

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

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 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 6 and 7.

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):

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

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 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 computational expensive, thus rendering their application in an Earth System Model framework prohibitive. An analytical solution of Eq. (1) provides an alternative and computationally 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 ofwere 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_{ox} , 3) a denitrification zone situated between z_{ox} 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 methanic zone situated below

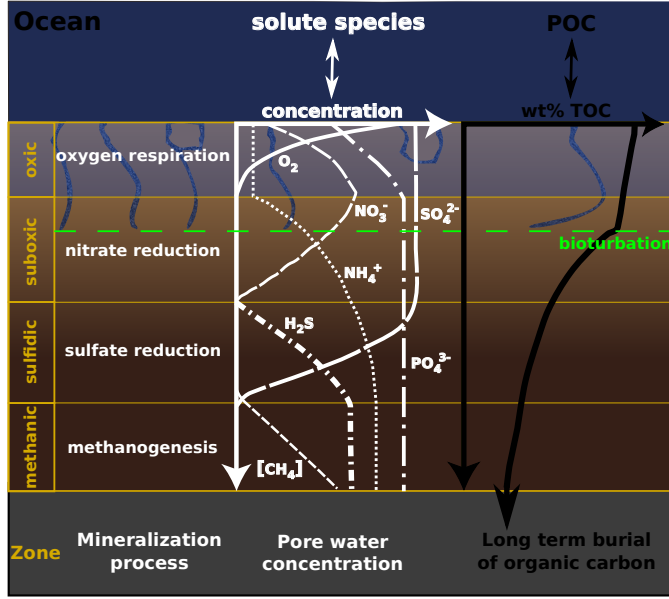


Figure 1. Schematic of the different modelled species and layers in our sediment model. Here showing the case $z_{\text{ox}} < z_{\text{bio}} < z_{\text{NO}_3} < z_{\text{SO}_4}$.

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 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 apparent diffusion coefficient, D_{i0} . In addition, the activity of infaunal organisms in the bioturbated zone of the sediment ($z < z_{\text{bio}}$) 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 diffusion coefficient, $D_{\text{mol},i}$ (hence, $D_{i,0} = D_{\text{mol},i} \cdot f_{ir}$, Soetaert et al., 1996a). The divergence of the flux is thus given by:

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

where D_i is the diffusion coefficient of species i ($D_i = D_{i,0} + D_{\text{bio}} = D_{\text{mol},i} \cdot f_{ir} + D_{\text{bio}}$ for dissolved species and $D_i = D_{\text{bio}}$ for solid species) and w is the burial rate. The bioturbation coefficient D_{bio} is set to zero below z_{bio} . In addition, infaunal activity ceases ($D_{\text{bio}} = 0$) once bottom waters become anoxic ($O_2 = 0.0 \text{ mol cm}^{-3}$). **last bit not like that in model**

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 $\text{Fe}(\text{OH})_3$, NH_4 adsorption, 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 O_2 , NO_3^- , $\text{Mn}(\text{VI})$, $\text{Fe}(\text{III})$ 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

Table 2. Boundary conditions for organic matter and oxygen.

Boundary	Condition	
$z = 0$	known concentration	1) $C_i(0) = C_{i0}$
$z = z_{\text{bio}}$	continuity	2) $C_i(z_{\text{bio}}^-) = C_i(z_{\text{bio}}^+)$ 3) $D_{\text{bio}} \cdot \frac{\partial C_i}{\partial z} \Big _{z_{\text{bio}}^-} = 0$
$z = 0$	known concentration	1) $O_2(0) = O_{20}$
$z = z_{\text{bio}}$	continuity	2) $O_2(z_{\text{bio}}^-) = O_2(z_{\text{bio}}^+)$ 3) $(D_{O_2,0} + D_{\text{bio}}) \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{bio}}^-} = D_{O_2,0} \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	O ₂ consumption	4) $O_2(z_{\text{ox}}) = 0$ and/or/at all??? $\frac{\partial O_2}{\partial z} \Big _{z_{\text{ox}}} = 0$
$z = z_{\text{ox}}$	Flux from below with: correct? & why ω at 5) (delete!?)	5) $-\omega D_{O_2} \cdot \frac{\partial O_2}{\partial z} \Big _{z_{\text{ox}}} = F_{\text{red}, z_{\text{ox}}}$ $F_{\text{red}, z_{\text{ox}}} = \frac{1-\phi}{\phi} \cdot \int_{z_{\text{ox}}}^{\infty} \sum_i (2\gamma_{\text{NH}_4} \text{NC}_i + \gamma_{\text{H}_2\text{S}} \text{SO}_4\text{C}) k_i C_i dz$

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

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

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_{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 (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:

$$\frac{\partial O_2}{\partial t} = 0 = D_{O_2} \frac{\partial^2 O_2}{\partial z^2} - w \frac{\partial O_2}{\partial z} - \frac{1-\phi}{\phi} \sum_i k_i \cdot [OC + 2\gamma_{NH_4} NC_i] \cdot C_i(z) \quad (4)$$

