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

Dominik Hülse[1], Sandra Arndt[1], Stuart Daines[2], and Andy J. Ridgwell[1, 3]

[1]School of Geographical Sciences, University of Bristol, Clifton, Bristol BS8 1SS, UK
[2]Earth System Science, University of Exeter, North Park Road, Exeter EX4 4QE, UK
[3]Department of Earth Sciences, University of California, Riverside, CA 92521, USA

Correspondence to: Sandra Arndt (s.arndt@bristol.ac.uk)

Abstract. TEXT

1   Introduction

Role of marine sediments for climate and global biogeochemical cycles

Diagenetic Models

How are sediment resolved in Earth System models

Problem with that

Alternative Model approaches, e.g. from coastal reserach

Solution presented here

2   Model Description

This section describes the formulation and solution of the model. A glossary of parameters along with their respective units is provided in Table **??**

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. Berner, 1980; Boudreau, 1997):

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

where C_i is the concentration of the biogeochemical species i, ξ equals the porosity ϕ 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, equilibrium reactions, mineral dissolution and precipitation, as well as adsorption and desorption processes.

State-of-the-art reaction-transport models generally solve Eq. (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 computational 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 complex analytical models describing the coupled dynamics of ....were developed (e.g. Billen, 1982; Goloway and Bender, 1982; Jahnke et al., 1982).

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 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_{bio}. In addition, it accounts for the dynamic redox zonation of marine sediments by dividing the sediment into: 2) an oxic zone situated between the SWI and a dynamically calculated penetration depth of oxygen z_{O_2}, 3) a denitrification zone situated between z_{O_2} and a dynamically calculated penetration depth of nitrate z_{NO_3}, 4) a sulfate reduction zone situated between z_{NO_3} and a dynamically calculated penetration depth of sulfate z_{SO_4} and 5) a methanogenic zone situated below

z_{SO_4} (Figure 1). Each zone is characterised by a set of diagenetic equations that encapsulate the most pertinent reaction and transport processes in the respective zone (see section **??** and **??** form more detail).
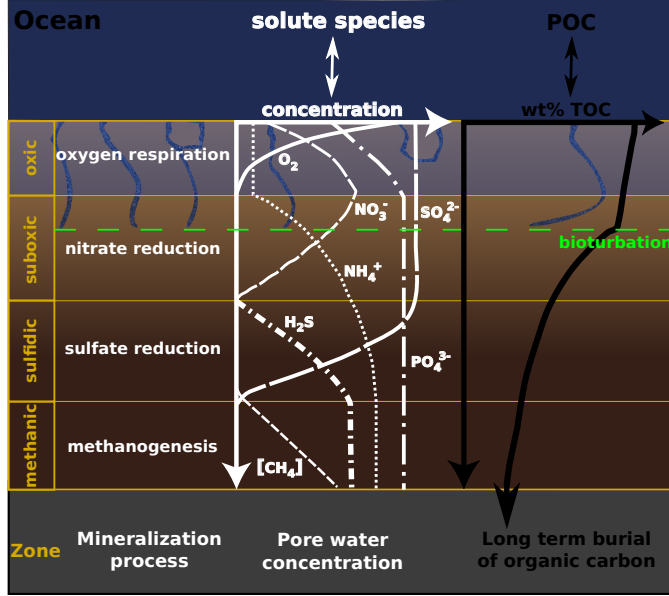

Figure 1. Schematic of the different modelled species and layers in our sediment model. Here showing the case $z_{ox} < z_{bio} < z_{NO_3} < z_{SO_4}$.

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 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, the so-called bioirrigation, is encapsulated in a factor, f_{ir} that enhances the molecular diffusion coefficient, $D_{mol,i}$ (hence, $D_{i,0} = D_{mol,i} \cdot f_{ir}$, Soetaert et al., 1996a). The divergence of the flux is thus given by:

$$\frac{\partial F}{\partial z} = -\frac{\partial}{\partial z}\left(-\xi D_i \frac{\partial C_i}{\partial z} + \xi w C_i\right)$$
(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 set to zero below z_{bio}. In addition, infaunnal activity ceases ($D_{bio} = 0$) once bottom waters become anoxic ($O_2 = 0.0$ mol cm^{-3}). last bit not like that in model

3

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 table **??** what to do here? provides an overview of the vertically resolved conservation equations for solid and dissolved species in each layer.

