# Modeling benthic–pelagic nutrient exchange processes and porewater distributions in a seasonally–hypoxic sediment: evidence for massive phosphate release by *Beggiatoa*?

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## Supplementary information for the bioirrigation experiment–model procedure

Throughout the duration of the sampling campaign, multi–cores (10 cm internal diameter) were taken to the home laboratory for manipulation experiments to determine bioirrigation rates. The procedure involves adding a large excess of a dissolved conservative tracer, in this case $Br^-$, to the water overlying the sediment and allowing the core to incubate for a known period of time. Posterior analytical determination of the depth distribution of $Br^-$ allows the rate of irrigation to be approximated by modeling the transient infiltration of $Br^-$ into the sediment using a numerical model (Martin and Banta, 1992).

Following delivery to the laboratory, the sediment cores were allowed to settle for a period of 24–48 h at 4 $^oC$ whilst stirring (60 rpm) the overlying water at approximately 20 cm above the sediment surface. Observed trajectories of small amounts of suspended particulate material at the bottom of the overlying water showed that this rate of stirring was sufficient to ventilate the surface of the sediment. It was not possible to control the dissolved $O_2$ concentration of the overlying water, and the cores were left open to the atmosphere except during September and October when bottom water $O_2$ concentration was < 5 μM. In these cases, the cores were bubbled with Ar for 2 h and sealed tightly with the stirrer mounted through a rubber stopper. After the settling period, an excess of NaBr dissolved in a small amount of seawater was then added to the cores whilst stirring, so that the final $Br^-$ concentration was ca. 20 mM. The cores were then allowed to incubate for 7 d (10 d on 22 March) in the dark with stirring, after which period the sediment cores were sectioned and sampled for analysis of $Br^-$ and porosity following the same procedures outlined above. By the end of the experiment, the $Br^-$ concentration in the overlying water had decreased by several mM due to uptake by the sediment. The incubation time was chosen based on results by Meile et al. (2005), who showed that the apparent rate of irrigation determined using excess $Br^-$ changes rapidly during the first few days of incubation and only reaches quasi–steady state after approximately 1 week when transient concentration gradients and fluxes associated with burrows are reduced (Boudreau and Marinelli, 1994). The presence of macrofauna in sieved (1 mm) sediment was noted but not measured quantitatively.

The measured $Br^-$ concentration profiles were simulated using a non–steady state model which accounts for solute transport into the sediments by molecular diffusion and bioirrigation using a non–local source sink function (Boudreau, 1984; Emerson et al., 1984). Assuming that porosity does not change during the incubation period, the 1D mass conservation equation which describes the change in $Br^-$ concentration (M) in the sediment with time is expressed as:

$$\varphi \frac{\partial \mathrm{Br}^-}{\partial t} = \frac{\partial}{\partial z}\left(\varphi D \frac{\partial \mathrm{Br}^-}{\partial \mathrm{z}}\right) + \alpha_{\mathrm{bi}}\varphi(\mathrm{Br}_{\mathrm{olw}} - \mathrm{Br}^-) \qquad \text{(S1)}$$

where z (cm) is depth in the sediment, $t$ (d) is time, $\alpha_{bi}$ ($d^{-1}$) is the depth–dependent bioirrigation coefficient describing solute pumping through animal burrows and $Br_{olw}$ (M) is the time–dependent

$Br^{-}$ concentration in the well mixed overlying water. The sediment porosity, $\varphi$, was defined by fitting the exponential function $\varphi = \varphi(L) + (\varphi(0) - \varphi(L))e^{-z/z_{por}}$ to the measured data on each date where the parameters $\varphi(0)$ and $\varphi(L)$ are the porosity at the sediment–water interface and in compacted sediments, respectively, and $z_{por}$ (cm) is the porosity attenuation length. $\varphi(0)$, $\varphi(L)$ and $z_{por}$ were determined by least squares fits to measured porosity profiles. The in situ molecular diffusion coefficient, $D$ ($cm^2\ d^{-1}$), was calculated from the value in seawater ($D_W = 1\ cm^2\ d^{-1}$) at the incubation temperature (4 °C) and salinity of 20 using $D = D_W(1 - \ln\varphi^2)^{-1}$ (Boudreau, 1997).