To solve Eq. 4 analytically (see section ??) boundary conditions at three depths are defined (Table 2). 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 nitrate is consumed by denitrification and ammonium is produced. 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 ($z \leq z_{ox}$)

$$\frac{\partial NO_3^I}{\partial t} = 0 = D_{NO_3} \frac{\partial^2 NO_3^I}{\partial z^2} - w \frac{\partial NO_3^I}{\partial z} + \gamma_{NH_4} \frac{1-\phi}{\phi} \cdot \sum_i NC_i \cdot k_i \cdot C_i(z) \quad (5)$$

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

2. Layer ($z_{ox} < z \leq z_{NO_3}$ [or z_{∞} for NH_4])

$$\frac{\partial NO_3^{II}}{\partial t} = 0 = D_{NO_3} \frac{\partial^2 NO_3^{II}}{\partial z^2} - w \frac{\partial NO_3^{II}}{\partial z} - \frac{1-\phi}{\phi} NO_3 C \cdot \sum_i k_i \cdot C_i(z) \quad (7)$$

$$\frac{\partial NH_4^{II}}{\partial t} = 0 = D_{NH_4} \frac{\partial^2 NH_4^{II}}{\partial z^2} - w \frac{\partial NH_4^{II}}{\partial z} + \frac{1-\phi}{\phi} \cdot \sum_i NC_i \cdot k_i \cdot C_i(z) \quad (8)$$

The boundary conditions to solve Equations 5 - 12 are summarized in Table 3. 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 3. Boundary conditions for nitrate and ammonium.

Boundary	Condition	
$z = 0$	known concentration	1) $NO_3(0) = NO_{30}$
$z = z_{\text{bio}}$	continuity	2) $NO_3(z_{\text{bio}}^-) = NO_3(z_{\text{bio}}^+)$
		3) $(D_{NO_3,0} + D_{\text{bio}}) \cdot \frac{\partial NO_3}{\partial z} \Big _{z_{\text{bio}}^-} = D_{NO_3,0} \cdot \frac{\partial NO_3}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	continuity	4) $NO_3(z_{\text{ox}}^-) = NO_3(z_{\text{ox}}^+)$
	where:	5) $-D_{NO_3} \cdot \frac{\partial NO_3}{\partial z} \Big _{z_{\text{ox}}^-} + \gamma_{\text{NH}_4} \cdot F_{\text{NH}_4} = -D_{NO_3} \cdot \frac{\partial NO_3}{\partial z} \Big _{z_{\text{ox}}^+}$
		$F_{\text{NH}_4} = \frac{1-\phi}{\phi} \cdot \int_{z_{\text{NO}_3}}^{\infty} \sum_i k_i \cdot \text{NC}_i \cdot C_i \, dz$
$z = z_{\text{NO}_3}$	NO_3 consumption	6) $NO_3(z_{\text{NO}_3}) = 0$ or $\frac{\partial NO_3}{\partial z} \Big _{z_{\text{NO}_3}} = 0$
$z = 0$	known concentration	1) $\text{NH}_4(0) = NH_{40}$
$z = z_{\text{bio}}$	continuity	2) $\text{NH}_4(z_{\text{bio}}^-) = \text{NH}_4(z_{\text{bio}}^+)$
		3) $(D_{\text{NH}_4,0} + D_{\text{bio}}) \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{bio}}^-} = D_{\text{NH}_4,0} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	continuity	4) $\text{NH}_4(z_{\text{ox}}^-) = \text{NH}_4(z_{\text{ox}}^+)$
not $+(1 - \gamma_{\text{NH}_4}) \cdot F_{\text{NH}_4}$?	where:	5) $-D_{\text{NH}_4} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{ox}}^-} - \gamma_{\text{NH}_4} \cdot F_{\text{NH}_4} = -D_{\text{NH}_4} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{ox}}^+}$
		$F_{\text{NH}_4} = \frac{1-\phi}{\phi} \cdot \int_{z_{\text{NO}_3}}^{\infty} \sum_i k_i \cdot \text{NC}_i \cdot C_i \, dz$
$z = z_{\text{NO}_3}$	continuity	6) $\text{NH}_4(z_{\text{NO}_3}^-) = \text{NH}_4(z_{\text{NO}_3}^+)$
	flux	7) $D_{\text{NH}_4} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{NO}_3}^-} = D_{\text{NH}_4} \cdot \frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\text{NO}_3}^+}$
$z = z_{\infty}$	NH_4 flux	8) $\frac{\partial \text{NH}_4}{\partial z} \Big _{z_{\infty}} = 0$

2.3.4 Sulfate and Sulfide

When nitrate is depleted, sulfate reduction is the pathway to mineralize organic matter, thus consuming sulfate (SO_4) and producing hydrogen sulfide (H_2S) until the sulfate penetration depth (z_{SO_4}). Sulfate and sulfide dynamics are thus described by:

1. Layer ($z \leq z_{\text{NO}_3}$)

$$\frac{\partial \text{SO}_4^I}{\partial t} = 0 = D_{\text{SO}_4} \frac{\partial^2 \text{SO}_4^I}{\partial z^2} - w \frac{\partial \text{SO}_4^I}{\partial z} \quad (9)$$

$$\frac{\partial \text{H}_2\text{S}^I}{\partial t} = 0 = D_{\text{H}_2\text{S}} \frac{\partial^2 \text{H}_2\text{S}^I}{\partial z^2} - w \frac{\partial \text{H}_2\text{S}^I}{\partial z} \quad (10)$$

2. Layer ($z_{\text{NO}_3} < z \leq z_{\text{SO}_4}$)

$$\frac{\partial \text{SO}_4^{II}}{\partial t} = 0 = D_{\text{SO}_4} \frac{\partial^2 \text{SO}_4^{II}}{\partial z^2} - w \frac{\partial \text{SO}_4^{II}}{\partial z} - \frac{1-\phi}{\phi} \cdot \sum_i \text{SO}_4\text{C} \cdot k_i \cdot C_i(z) \quad (11)$$

$$\frac{\partial \text{H}_2\text{S}^{II}}{\partial t} = 0 = D_{\text{H}_2\text{S}} \frac{\partial^2 \text{H}_2\text{S}^{II}}{\partial z^2} - w \frac{\partial \text{H}_2\text{S}^{II}}{\partial z} + \frac{1-\phi}{\phi} \cdot \sum_i \text{SO}_4\text{C} \cdot k_i \cdot C_i(z) \quad (12)$$

To solve equations 9 - 12 the model assumes known concentrations at the sediment-water interface and continuity across the bioturbation depth (z_{bio}) and the nitrate penetration depth (z_{NO_3}) (see Table

Table 4. Boundary conditions for sulfate and sulfide. As in MATLAB (in red my suggestions).

Boundary	Condition	
$z = 0$	known concentration	1) $SO_4(0)=SO_{40}$
$z = z_{bio}$	continuity	2) $SO_4(z_{bio}^-)=SO_4(z_{bio}^+)$
	flux	3) $(D_{SO_4,0} + D_{bio}) \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{bio}^-} = D_{SO_4,0} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{bio}^+}$
$z = z_{ox}$	continuity	4) $SO_4(z_{ox}^-)=SO_4(z_{ox}^+)$
	flux γ_{H_2S} below?	5) $-D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{ox}^-} + F_{H_2S}(z_{ox}) = -D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{ox}^+}$
	where: $\int_{z_{SO_4}}^{\infty}$ here?	$F_{H_2S}(z_{ox}) = \frac{1-\phi}{\phi} \cdot \gamma_{H_2S} \cdot \left(\int_{z_{NO_3}}^{SO_4} \sum_i SO_4 C \cdot k_i \cdot C_i dz + \gamma_{CH_4} \cdot \int_{z_{SO_4}}^{\infty} \sum_i SO_4 C \cdot k_i \cdot C_i dz \right)$
$z = z_{NO_3}$	continuity	6) $SO_4(z_{NO_3}^-)=SO_4(z_{NO_3}^+)$
	flux	7) $D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{NO_3}^-} = D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{NO_3}^+}$
$z = z_{SO_4}$	SO_4 consumption	8) $SO_4(z_{SO_4}) = 0$
	Flux from below	9) $-D_{SO_4} \cdot \frac{\partial SO_4}{\partial z} \Big _{z_{SO_4}} = F_{SO_4}(z_{SO_4})$
	with: $SO_4 C \cdot \gamma_{CH_4}$?	$F_{SO_4}(z_{SO_4}) = \frac{1-\phi}{\phi} \cdot \int_{z_{SO_4}}^{\infty} \sum_i SO_4 C \cdot \gamma_{CH_4} \cdot k_i \cdot C_i dz$ not rather MC instead SO4C?
$z = 0$	known concentration	1) $H_2S(0) = H_{2S0}$
$z = z_{bio}$	continuity	2) $H_2S(z_{bio}^-)=H_2S(z_{bio}^+)$
	flux	3) $(D_{H_2S,0} + D_{bio}) \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{bio}^-} = D_{H_2S,0} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{bio}^+}$
$z = z_{ox}$	continuity	4) $H_2S(z_{ox}^-)=H_2S(z_{ox}^+)$
	flux	5) $-D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{ox}^-} + F_{H_2S}(z_{ox}) = -D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{ox}^+}$
not as SO4!?	where: $1 - \gamma_{H_2S}$?	$F_{H_2S}(z_{ox}) = \frac{1-\phi}{\phi} \cdot (1 - \gamma_{H_2S}) \cdot \int_{z_{NO_3}}^{\infty} \sum_i SO_4 C \cdot k_i \cdot C_i dz$
$z = z_{NO_3}$	continuity	6) $H_2S(z_{NO_3}^-)=H_2S(z_{NO_3}^+)$
	flux	7) $D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{NO_3}^-} = D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{NO_3}^+}$
$z = z_{SO_4}$	continuity	8) $H_2S(z_{SO_4}^-)=H_2S(z_{SO_4}^+)$
	flux (with AOM)	9) $-D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{SO_4}^-} + F_{H_2S}(z_{SO_4}) = -D_{H_2S} \cdot \frac{\partial H_2S}{\partial z} \Big _{z_{SO_4}^+}$
correct???	where:	$F_{H_2S}(z_{SO_4}) = \frac{1-\phi}{\phi} \cdot \int_{z_{SO_4}}^{\infty} \sum_i SO_4 C \cdot k_i \cdot C_i dz$
$z = z_{\infty}$	flux	10) $\frac{\partial H_2S}{\partial z} \Big _{z_{\infty}} = 0$