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 O_2, NO_3^-, Mn(VI), Fe(III) and SO_4^{2-} followed by methanogenesis and/or fermentation. Organic matter degradation is described via a multi-G model approach (Arndt et al., 2013, 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 burial. Each compound class is degraded according to first-order kinetics. Organic matter dynamics are thus described by:

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

where:

$$D_{C_i} = D_{bio} \qquad\qquad\qquad \text{if } (z \leq z_{bio}) \tag{4}$$

$$D_{C_i} = 0 \qquad\qquad\qquad \text{if } (z > z_{bio}) \tag{5}$$

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_{bio} (Table 1).

Table 1. Boundary conditions for organic matter and oxygen.

Boundary	Condition	
$z = 0$	known concentration	1) $C_i(0) = C_{i0}$
$z = z_{bio}$	continuity	2) $C_i(z_{bio}^-) = C_i(z_{bio}^+)$
		3) $D_{bio} \cdot \frac{\partial C_i}{\partial z}\big|_{z_{bio}^-} = 0$
$z = 0$	known concentration	1) $O_2(0) = O_{20}$
$z = z_{bio}$	continuity	2) $O_2(z_{bio}^-) = O_2(z_{bio}^+)$
		3) $(D_{O_2,0} + D_{bio}) \cdot \frac{\partial O_2}{\partial z}\big|_{z_{bio}^-} = D_{O_2,0} \cdot \frac{\partial O_2}{\partial z}\big|_{z_{bio}^+}$
$z = z_{ox}$	O_2 consumption	4) $O_2(z_{ox}) = 0$ or $\frac{\partial O_2}{\partial z}\big|_{z_{ox}} = 0$
$z = z_{ox}$	Flux from below	5) $-\omega D_{O_2} \cdot \frac{\partial O_2}{\partial z}\big|_{z_{ox}} = F_{red,z_{ox}}$
	with:correct? &	$F_{red,z_{ox}} = \frac{1-\phi}{\phi} \cdot \int_{z_{ox}}^{\infty} \sum_i (2\gamma_{NH_4} NC_i + \delta SC_i) k_i C_i \, dz$
	why ω at 5) (delete!?)	

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 reduces 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. In addition, the oxygen consumption through the oxidation of reduced species (Fe^{2+}, Mn^{2+}, NH_4, H_2S) 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_{ox}. This simplification can be justified as it has been shown that these secondary redox reactions mainly occur at the oxic/suboxic interface (Soetaert et al., 1996b). Oxygen is described in $mol \ cm^{-3}$ liquid and conversion from the solid phase of mineralized organic matter (expressed in $mol \ cm^{-3}$ bulk sediment) to consumption of dissolved oxygen (or later nutrients) introduce a factor of $\frac{1-\phi}{\phi}$, where ϕ is the sediment porosity. Oxygen dynamics are thus described by:

$$\frac{\partial O_2}{\partial t} = 0 = D_{O_2} \frac{\partial^2 O_2}{\partial z^2} - w \frac{\partial O_2}{\partial z} - \frac{1-\phi}{\phi} \sum_i k_i \cdot [OC + 2\gamma_{NH_4} NC_i] \cdot C_i(z) \tag{6}$$

where:

$$D_{O_2} = D_{O_2,0} + D_{bio} \qquad\qquad \text{if } (z \leq z_{bio}) \tag{7}$$

$$D_{O_2} = D_{O_2,0} \qquad\qquad \text{if } (z > z_{bio}) \tag{8}$$

To solve Eq. 6 analytically (see section **??**) boundary conditions at three depths are defined (Table 1). The model assumes a known bottom water concentration and the complete consumption of oxygen at the oxygen penetration depth (or zero flux if $z_{ox} = z_{\infty}$). It considers equal oxygen concentration and

diffusive flux above (z_{bio}^-) and below (z_{bio}^+) the bioturbation boundary. In addition, the model imposes a flux of reduced species through the bottom of the oxic zone that is calculated as the reduced substances produced through anoxic mineralization of organic matter below z_{ox}. Thus, assuming that fractions (γ_{NH_4} and δ) of these reduced species are oxidised at the oxic/suboxic interface.

