RADI.jl

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Abstract

RADI.jl is a Julia implementation of RADI: the 1-D Reaction-Advection-Diffusion-Irrigation Diagenetic Sediment Module **(Q1: is there already a citation for RADI?)**. Here, we define the variables and the equations used in this implementation. So far, only one solute (dissolved oxygen) and one solid (particulate organic carbon) are included and documented here. This document focuses on the mathematics of the model and this specific implementation in Julia. It is not intended to explain the underlying science.

1 Parameters

1.1 Time

Time units are always in years.

- T (`stoptime` in a) is the total time that the model runs for.
- $\mathrm{d}t$ (`interval` in a) is the time resolution (i.e. the interval between each timestep).
- t (`timesteps` in a) refers to the array of modelled timepoints.

The model therefore runs from time 0 to T in intervals of $\mathrm{d}t$.

1.2 Sediments and porewaters

1.2.1 Structure

Depth units are always in metres.

- Z (`z_max` in m) is the total height of the sediment column being modelled.
- $\mathrm{d}z$ (`z_res` in m) is the depth resolution (i.e. the height of each model layer).
- z (`depths` in m) refers to the array of modelled depths within the sediment.

The model layers are therefore at depths within the sediment from 0 to Z in increments of $\mathrm{d}z$, where 0 represents the interface between the surface sediment and overlying seawater.

1.2.2 Overlying water

Properties of the overlying water can be set by the user:

- $[O_2]_w$ (`oxy_w` in $\mathrm{mol \cdot m^{-3}}$) is the seawater dissolved oxygen concentration.
- F_c (`Foc` in $\mathrm{mol{\cdot}m^{-1}{\cdot}a^{-1}}$) is the flux of particulate organic carbon arriving at the seafloor.
- δ (`dbl` in m) is the diffusive boundary layer thickness.
- T_w (`T` in °C) is the water temperature.

Note that T is also used for the total model runtime...

1.2.3 Sediment properties

In the current set-up of RADI.jl, the porosity parameters ϕ_∞ and ϕ_0 are set to 0.74 and 0.85 respectively (`phiInf` and `phi0`, both dimensionless), and $\beta = 33$ $\mathrm{m^{-1}}$ (`beta`). These values were obtained by fitting real data from station 7, mooring 3 of cruise NBP98-2 [Sayles et al., 2001]. **Q2: Should these (ϕ_0, ϕ_∞ and β) be inputs that the user can easily adjust?**

The porosity profile (ϕ, `phi`, dimensionless) is parameterised following Boudreau [1996b]:

$$\phi = \phi_\infty + (\phi_0 - \phi_\infty)\exp(-\beta z) \tag{1}$$

The corresponding "solid porosity" (ϕ_s, `phiS`, dimensionless) is:

$$\phi_s = 1 - \phi \tag{2}$$

RADI.jl also uses the related convenience variable `phiS_phi` $= \phi_s/\phi$.

Following Boudreau [1996a], the sediment tortuosity (θ, `tort`, dimensionless) is:

$$\theta = \sqrt{1 - 2\log\phi} \tag{3}$$

RADI.jl also uses the related convenience variable `tort2` $= \theta^2$.

Following Archer et al. [2002], the surface sediment bioturbation coefficient B_0 (`D_bio_0` in $\mathrm{m^2{\cdot}a^{-1}}$) is:

$$B_0 = (0.0232 \cdot 10^{-4})(F_c \cdot 10^2)^{0.85} \tag{4}$$

Q3: Eq. (4): where do the 10^{-4} and 10^2 multipliers come from? Are they just unit conversions?

The bioturbation coefficient propagates down through the sediment as B_z (`D_bio` in $\mathrm{m^2{\cdot}a^{-1}}$):

$$B_z = B_0 \exp(-z/\lambda_b)[O_2]_w/([O_2]_w + 0.02\,\mathrm{mol \cdot m^{-3}}) \tag{5}$$

where λ_b (`lambda_b` in m) is the characteristic depth of 0.08 m, following Sayles et al. [2001]. **Q4: Where does the magic 0.02 number come from?**

The rate constant for organic matter degradation (k_z, `krefractory` in $\mathrm{a^{-1}}$) is [Archer et al., 2002]:

$$k_z = 80.25\,B_0\exp(-z) \tag{6}$$

2 Variables

2.1 Porewater solutes

Within the sediment porewaters:

- $[O_2]$ (`oxy` in $\mathrm{mol \cdot m^{-3}}$) is the dissolved oxygen concentration.

2.2 Solids

Within the sediment itself:

- [POC] (`poc` in $\mathrm{mol \cdot m^{-3}}$) is the particulate organic carbon concentration.