4). The re-oxidation of reduced H_2S from below is considered in the oxic-suboxic boundary condition for both species. At the sulfate penetration depth (z_{SO_4}) sulfate is used for anaerobic oxidation of methane (AOM) which is produced below z_{SO_4} . Therefore sulfate concentration is zero and its diffusive flux must equal the amount of methane produced below. Additionally H_2S is produced by AOM which is considered in the flux boundary condition at z_{SO_4} . **correct??**

Sulfate:

BC (5): Diffusive flux at z_{ox} is equal, considering the flux of reduced substances (H_2S) from below (SD, matlab): flux discontinuity from H_2S source; include methane region as AOM will produce sulfide as well(?)

BC(9): matlab: Calculate SO_4 consumption below z_{SO_4} , by organic matter and indirectly via methane

oxidation, should it not be MC (methane to carbon ratio instead of SO_4C ???)

Sulfide:

BC (5): Match at zox, layer 1 - layer 2 (continuity, flux discontinuity from H_2S source), flux of H_2S to oxic interface (from all sources of H_2S below), NB: include methane region as AOM will produce sulphide as well should it be not the same as in SO_4 ???

BC (9): (flux with AOM production) flux of H_2S produced by AOM interface (Source of H_2S), don't think the reaction constants are correct in matlab!

2.3.5 Phosphate

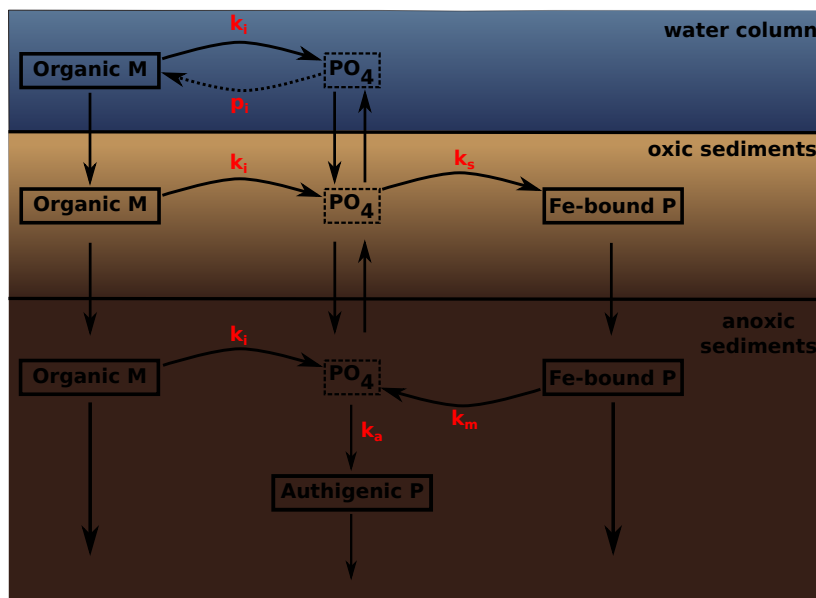


Figure 2. A schematic of the sedimentary P cycle in SED (1.0). Red numbers represent kinetic rate constants for phosphorus dynamics (compare Table 7; p_i represents uptake rate of PO_4 via primary production in shallow environments). Adapted from Slomp et al. (1996).

To model phosphorus (P) in the sediments the model takes into account the change with depth of phosphate (PO_4) and iron-bound P, thereby mainly following the description of Slomp et al. (1996) and Gypens et al. (2008). Throughout the sediment column organic matter is mineralized resulting in a release of phosphate to the pore water. In the oxic part of the sediment, this PO_4 either diffuses upward to the water column or is adsorbed to Fe oxides forming Fe-bound P (or M)(Slomp et al., 1998). In the suboxic/anoxic zone, PO_4 is not only produced through organic matter degradation but is also released from the Fe-bound P pool due to the reduction of Fe oxides. Furthermore, phosphate concentrations can become high enough in this layer for authigenic mineral formation to occur