2.3.3 Nitrate and Ammonium

To model nitrate and ammonium dynamics the sediment is partitioned into two geochemical layers (oxic and suboxic), where different equations describe the biogeochemical processes. Above the oxygen penetration depth organic matter mineralization produces ammonium, which is partly nitrified to nitrate (the fraction γ_{NH_4}). In the suboxic zone ($z > z_{ox}$), oxygen concentration is zero and nitrate serves as the electron acceptor to respire organic matter, thus consuming nitrate and producing ammonium. Below the nitrate penetration depth z_{NO_3}, ammonium is still produced through OM mineralization. Therefore the diagenetic equations for nitrate and ammonium are given by:

1. Layer ($z \leq z_{ox}$)

$$\frac{\partial NO_3^I}{\partial t} = 0 = D_{NO_3}\frac{\partial^2 NO_3^I}{\partial z^2} - w\frac{\partial NO_3^I}{\partial z} + \gamma_{NH_4}\frac{1-\phi}{\phi} \cdot \sum_i NC_i \cdot k_i \cdot C_i(z) \tag{9}$$

$$\frac{\partial NH_4^I}{\partial t} = 0 = D_{NH_4}\frac{\partial^2 NH_4^I}{\partial z^2} - w\frac{\partial NH_4^I}{\partial z} + (1-\gamma_{NH_4})\frac{1-\phi}{\phi} \cdot \sum_i NC_i \cdot k_i \cdot C_i(z) \tag{10}$$

2. Layer ($z_{ox} < z \leq z_{NO_3}$ [or z_∞ for NH$_4$])

$$\frac{\partial NO_3^{II}}{\partial t} = 0 = D_{NO_3}\frac{\partial^2 NO_3^{II}}{\partial z^2} - w\frac{\partial NO_3^{II}}{\partial z} - \frac{1-\phi}{\phi}NO_3CR \cdot \sum_i k_i \cdot C_i(z) \tag{11}$$

$$\frac{\partial NH_4^{II}}{\partial t} = 0 = D_{NH_4}\frac{\partial^2 NH_4^{II}}{\partial z^2} - w\frac{\partial NH_4^{II}}{\partial z} + \frac{1-\phi}{\phi} \cdot \sum_i NC_i \cdot k_i \cdot C_i(z) \tag{12}$$

where

$$D_i = D_{i,0} + D_{bio} \qquad\qquad \text{if } (z \leq z_{bio}) \tag{13}$$

$$D_i = D_{i,0} \qquad\qquad \text{if } (z > z_{bio}) \tag{14}$$

and $i \in \{NO_3, NH_4\}$. The boundary conditions to solve Equations 9 - 12 are summarized in Table 2. The model assumes known bottom water concentrations for both species, the complete consumption of nitrate at the nitrate penetration depth (or zero flux if $z_{NO_3} = z_\infty$) and no change in ammonium flux at z_∞. It considers equal concentrations and diffusive fluxes at z_{bio} and z_{ox}. In addition, the re-oxidation of upward-diffusing reduced ammonium is considered in the oxic-suboxic boundary condition for nitrate and ammonium.

Table 2. Boundary conditions for nitrate and ammonium.

