species and  $D_i = D_{bio}$  for solid species) and  $w$  is the burial rate. The bioturbation coefficient  $D_{bio}$  is  
 65 set to zero below  $z_{bio}$ . In addition, infaunal activity ceases ( $D_{bio} = 0$ ) once bottom waters become anoxic ( $O_2 = 0.0 \text{ mol cm}^{-3}$ ). **add if-query in code!!**

**Table 1.** Reactions and variables implemented in the Reaction Network of SED (1.0). The primary and secondary redox reactions are listed in the sequence they occur with increasing sediment depth.

	Description
Primary redox reactions	Degradation of organic matter via aerobic respiration, denitrification, sulfate reduction, methanogenesis (implicit)
Secondary redox reactions	Oxidation of ammonium and sulfide by oxygen, anaerobic oxidation of methane by sulfate
Adsorption/Desorption	Ad-/Desorption of P on/from $\text{Fe}(\text{OH})_3$ , $\text{NH}_4$ adsorption, $\text{PO}_4$ adsorption
Mineral precipitation	Formation of authigenic P
Variables	Organic matter, oxygen, nitrate, ammonium, sulfate, sulfide (hydrogen sulfide), phosphate, Fe-bound P, DIC, ALK

## 2.3 Reaction Network

Earth System models generally track the evolution of the global biogeochemical cycles of organic and inorganic carbon, the essential nutrients (nitrogen, phosphorus) and oxygen with the aim of investigating the evolution of the ocean’s redox structure and carbonate system and its feedbacks on global climate. This general aim thus defines a minimum set of state variables and reaction processes that need to be resolved for an efficient representation of the benthic-pelagic coupling in Earth System Models. The sediment model has to provide robust quantifications of organic and inorganic carbon burial fluxes, growth-limiting nutrient, equilibrium invariant and reduced species return fluxes, and oxygen uptake fluxes. As a consequence, the reaction network must explicitly or implicitly account for the most important primary and secondary redox reactions, equilibrium reactions, mineral precipitation/dissolution and adsorption/desorption, resulting in a complex set of coupled reaction-transport equations. The following subsections provide a short discussion of the reaction processes included in the model and give an overview of the vertically resolved conservation equations and boundary conditions for solid and dissolved species in each layer. Table 1 states the reactions and variables considered in the reaction network.

### 2.3.1 Organic matter

In marine sediments, organic matter (OM) is degraded by heterotrophic activity coupled to the sequential utilisation of terminal electron acceptors (TEAs), typically in the order of  $\text{O}_2$ ,  $\text{NO}_3^-$ ,  $\text{Mn}(\text{VI})$ ,  $\text{Fe}(\text{III})$  and  $\text{SO}_4^{2-}$  followed by methanogenesis and/or fermentation. Organic matter degradation is described via a multi-G model approach (?, and references therein), assuming that the bulk OM is divided into discrete compound classes  $C_i$  characterised by specific degradation rate constants  $k_i$ . Such a multi-G approach allows for selective preservation of compound classes according to their degradability,  $k_i$  and, thus, accounts for the change in organic matter degradability with

**Table 2.** Boundary conditions for organic matter and oxygen.

Boundary	Condition	
$z = 0$ $z = z_{\text{bio}}$	known concentration continuity	1) $C_i(0) = C_{i0}$ 2) $C_i(z_{\text{bio}}^-) = C_i(z_{\text{bio}}^+)$ 3) $-D_{\text{bio}} \cdot \frac{\partial C_i}{\partial z} \Big _{z_{\text{bio}}^-} = 0$
$z = 0$ $z = z_{\text{bio}}$  $z = z_{\text{ox}}$	known concentration continuity  O <sub>2</sub> consumption ( $z_{\text{ox}} = z_{\infty}$ )  ( $z_{\text{ox}} < z_{\infty}$ ) with flux from below	1) $O_2(0) = O_{20}$ 2) $O_2(z_{\text{bio}}^-) = O_2(z_{\text{bio}}^+)$ 3) $-(D_{O_2,0} + D_{\text{bio}}) \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{bio}}^-} = -D_{O_2,0} \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{bio}}^+}$ 4) <b>IF</b> ( $O_2(z_{\infty}) > 0$ ) $\frac{\partial O_2}{\partial z} \Big _{z_{\text{ox}}} = 0$ <b>ELSE</b> $O_2(z_{\text{ox}}) = 0$ and $-D_{O_2} \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{ox}}} = F_{\text{red}}(z_{\text{ox}})$ $F_{\text{red}}(z_{\text{ox}}) = \frac{1-\phi}{\phi} \cdot \int_{z_{\text{ox}}}^{\infty} \sum_i (2\gamma_{\text{NH}_4} \text{NC}_i + \gamma_{\text{H}_2\text{S}} \text{SO}_4\text{C}) k_i C_i dz$

90 burial. Each compound class is degraded according to first-order kinetics. Organic matter dynamics are thus described by:

$$\frac{\partial C_i}{\partial t} = 0 = D_{C_i} \frac{\partial^2 C_i}{\partial z^2} - w \frac{\partial C_i}{\partial z} - k_i \cdot C_i \quad (3)$$

The solution of Eq. 3 (see section ?? for details) requires the definition of boundary conditions. The model assumes a known concentration/flux at the sediment-water interface and continuity across the bottom of the bioturbated zone,  $z_{\text{bio}}$  (Table 2).

### 2.3.2 Oxygen

Oxygen serves as the most powerful terminal electron acceptor for the heterotrophic degradation of organic carbon. In addition, the oxidation of reduced species produced through microbial activity throughout the sediment column further contributes to the consumption of oxygen. The model explicitly accounts for the consumption of oxygen by heterotrophic degradation and nitrification of ammonium in the oxic layer of the sediment. The nitrification of 1 mol of ammonium in the oxic layer consumes 2 mol of oxygen. In addition, the oxygen consumption through the oxidation of reduced species ( $\text{Fe}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{NH}_4$ ,  $\text{H}_2\text{S}$ ) produced in the suboxic and anoxic layers of the sediment is implicitly taken into account through the flux boundary condition at the dynamic oxygen penetration depth  $z_{\text{ox}}$ . This simplification can be justified as it has been shown that these secondary redox reactions mainly occur at the oxic/suboxic interface (?). Oxygen is described in  $\text{mol cm}^{-3}$  liquid and conversion from the solid phase of mineralized organic matter (expressed in  $\text{mol cm}^{-3}$  bulk sediment) to consumption of dissolved oxygen (or later nutrients) introduce a factor of  $\frac{1-\phi}{\phi}$ , where  $\phi$  is