(Cappellen and Berner, 1988). This phosphorus bound in authigenic minerals represents a permanent sink for reactive phosphorus (Slomp et al., 1996). See Figure 2 for a schematic overview of the sedimentary P cycle. Therefore the diagenetic equations for phosphorus are written:

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

$$\begin{aligned} \frac{\partial \text{PO}_4^I}{\partial t} = & \frac{D_{\text{PO}_4}}{1 + K_{\text{PO}_4}^I} \frac{\partial^2 \text{PO}_4^I}{\partial z^2} - w \frac{\partial \text{PO}_4^I}{\partial z} + \frac{1 - \phi}{\phi \cdot (1 + K_{\text{PO}_4}^I)} \sum_i (\text{PC}_i \cdot k_i \cdot C_i(z)) \\ & - \frac{k_s}{1 + K_{\text{PO}_4}^I} (\text{PO}_4^I - \text{PO}_4^s) \end{aligned} \quad (13)$$

$$\frac{\partial M^I}{\partial t} = D_M \frac{\partial^2 M^I}{\partial z^2} - w \frac{\partial M^I}{\partial z} + k_s \frac{\phi}{1 - \phi} (\text{PO}_4^I - \text{PO}_4^s) \quad (14)$$

2. Layer ($z_{\text{ox}} < z$)

$$\frac{\partial M^{II}}{\partial t} = D_M \frac{\partial^2 M^{II}}{\partial z^2} - w \frac{\partial M^{II}}{\partial z} - k_m (M^{II} - M^\infty) \quad (15)$$

$$\begin{aligned} \frac{\partial \text{PO}_4^{II}}{\partial t} = & \frac{D_{\text{PO}_4}^{II}}{1 + K_{\text{PO}_4}^{II}} \frac{\partial^2 \text{PO}_4^{II}}{\partial z^2} - w \frac{\partial \text{PO}_4^{II}}{\partial z} + \frac{1 - \phi}{\phi \cdot (1 + K_{\text{PO}_4}^{II})} \sum_i (\text{PC}_i \cdot k_i \cdot C_i(z)) \\ & - \frac{k_a}{1 + K_{\text{PO}_4}^{II}} (\text{PO}_4^{II} - \text{PO}_4^a) + \frac{(1 - \phi)k_m}{\phi(1 + K_{\text{PO}_4}^{II})} (M^{II} - M^\infty) \end{aligned} \quad (16)$$

$$(17)$$

The boundary conditions to solve Equations 13 - 16 are summarized in Table 5. The model assumes known bottom water concentrations and equal concentrations and diffusive fluxes at z_{bio} and z_{ox} for both species. Additionally it considers no change in phosphate flux and an asymptotic Fe-bound P concentration at z_∞ .

2.4 Model Parameters

This section describes the parameters used in SED (1.0) to describe sediment transport and biogeochemical reactions related to the burial and mineralization of organic matter under a wide range of environmental conditions. Table 6 states the parameters for sediment characteristics and Table 7 summarizes the stoichiometric factors and secondary reaction parameters used in the model.

2.4.1 Transport Parameters

Advection is the bulk flow of sediments and can be directly related to the accumulation of new material on the seafloor (i.e. sedimentation, Burdige, 2006). This results in a downward flux of older sediment material and porewater in relation to the sediment-water interface. SED (1.0) uses the empirical global relationship between sediment accumulation rate (cm yr^{-1}) and seafloor depth (m) of Middelburg et al. (1997):

$$w = 3.3 \cdot 10^{-0.87478367 - 0.00043512 \cdot \text{depth}} \quad (18)$$

Table 5. Boundary conditions for phosphate and Fe-bound P (M).

Boundary	Condition	
$z = 0$	known concentration	1) $\text{PO}_4(0) = \text{PO}_{40}$
$z = z_{\text{bio}}$	continuity	2) $\text{PO}_4(z_{\text{bio}}^-) = \text{PO}_4(z_{\text{bio}}^+)$
	flux	3) $(D_{\text{PO}_4,0} + D_{\text{bio}}) \cdot \frac{\partial \text{PO}_4}{\partial z} \Big _{z_{\text{bio}}^-} = D_{\text{PO}_4,0} \cdot \frac{\partial \text{PO}_4}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	continuity	4) $\text{PO}_4(z_{\text{ox}}^-) = \text{PO}_4(z_{\text{ox}}^+)$
	flux	5) $-\frac{D_{\text{PO}_4}}{1+K_{\text{PO}_4}^I} \cdot \frac{\partial \text{PO}_4}{\partial z} \Big _{z_{\text{ox}}^-} = -\frac{D_{\text{PO}_4}}{1+K_{\text{PO}_4}^{II}} \cdot \frac{\partial \text{PO}_4}{\partial z} \Big _{z_{\text{ox}}^+}$
$z = z_{\infty}$	flux	10) $\frac{\partial \text{PO}_4}{\partial z} \Big _{z_{\infty}} = 0$
$z = 0$	known concentration	1) $M(0) = M_0$
$z = z_{\text{bio}}$	continuity	2) $M(z_{\text{bio}}^-) = M(z_{\text{bio}}^+)$
correct???	flux	3) $\frac{\partial M}{\partial z} \Big _{z_{\text{bio}}^-} = \frac{\partial M}{\partial z} \Big _{z_{\text{bio}}^+}$
$z = z_{\text{ox}}$	continuity	4) $M(z_{\text{ox}}^-) = M(z_{\text{ox}}^+)$
correct???	flux	5) $\frac{\partial M}{\partial z} \Big _{z_{\text{ox}}^-} = \frac{\partial M}{\partial z} \Big _{z_{\text{ox}}^+}$
$z = z_{\infty}$	asymptotic concentration	10) $M(z_{\infty}) = M_{\infty}$