The lower boundary condition was defined as a zero gradient ($\partial Br^{-}/\partial z = 0$). The $Br^{-}$ concentration at the sediment surface was calculated dynamically considering a diffusive boundary layer of thickness $z_{diff}$:

$$\varphi D \left.\frac{\partial \mathrm{Br}^{-}}{\partial z}\right|_{z=0} = D_W \frac{\mathrm{Br_{olw}} - \mathrm{Br}^{-}(0)}{z_{diff}} \tag{S2}$$

where $Br^{-}(0)$ (M) is the $Br^{-}$ concentration in the surface sediment layer directly below the diffusive sublayer (Boudreau, 1996). A value of 0.04 cm was chosen for $z_{diff}$ (Forster et al., 1999).

Transport of $Br^{-}$ into the sediments results in a decrease in $Br^{-}$ concentration in the overlying water column. This is accounted for by dynamically modeling $Br_{olw}$ at each time step by integrating the tracer concentration over the entire depth of the sediment ($z_{max}$):

$$\mathrm{Br_{olw}} = \mathrm{Br_{olw}}(\mathrm{t} = 0) - \frac{1}{h}\int_0^{z_{max}} \varphi \mathrm{Br}^{-}\ dz \tag{S3}$$

where $h$ is the height of the overlying water column (ca. 20 to 30 cm). $Br_{olw}$ also serves as the upper boundary condition for $Br^{-}$, from which $Br^{-}(0)$ is calculated at each time step.

The depth–dependence of $\alpha_{bi}$ was described using the function:

$$\alpha_{\mathrm{bi}} = \alpha_{\mathrm{bi1}} \frac{\exp(\alpha_{\mathrm{bi2}} - z)}{1 + \exp(\alpha_{\mathrm{bi2}} - z)} \tag{S4}$$

where $\alpha_{bi1}$ ($d^{-1}$) is approximately equal to the rate of bioirrigation at the sediment surface and $\alpha_{bi2}$ (cm) controls the irrigation depth. This type of formulation allows for a constant rate of irrigation in the sediment down to a depth equal to ca. $\alpha_{bi2}$ (Dale et al., 2011) and better describes the data from Boknis Eck compared to the more commonly employed single exponential function (e.g. Martin and Banta, 1992).

To solve the model, the continuous spatial derivatives in Eq. (S1) were replaced with finite differences (Boudreau, 1997). The resulting set of ODEs was solved using the NDSolve algorithm in MATHEMATICA 7.0 using the method of lines over 100 discrete depth intervals with a grid spacing increasing from sub–mm scale at the top of the model domain to sub–cm scale at the bottom (30 cm). The initial $Br^-$ concentration in the sediment was assumed to be constant and set to the value measured in sediments below 20 cm in the parallel cores sectioned for geochemical analysis. This approach disregards the obvious concentration gradients in background $Br^-$ in the upper 10 cm due to irrigation and seasonal salinity changes (see Results). Yet, since the $Br^-$ tracer concentration in the overlying water was ca. 50 times greater than the ambient background concentration (0.4 mM), failure to account for these seasonal trends of $Br^-$ in the initial condition creates a negligible error in the results. The model solutions were >99 % mass conservative.

The bioirrigation constants $\alpha_{bi1}$ and $\alpha_{bi2}$ were quantified by running the model transiently for the length of the incubation period and tuning their values until a good fit with the measured $Br^-$ concentrations was obtained. To make this approach as objective as possible, a simple optimization routine was used. This consisted of running the model 10000 times using random values of $\alpha_{bi1}$ and $\alpha_{bi2}$ chosen with the RandomReal function in MATHEMATICA. After each simulation, the root mean squared error (RMSE) of the modeled results versus the observations was calculated. The final parameter values were those giving the lowest RMSE (typically less than 1 mM).

Quantifying bioirrigation rates using this approach relies on several underlying assumptions, such as (i) addition of NaBr does not affect sediment respiration or irrigation rates, (ii) accumulation of $Br^-$ released during POM mineralization is negligible compared to the addition of the tracer, (iii) transfer of the cores from local in situ temperature to the constant cool room temperature of 4 $^{o}$C does not significantly affect bioirrigation, (iv) cumulative error due to uncertainty in porosity, water height and diffusive boundary layer thickness is small (<10%), and (v) no artifacts arise due to changes in dissolved $O_2$ concentration over the course of the experiment. With the exception of the latter, which is the most tenuous in our case, these assumptions have been substantiated on numerous occasions (Martin and Banta, 1992; Forster et al., 1999; 2003; Rao and Janhke, 2004; Sayles and Martin, 1995).