Boundary	Condition	
$z = 0$	known concentration	1) $NO_3(0) = NO_{30}$
$z = z_{bio}$	continuity	2) $NO_3(z_{bio}^-) = NO_3(z_{bio}^+)$
		3) $(D_{NO3,0} + D_{bio}) \cdot \frac{\partial NO_3}{\partial z}\big|_{z_{bio}^-} = D_{NO3,0} \cdot \frac{\partial NO_3}{\partial z}\big|_{z_{bio}^+}$
$z = z_{ox}$	continuity	4) $NO_3(z_{ox}^-) = NO_3(z_{ox}^+)$
		5) $-D_{NO3} \cdot \frac{\partial NO_3}{\partial z}\big|_{z_{ox}^-} + \gamma_{NH4} \cdot F_{NH4} = -D_{NO3} \cdot \frac{\partial NO_3}{\partial z}\big|_{z_{ox}^+}$
	where:	$F_{NH4} = \frac{1-\phi}{\phi} \cdot \int_{z_{NO3}}^{\infty} \sum_i k_i \cdot NC_i \cdot C_i \, dz$
$z = z_{NO3}$	NO_3 consumption	6) $NO_3(z_{NO3}) = 0$ or $\frac{\partial NO_3}{\partial z}\big|_{z_{NO3}} = 0$
$z = 0$	known concentration	1) $NH_4(0) = NH_{40}$
$z = z_{bio}$	continuity	2) $NH_4(z_{bio}^-) = NH_4(z_{bio}^+)$
		3) $(D_{NH4,0} + D_{bio}) \cdot \frac{\partial NH_4}{\partial z}\big|_{z_{bio}^-} = D_{NH4,0} \cdot \frac{\partial NH_4}{\partial z}\big|_{z_{bio}^+}$
$z = z_{ox}$	continuity	4) $NH_4(z_{ox}^-) = NH_4(z_{ox}^+)$
		5) $-D_{NH4} \cdot \frac{\partial NH_4}{\partial z}\big|_{z_{ox}^-} + (1 - \gamma_{NH4}) \cdot F_{NH4} = -D_{NH4} \cdot \frac{\partial NH_4}{\partial z}\big|_{z_{ox}^+}$
	where:	$F_{NH4} = \frac{1-\phi}{\phi} \cdot \int_{z_{NH4}}^{\infty} \sum_i k_i \cdot NC_i \cdot C_i \, dz$
$z = z_{NH4}$	NO_3 consumption	6) $\frac{\partial NH_4}{\partial z}\big|_{z_{NH4}} = 0$

2.3.4 Sulfate

Processes considered

General equation

Solution

2.3.5 Phosphate

Processes considered

general equation

solution

2.3.6 Sulfide

Processes considered

general equation

solution

2.4 Model Parameters

2.4.1 Transport Parameters

Sedimentation rate
Diffusion coefficients
Bio-irrigation coefficients

2.5 Reaction Parameters

short description

2.6 Module Structure

technical description, e.g. how is it implemented and how can it be coupled to model

3 Test Cases

3.1 Benthic fluxes on a global scale

Application to Seitert, 2004 OM, burwiczk see rate data and evaluation based on global data (Archer)

3.2 HILDA-like test

3.3 GENIE-Cretaceous test?

4 Scope of applicability and model limitations

5 Conclusions

TEXT

6 Code Availability

Appendix A

A1

References

Arndt, S., Jørgensen, B., LaRowe, D., Middelburg, J., Pancost, R., and Regnier, P. (2013). Quantifying the degradation of organic matter in marine sediments: A review and synthesis. *Earth-Science Reviews*, 123:53–86.

Berner, R. A. (1980). *Early Diagenesis: A Theoretical Approach*. Princeton University Press.

Billen, G. (1982). Modelling the processes of organic matter degradation and nutrients recycling in sedimentary systems. *Sediment microbiology*, pages 15–52.

Boudreau, B. P. (1997). *Diagenetic models and their implementation*, volume 505. Springer Berlin.

Goloway, F. and Bender, M. (1982). Diagenetic models of interstitial nitrate profiles in deep sea suboxic sediments. *Limnol. Oceanogr*, 27(4):624–638.

Jahnke, R. A., Emerson, S. R., and Murray, J. W. (1982). A model of oxygen reduction, denitrification, and organic matter mineralization in marine sediments. *Limnol. Oceanogr*, 27(4):6–10.

Soetaert, K., Herman, P. M., and Middelburg, J. J. (1996a). Dynamic response of deep-sea sediments to seasonal variations: a model. *Limnology and Oceanography*, 41(8):1651–1668.

Soetaert, K., Herman, P. M. J., and Middelburg, J. J. (1996b). A model of early diagenetic processes from the shelf to abyssal depths. *Geochimica et Cosmochimica Acta*, 60(6):1019–1040.