As discussed before (Sec. 2.2), the diffusion coefficient of species i is calculated as $D_i = D_{i,0} + D_{\text{bio}} = D_{\text{mol},i} \cdot f_{ir} + D_{\text{bio}}$ for dissolved species and $D_i = D_{\text{bio}}$ for solid species. The bioturbation coefficient D_{bio} ($\text{cm}^2 \text{ yr}^{-1}$) is constant in the bioturbated zone and also follows the empirical relationship by Middelburg et al. (1997):

$$D_{\text{bio}} = 5.2 \cdot 10^{0.76241122 - 0.00039724 \cdot \text{depth}} \quad (19)$$

Studies showed that bioturbational effects on a global scale are largely restricted to the upper 10 cm of the sediments and are only marginally related to seafloor depth (e.g. Boudreau, 1998; Teal et al., 2010). Therefore, SED (1.0) imposes a globally invariant bioturbation depth of 10cm. Bioirrigation can enhance the molecular diffusion coefficient $D_{i,0} = D_{\text{mol},i} \cdot f_{ir}$ (Soetaert et al., 1996a). However, here we do not consider this effect and set f_{ir} to a constant value of 1. The specific molecular diffusion coefficients $D_{\text{mol},i}$ are corrected for sediment porosity ϕ , tortuosity F and are linearly interpolated for an ambient temperature T using zero-degree coefficients D_i^0 and temperature dependent diffusion coefficients D_i^T (compare Gypens et al., 2008):

$$D_{\text{mol},i} = (D_i^0 + D_i^T \cdot T) \cdot \frac{1}{\phi \cdot F}$$

Tortuosity can be expressed in terms of porosity as $F = \frac{1}{\phi^m}$ (Ullman and Aller, 1982) with the exponent m varying according to the type of sediment (here we use $m=3$). Values for D_i^T and D_i^0 are summarized in Table 6 and are adapted from Li and Gregory (1974) and Gypens et al. (2008).

2.4.2 Reaction Parameters

The applied multi-G approach for organic matter degradation considers specific degradation rate constants k_i (yr^{-1}) for each compound class. The degradation constants are generally taken from

Table 6. Fixed sediment characteristics and transport parameters. **TODO: Update table!**

Parameter	Unit	Value	Description/Source
ρ_{sed}	g cm^{-3}	2.5	Sediment density
w	cm yr^{-1}	0.03	Advection/ Sediment accumulation rate
z_{bio}	cm	10	Bioturbation depth Boudreau (1998); Teal et al. (2010)
D_{bio}	$\text{cm}^2 \text{yr}^{-1}$	Fct. of seafloor depth	Bioturbation coefficient Middelburg et al. (1997)
ϕ	-	0.8	Porosity
F	-	$\frac{1}{\phi^m}$	Tortuosity, here $m=3$
f_{ir}	-	1	Irrigation factor
PO_4^s	mol cm^{-3}	$1 \cdot 10^{-9}$	equilibrium conc. for P sorption Slomp et al. (1996)
PO_4^a	mol cm^{-3}	$3.7 \cdot 10^{-9}$	equilibrium conc. for authigenic P precipitation Slomp et al. (1996)
M^∞	mol cm^{-3}	$1.99 \cdot 10^{-9}$	asymptotic concentration for Fe-bound P Slomp et al. (1996)
Diffusion coefficients (Li and Gregory, 1974; Gypens et al., 2008)			
$D_{\text{O}_2}^0$	$\text{cm}^2 \text{yr}^{-1}$	348.62172	Molecular diffusion coefficient of oxygen at 0°C
$D_{\text{O}_2}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$	14.08608	Diffusion coefficient for linear temp. dependence of oxygen
$D_{\text{NO}_3}^0$	$\text{cm}^2 \text{yr}^{-1}$	308.42208	Molecular diffusion coefficient of nitrate at 0°C
$D_{\text{NO}_3}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$	12.2640	Diffusion coefficient for linear temp. dependence of nitrate
$D_{\text{NH}_4}^0$	$\text{cm}^2 \text{yr}^{-1}$	308.42208	Molecular diffusion coefficient of ammonium at 0°C
$D_{\text{NH}_4}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$	12.2640	Diffusion coefficient for linear temp. dependence of ammonium
$D_{\text{SO}_4}^0$	$\text{cm}^2 \text{yr}^{-1}$	157.68	Molecular diffusion coefficient of sulfate at 0°C
$D_{\text{SO}_4}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$	7.884	Diffusion coefficient for linear temp. dependence of sulfate
$D_{\text{H}_2\text{S}}^0$	$\text{cm}^2 \text{yr}^{-1}$???	Molecular diffusion coefficient of sulfide at 0°C
$D_{\text{H}_2\text{S}}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$???	Diffusion coefficient for linear temp. dependence of sulfide
$D_{\text{PO}_4}^0$	$\text{cm}^2 \text{yr}^{-1}$	112.90764	Molecular diffusion coefficient of phosphate at 0°C
$D_{\text{PO}_4}^T$	$\text{cm}^2 \text{yr}^{-1} \text{ }^\circ\text{C}^{-1}$	5.586252	Diffusion coefficient for linear temp. dependence of phosphate