## Supplementary information for the diagenetic model

Parameters used in the biogeochemical model not listed in Table 3 are provided in Table S1. Boundary conditions are given in Table S2. Constitutive equations which define the transport terms, temperature corrections and conversion factors are given in Table S3. General details of these functions are presented in Dale et al. (2011).

The parameters for the porosity function were determined from the measured porosity values for all geochemical cores analyzed using the function described in the bioirrigation section above. Porosity was used, amongst others, to calculate in situ diffusion coefficients, $D$, from the molecular diffusion coefficients in porewater, $D_W$, for the bottom water temperature and mean salinity of 20 using data provided by Boudreau (1997) and Schulz (2006). $D$ was therefore time dependent through the temperature.

The depth–dependent fluid velocity, $v_a$(z), was calculated assuming steady state compaction (Berner, 1980). To account for the enhanced advection of dissolved $CH_4$ following gas eruption from the sediment, the upward velocity, $v_a(0,t)$, is subtracted from the downward movement of porewater due to burial. For all other solutes $v_a(0,t) = 0$.

Changes have been made with regard to the bioirrigation coefficient, $\alpha_{bi}$ (Eq. (S4)), which was assumed to vary among solutes. This reasoning is based on previous observations by Aller (2001) and model simulations by Berg et al. (2003) and Meile et al. (2005) who showed that diffusion gradients across burrow walls can lead to unique irrigation coefficients for different species. The approach of Meile et al. (2005) is particularly insightful since they derived 1D irrigation coefficients from a virtual porewater data set generated using a 3D model which accounted for burrow geometry and reactions.

They demonstrated that highly redox sensitive species such as $Fe^{2+}$ tend to be oxidized on burrow walls, leading to zero apparent irrigation rates when analyzed using a 1D model (Meile et al., 2005). Similarly, owing to their reactivity, $O_2$ and $TH_2S$ tend to be irrigated at about twice the rate of less reactive species such as $SO_4^{2-}$, $NH_4^+$ and $TCO_2$. Bioirrigation coefficients determined using the $Br^-$ tracer experiment for an incubation length of around 7 days approximate those of $SO_4^{2-}$, $TCO_2$ and $NH_4^+$. This is because the radial concentration gradient of $Br^-$ after this period displays vertical and radial concentration gradients around burrows characteristic of $SO_4^{2-}$, $TCO_2$ and $NH_4^+$. Therefore, in this study the coefficient $\gamma_{bi}$ (Eq. (3a) in main text) was set equal to 1 for all solutes with the exception of $O_2$, $TH_2S$ and $Fe^{2+}$, which were equal to 2 (for $O_2$ and $TH_2S$) and 0 (for $Fe^{2+}$).

The same first–order rate constant values for G1 ($k_{G1} = 1.4\times10^{-4}$ d$^{-1}$), G2 ($k_{G2} = 4.1\times10^{-6}$ d$^{-1}$) and G3 ($k_{G3} = 1.1\times10^{-6}$ d$^{-1}$) mineralization were used as in (Dale et al., 2011). $k_{G1}$ was constrained using SR rates measured ex situ with $^{35}SO_4^{2-}$, whereas $k_{G2}$ and $k_{G3}$ were constrained using data from a gravity core taken at the same site. The reactivity of the G0 fraction representing fresh phytodetritus was set to 0.016 d$^{-1}$ based on results by Graf et al. (1983) who determined that the spring bloom in Boknis Eck was consumed within 5–6 weeks of being deposited in the seabed. The data presented by Dale et al. (2011) correspond to the pre–spring bloom winter situation and consideration of this fraction was unnecessary in that study. Due to a lack of data, the N:C ratio of G0 was set to that of the G1 fraction (9.5/106) determined previously (Dale et al., 2011) which is close to the experimentally determined composition of organic matter of 8.9/106 (Balzer et al., 1983). $(N:C)_i$ for G1, G2 and G3 were unchanged from Dale et al. (2011). A Redfield $P:C$ value of 1/106 estimated from porewater data and benthic chamber fluxes was prescribed for all carbon fractions (Balzer et al., 1983).

All reaction rate expressions include an additional term to allow for the widely–observed fact that biogeochemical reactions in marine sediments are sensitive to changes in temperature. All POM mineralization rate constants, with the exception of aerobic respiration and denitrification, were allowed to increase by a factor of 3 for every 10 °C increase in temperature, that is, using a $Q_{10}$ value of 3 (Westrich and Berner, 1988; Klump and Martens, 1989). Aerobic respiration and denitrification were assigned a $Q_{10}$ of 1.8 based on data presented by Thamdrup et al. (1998) and Rysgaard et al. (2004) for the temperature range characteristic of Boknis Eck bottom waters (0 to 10 °C). Anammox was better described with a $Q_{10}$ of 2.5 since it responds more rapidly to rises in temperature over this range than denitrification (Dalsgaard and Thamdrup, 2002; Rysgaard et al., 2004). AOM was assigned a $Q_{10}$ of 2 based on slurry incubations using sediment from the same site (Treude et al., 2005). Data on the temperature response of the other secondary redox reactions is, to our knowledge, not well established and these were assigned a $Q_{10}$ of 2 (Fossing et al., 2004).

Table S1. Additional parameters used in the biogeochemical model.

| Parameter | Description | Value | Unit | Main constraint |
|---|---|---|---|---|
| $\rho_s$ | Dry sediment density | 2.5 | g $cm^{-3}$ | Assumed (Dale et al., 2011) |
| $\varphi(0)$ | Porosity at $z = 0$ | 0.94 | 1 | Measured (this study) [a] |
| $\varphi(L)$ | Porosity at $z = L$ (60 cm) | 0.87 | 1 | Measured (this study) [a] |
| $z_{por}$ | Porosity attenuation length | 1.25 | cm | Measured (this study) [a] |
| $v_s(L)$ | Sediment burial velocity | $1.1\times10^{-3}$ | cm $d^{-1}$ | Excess $^{210}$Pb (Nittrouer et al., 1998) |
| $z_{bt}$ | Bioturbation attenuation coefficient | 2 | cm | Assumed based on steady state model (Dale et al., 2011) |
| $Q_{10}$ | Temperature rate increase for POM mineralization | 3.0 | 1 | Experimentally determined (Westrich and Berner, 1988; Klump and Martens, 1989) |
| $Q_{10}$ | Temperature rate increase for aerobic respiration and denitrification | 1.8 | 1 | Experimentally determined (Rysgaard et al., 2004; Thamdrup et al., 1988) |
| $Q_{10}$ | Temperature rate increase for anammox | 2.5 | 1 | Experimentally determined (Rysgaard et al., 2004) |
| $Q_{10}$ | Temperature rate increase for all other reactions | 2 | 1 | Assumed, based on Fossing et al. (2004) |
| $T_{ref}$ | Reference temperature for reaction rates | 2.1 | $^{o}$C | Lowest temperature where SR was measured |
| $k_{G0}$ | Rate constant for G0 degradation | 0.016 | $d^{-1}$ | Protein content and ATP turnover (Graf et al., 1983) |
| $k_{G1}$ | Rate constant for G1 degradation | $1.4\times10^{-4}$ | $d^{-1}$ | Measured SR rates (Bertics et al., 2012) |
| $k_{G2}$ | Rate constant for G2 degradation | $4.1\times10^{-6}$ | $d^{-1}$ | Gravity core porewater data (Dale et al., 2011) |
| $k_{G3}$ | Rate constant for G3 degradation | $1.15\times10^{-6}$ | $d^{-1}$ | Gravity core porewater data (Dale et al., 2011) |
| $f_{ox}$ | Enhancement factor for POM degradation by $O_2$ | 10 | 1 | $O_2$ penetration depths from Preisler et al. (2007) |
| $K_{O2}$ | Half–saturation constant for $O_2$ | 1 | μM | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $K_{NO3}$ | Half–saturation constant for $NO_3^-$ | 10 | μM | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $K_{NO2}$ | Half–saturation constant for $NO_2^-$ | 10 | μM | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $K_{Fe}$ | Half–saturation constant for $Fe(OH)_{3\text{–}A}$ | 0.028 | wt–% | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $K_{SO4}$ | Half–saturation constant for sulfate | 0.5 | mM | Flow through reactor experiments (Pallud and Van Cappellen, 2006) |
| $K_{PO4}$ | Half–saturation constant for $TPO_4$ during $R_{Fe2ox}$ | 10 | μM | Assumed (this study) [b] |
| $k_{NH4ox}$ | Rate constant for aerobic oxidation of $NH_4^+$ | $2.7\times10^{4}$ | $M^{-1}$ $d^{-1}$ | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $k_{NO2ox}$ | Rate constant for aerobic oxidation of $NO_2^-$ | $2.7\times10^{4}$ | $M^{-1}$ $d^{-1}$ | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $k_{amx}$ | Rate constant for anammox | $2.7\times10^{4}$ | $M^{-1}$ $d^{-1}$ | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $k_{DNRA}$ | Rate constant for DNRA | $2.7\times10^{5}$ | $M^{-1}$ $d^{-1}$ | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $k_{H2Sox}$ | Rate constant for aerobic oxidation of $TH_2S$ | $2.7\times10^{4}$ | $M^{-1}$ $d^{-1}$ | Benthic fluxes and porewater modeling (Bohlen et al., 2011; Dale et al., 2011) |
| $k_{AOM}$ | Rate constant for AOM | 0.27 | $d^{-1}$ | $SO_4^{2-}$ concentration profile (this study) |
| $(N{:}C)_0$ | Molar mineralization ratio of N:C in G0 | 9.5/106 | mol N (mol $C)^{-1}$ | Assumed equal to $(N{:}C)_1$ and measured by Balzer et al. (1983) |
| $(N{:}C)_1$ | Molar mineralization ratio of N:C in G1 | 9.5/106 | mol N (mol $C)^{-1}$ | Steady–state model (Dale et al., 2011) |
| $(N{:}C)_2$ | Molar mineralization ratio of N:C in G2 | 8/106 | mol N (mol $C)^{-1}$ | Steady–state model (Dale et al., 2011) |
| $(N{:}C)_3$ | Molar mineralization ratio of N:C in G3 | 27/106 | mol N (mol $C)^{-1}$ | Steady–state model (Dale et al., 2011) |