Table 7. Values for biogeochemical parameters used in SED (1.0).

Parameter/Variable	Unit	Value	Description
Stoichiometric factors and molecular ratios			
NC ₁	mol/mol	0.1509	nitrogen to carbon ratio refractory fraction, two different ones? why these values?
NC ₂	mol/mol	0.13333	nitrogen to carbon ratio labile fraction
PC _i	mol/mol	0.0094	phosphorus to carbon ratio
MC	mol/mol	0.5	methane to carbon ratio produced during methanogenesis
OC	mol/mol	1.0	oxygen to carbon ratio
NO ₃ C	mol/mol	94.4/106	nitrate to carbon ratio
SO ₄ C	mol/mol	0.5	sulfate to carbon ratio
Secondary reaction parameters			
γ_{NH_4}	-	1.0	fraction of NH ₄ that is oxidised in oxic layer
$\gamma_{\text{H}_2\text{S}}$	-	0.8	fraction of H ₂ S that is oxidised in oxic layer
γ_{CH_4}	-	1.0	fraction of CH ₄ that is oxidised at z_{SO_4}
Rate constants			
k_i	yr ⁻¹	from Earth System Model	OM degradation rate constants
k_s	yr ⁻¹	???	rate constant for P sorption
k_m	yr ⁻¹	???	rate constant for Fe-bound P release
k_a	yr ⁻¹	???	rate constant for authigenic P formation

the coupled Earth System model and are assumed invariant along the sediment column, therefore independent of the nature of the terminal electron acceptor. The stoichiometry of organic matter is represented by the factors NC_i and PC_i denoting the molecular nitrogen to carbon and phosphorus to carbon ratio. In the sulfidic and methanic zone the reduction of 1 mol organic matter additionally produces 0.5 mol of hydrogen sulfide (SO₄C) and 0.5 mol of methane (MC). In the total sediment column organic matter mineralization consumes the specific terminal electron acceptor with a fixed ratio (OC, NO₃C and SO₄C respectively). See Table 7 for a complete summary of the parameters and their values.

2.5 Module Structure

TODO: An analytical steady-state solution is found for the reaction-transport equation of each chemical species in each layer. At each boundary (i.e. z_{ox} , z_{bio} , z_{NO_3} and z_{SO_4}) the model has to

match continuity and flux for different ODE solutions of the layer above and below the specific boundary. In particular the bioturbation boundary is problematic as it can theoretically occur in any geochemical layer. In order to simplify this recurring boundary matching problem it is implemented in an independent algorithm which is described in Section 2.5.1. Instructions and requirements for coupling SED (1.0) to a global Earth Sytem Model are given in Section 2.5.2.

2.5.1 Generic boundary condition matching (GBCM)

A general steady-state advection-diffusion-reaction (ADR) diagenetic equation looks like:

$$\frac{\partial C}{\partial t} = 0 = D \frac{\partial^2 C}{\partial z^2} - w \frac{\partial C}{\partial z} - \sum_i \alpha_i \exp(-\beta_i z) - k \cdot C + Q. \quad (20)$$

where z is the sediment depth, t the time, D is the diffusion coefficient and w is the advection rate. The ODE solution is of the general form:

$$C(z) = A \exp(az) + B \exp(bz) + \sum_i \frac{\alpha_i}{D\beta_i^2 - w\beta_i - k} \cdot \exp(-\beta_i z) + \frac{Q}{k} \quad (21)$$

and can therefore be expressed as:

$$C(z) = A \cdot E(z) + B \cdot F(z) + G(z) \quad (22)$$

where $E(z)$, $F(z)$ are the homogeneous solutions of the ODE, $G(z)$ the particular integral, and A, B are the integration constants.