[a] Mean porosity values from measurements in all multiple cores in Table 1 (main text)

[b] The $TPO_4$ concentration is relatively insensitive to this parameter, and is included to avoid negative $TPO_4$ concentrations (see main text).

Table S2: Boundary conditions used in the model. Time–dependent boundary conditions denoted ‘variable’ are shown in Fig. 1.

| Variable | Value | Unit | Constraint |
|---|---|---|---|
| Upper solutes | | | |
| $O_2$ | Variable | μM | Measured (Dale et al., 2011) |
| $NO_3^-$ | 6 | μM | Measured (Dale et al., 2011) |
| $NO_3^-{}_{bac}$ | 150 | μM | Measured (Preisler et al., 2007) |
| $NO_2^-$ | 0.5 | μM | Measured (Dale et al., 2011) |
| $SO_4^{2-}$ | Variable | mM | Scaled to salinity (this study) |
| $Fe^{2+}$ | 0.1 | μM | Assumed |
| $NH_4^+$ | 3 | μM | Measured (Dale et al., 2011) |
| $TPO_4$ | 1.5 | μM | Measured (this study) |
| $CH_4$ | 10 | nM | Measured (Bange et al., 2010), assumed constant. |
| $TCO_2$ | 2 | mM | Measured (this study) |
| $TH_2S$ | 0.1 | μM | Measured (this study) |
| $Br^-$ | Variable | mM | Scaled to salinity (this study) |
| Upper solids | | | |
| G0 | Variable | mmol $m^{-2}$ $d^{-1}$ | POC flux (Balzer et al., 1986) minus G1, G2 and G3 |
| G1 | Variable | mmol $m^{-2}$ $d^{-1}$ | SR rates (this study) |
| G2 | 1.34 | mmol $m^{-2}$ $d^{-1}$ | Gravity core porewater data (Dale et al., 2011) |
| G3 | 1.81 | mmol $m^{-2}$ $d^{-1}$ | Gravity core porewater data (Dale et al., 2011) |
| $Fe(OH)_{3-A}$ | 0.41 | mmol $m^{-2}$ $d^{-1}$ | [a] |
| $Fe(OH)_{3-B}$ | 0.41 | mmol $m^{-2}$ $d^{-1}$ | [a] |
| ΣFe–P | $0.82 \times \varepsilon$ | mmol $m^{-2}$ $d^{-1}$ | [b] |
| $FeS_2$ | 0 | mmol $m^{-2}$ $d^{-1}$ | Assumed |
| Lower solutes | | | |
| $O_2$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| $NO_3^-$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| $NO_2^-$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| $SO_4^{2-}$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| $Fe^{2+}$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| $NH_4^+$ | 2500 | μM | Measured data |
| $TPO_4$ | 500 | μM | Measured data |
| $CH_4$ | 500 | μM | Assumed based on model results (Dale et al., 2011) |
| $TCO_2$ | 30 | mM | Measured data |
| $TH_2S$ | 4000 | μM | Measured data |
| $Br^-$ | $\partial/\partial z=0$ | mmol $m^{-4}$ | Measured data |
| Lower solids | | | |
| All solids | $\partial/\partial z=0$ | mmol $m^{-2}$ | Assumed |