Each boundary matching problem involves matching continuity and flux for the two solutions $C_U(z)$ (= 'upper') and $C_L(z)$ (= 'lower') across a boundary at $z = z_b$. Therefore, we get two ODE solutions of the genral form:

$$C_U(z) = A_U \cdot E_U(z) + B_U \cdot F_U(z) + G_U(z) \quad (23)$$

$$C_L(z) = A_L \cdot E_L(z) + B_L \cdot F_L(z) + G_L(z). \quad (24)$$

The two boundary conditions are: for continuity (where for generality we allow a discontinuity V_b)

$$C_U(z_b) = C_L(z_b) + V_b \quad (25)$$

and for flux

$$D_U C'_U(z_b) + w C_U(z_b) = D_L C'_L(z_b) + w C_L(z_b) + F_b \quad (26)$$

where w is advection, D are the diffusion coefficients and F_b is any flux discontinuity.

In terms of the ODE solutions (23), (24), the boundary conditions represent two equations connecting

the four integration constants:

$$\begin{pmatrix} E_U & F_U \\ D_U E'_U & D_U F'_U \end{pmatrix} \begin{pmatrix} A_U \\ B_U \end{pmatrix} = \begin{pmatrix} E_L & F_L \\ D_L E'_L & D_L F'_L \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix} + \begin{pmatrix} G_L - G_U + V_b \\ D_L G'_L - D_U G'_U + F_b - wV_b \end{pmatrix} \quad (27)$$

where the ODE solutions E , F , G are all evaluated at z_b .

Equation (27) can be solved to give A_U and B_U as a function of the integration constants from the layer below (A_L and B_L), thereby constructing a piecewise solution for the whole region, with now just two integration constants A_L and B_L .

In the code the function **benthic_utils.matchsoln** provides this solution in the form:

$$\begin{pmatrix} A_U \\ B_U \end{pmatrix} = \begin{pmatrix} c_1 & c_2 \\ c_3 & c_4 \end{pmatrix} \begin{pmatrix} A_L \\ B_L \end{pmatrix} + \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}. \quad (28)$$

Using (28) we can now rewrite $C_U(z)$ in (23) as a function of A_L and B_L :

$$C_U(z) = (c_1 A_L + c_2 B_L + d_1) \cdot E_U(z) + (c_3 A_L + c_4 B_L + d_2) \cdot F_U(z) + G_U(z)$$

and hence define the “transformed” basis functions $E_U^*(z)$, $F_U^*(z)$, $G_U^*(z)$ such that:

$$C_U(z) = A_L \cdot E_U^*(z) + B_L \cdot F_U^*(z) + G_U^*(z) \quad (29)$$

where

$$\begin{aligned} E_U^*(z) &= c_1 E_U(z) + c_3 F_U(z) \\ F_U^*(z) &= c_2 E_U(z) + c_4 F_U(z) \\ G_U^*(z) &= G_U(z) + d_1 E_U(z) + d_2 F_U(z) \end{aligned} \quad (30)$$

(in the code this is done by **benthic_utils.xformsoln**).

Solving the sediment layer stack

Equations (28), (29) and (30) can now be applied for each layer boundary, working up from the bottom of the sediments. The net result is to construct a piecewise solution with just two integration constants (coming from the lowest layer), which can then be solved for by applying one boundary condition for the sediment-water interface and one for the bottom of the sediments (e.g. a concentration condition at the bottom of the sediments, and a flux condition at the SWI).

TODO: Add figure, illustrating this e.g. for nitrate...

Abstracting out the bioturbation boundary

The bioturbation boundary affects the diffusion coefficient of the modelled solutes and the conservation equation of organic matter which is available for mineralization. The boundary is particularly inconvenient as it can in principle occur in the middle of any “geochemical” layer and therefore generates multiple cases. To simplify this for solutes, the “piecewise solution construction” above is used to abstract out the bioturbation boundary. An initial test for each layer is made to identify its “bioturbation-status” (fully bioturbated, fully non-bioturbated or crossing the bioturbation boundary) and (if needed) a piecewise solution is constructed by matching boundary conditions across the bioturbation boundary. The “outside” code therefore never needs to know whether it is dealing with a piecewise solution (i.e. matched across a bioturbation boundary) or a “simple” solution (i.e. the layer is fully bioturbated or fully non-bioturbated).

In the code, this is performed by **zTOC.prepfg_I12** which hands back a structure **ls** containing the “bioturbation-status” for each layer and (if needed) the description of the piecewise solution (coefficients $c_1, c_2, c_3, c_4, d_1, d_2$ as above). So e.g. for sulfate, **zTOC.prepfg_I12** is called three times at the beginning of **zSO4.calcbbc** (one for each “geochemical” layer: oxic, suboxic, sulfidic) handing back three structures **ls** describing the layer’s “bioturbation-status”, abstracting away the bioturbation boundary and all associated conditional logic. When calculating the solutions for the different layers, the pre-calculated structure **ls** is passed to the function **zTOC.calcfg_I12** which sorts out the correct solution type to use.

2.5.2 Coupling to an Earth System Model

3 Test Cases

3.1 Benthic fluxes on a global scale

Application to Seitert, 2004 OM, burwicz 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

Acknowledgements. TEXT

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