[a] The total iron oxide flux is calculated from mass accumulation rates and iron concentrations (Balzer, 1982; Lapp and Balzer, 1993). The partitioning of the flux between the two pools is assumed to be equal.

[b] P:Fe molar ratio in iron oxyhydroxides ($\varepsilon$) based on model simulations by Slomp et al. (1996). Both $Fe(OH)_{3-A}$ and $Fe(OH)_{3-B}$ deposited on the seabed have an associated P fraction.

Table S3: Depth–dependent constitutive equations used in the biogeochemical model.

| Parameter | Constitutive equation |
|---|---|
| Porosity | $\varphi(\mathrm{z}) = \varphi(L) + \left(\varphi(0) - \varphi(\mathrm{L})\right) \cdot \exp\left(-\frac{z}{z_{por}}\right)$ |
| Molecular diffusion in sediment [a] | $D(z,T) = \frac{D_W(T)}{1-\ln(\varphi(z)^2)}$ |
| Burial of solids | $v_\mathrm{s}(z) = \frac{\left(1-\varphi(L)\right)\cdot v_\mathrm{S}(L)}{\left(1-\varphi(z)\right)}$ |
| Burial of solutes [b] | $v_\mathrm{a}(z,t) = \frac{v_S(L)\cdot\varphi(L)-v_a(0,t)\cdot\varphi(0)}{\varphi(\mathrm{z})}$ |
| Bioturbation | $D_b(z,t) = D_b(0,t) \cdot \exp\left(-\frac{z^2}{2\cdot z_{\mathrm{bt}}{}^2}\right)$ |
| Bioirrigation | $\alpha_{\mathrm{bi}}(z,t) = \alpha_{\mathrm{bi1}}(t) \cdot \frac{\exp(\alpha_{\mathrm{bi2}}(t)-z)}{1+\exp(\alpha_{\mathrm{bi2}}(t)-z)}$ |
| Intracellular nitrate transport | $\alpha_{\mathrm{b}}(z,t) = \alpha_{\mathrm{b1}}(t) \cdot \frac{\exp(\alpha_{\mathrm{b2}}-z)}{1+\exp(\alpha_{\mathrm{b2}}-z)}$ |
| Temperature correction for rates [a] | $f(T) = Q_{10}{}^{\left(\frac{T(t)-T_{\mathrm{ref}}}{10}\right)}$ |
| Conversion between solid (wt %) and dissolved species (mmol cm$^{-3}$) [c] | $f_\mathrm{X}(\mathrm{z}) = \frac{100\ \% \cdot M_W \cdot \varphi(z)}{\frac{10^3\mathrm{mmol}}{\mathrm{mol}} \cdot \rho_S\cdot(1-\varphi(z))}$ |

[a] Depends on time through the temperature ($T$) dependency.

[b] Upward advection of solutes, $v_\mathrm{a}(0,t)$, is used for $CH_4$ only. For all other species $v_\mathrm{a}(0) = 0$.

[c] $f_\mathrm{X}$ where X = POC, Fe or P and $M_W$ is the molecular weight in g mol$^{-1}$.

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