3 Master equation

For each modelled variable v at time t and depth z:

$$v_{(t+\mathrm{d}t),z} = v_{t,z} + [R(v_{t,z}) + A(v_{t,z}) + D(v_{t,z}) + I(v_{t,z})] \cdot \mathrm{d}t \tag{7}$$

where:

- $R(v_{t,z})$ quantifies the rate of change of $v_{t,z}$ due to **reactions** (section 4).
- $A(v_{t,z})$ quantifies the rate of change of $v_{t,z}$ due to **advection** (section 5).
- $D(v_{t,z})$ quantifies the rate of change of $v_{t,z}$ due to **diffusion** (section 6).
- $I(v_{t,z})$ quantifies the rate of change of $v_{t,z}$ due to **irrigation** (section 7).

In the subsequent sections, only the subscript z's are explicitly written out; the t's are excluded, for clarity.

4 Reaction

Biogeochemical reactions operate on solutes and solids throughout the entire sediment column, including the very top and bottom layers. $R(v_t)$ is the net rate at which v is being consumed (negative R) or created (positive R) by these reactions.

4.1 Organic matter degradation

Organic matter degradation affects dissolved oxygen and particulate organic carbon:

$$R(\mathrm{POC}) = -k_z[\mathrm{POC}] \tag{8}$$

$$R(\mathrm{O_2}) = r(\mathrm{POC}) \cdot \phi_s/\phi \tag{9}$$

where the rate constant k_z was defined in Eq. (6), and porosity coefficients ϕ and ϕ_s in Eqs. (1) and (2) respectively. **Q5: Eq. (9): should there not be a photosynthetic quotient ($C{:}O_2$ ratio) in here?**

5 Advection

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Q6: By "advection" do we mean things literally moving around within a static sediment (i.e. porewater is advecting relative to the centre of the Earth), or is it that things to move relatively speaking because the sediment surface moves up as new material settles onto it (i.e. porewater is static relative to the centre of the Earth, but advecting relative to the sediment-water interface)?

Advection is modelled differently (1) at the sediment-water interface (i.e. where $z = 0$), (2) within the sediment ($0 < z < Z$), and (3) at the bottom of the sediment ($z = Z$).

5.1 Advection at the sediment-water interface

At sediment depth $z = 0$ only, for solutes (e.g. O_2):

$$A(v_0) = u_0(v_w - v_0)\theta^2/\delta \tag{10}$$

and for solids (e.g. POC):

$$A(v_0) = w_0(F_c - \phi_s w_0 v_0)/(B_0\phi_s) \tag{11}$$

5.2 Advection within the sediment

At sediment depth z, where $0 < z < Z$, for solutes (e.g. O_2):

$$A(v_z) = -[u_z - (\theta^2 \mathrm{d}\phi/\phi - \mathrm{d}\{\theta^2\})d(v_z)/\theta^2][v_{(z+\mathrm{d}z)} - v_{(z-\mathrm{d}z)}]/2\mathrm{d}z \tag{12}$$

where $d(v_z)$ is the relevant diffusion coefficient given in section 6.

For solids (e.g. POC):

$$\begin{aligned} A(v_z) = -\,&[(1-\sigma_z)v_{(z+\mathrm{d}z)} + 2\sigma_z v_z - (1+\sigma_z)v_{(z-\mathrm{d}z)}]\cdot \\ &[w_z - \mathrm{d}B_z - \mathrm{d}\phi_s B_z/\phi_s]/2\mathrm{d}z \end{aligned} \tag{13}$$

where σ_z (`sigma`) is given by:

$$\sigma_z = 1/\tanh(P_{e_h}) - 1/P_{e_h} \tag{14}$$

in which P_{e_h} (`Peh`) is:

$$P_{e_h} = w_z \mathrm{d}z/(2B_z) \tag{15}$$

5.3 Advection at the bottom of the sediment

Solutes (e.g. O_2) are not affected by advection at the bottom of the sediment.

At sediment depth $z = Z$ only, and for solids only (e.g. POC):

$$A(v_Z) = -(w_Z - \mathrm{d}B_Z - \mathrm{d}\phi_s B_Z/\phi_s)(v_Z - v_{(Z-\mathrm{d}z)})\sigma_Z/\mathrm{d}z \tag{16}$$

6 Diffusion

6.1 Effective diffusion coefficients

Diffusion is controlled by each variable's effective diffusion coefficient, which varies with depth in the sediment (generically denoted $d_z(v)$ for variable v, `D_var`, always in $\mathrm{m}^2{\cdot}\mathrm{a}^{-1}$).

6.1.1 Effective diffusion coefficients for solutes

Each solute has a "free-solution" molecular/ionic diffusion coefficient $d^\circ(v)$, which can be estimated from temperature, salinity and pressure. For dissolved oxygen, following Li and Gregory [1974]:

$$d^\circ(\mathrm{O_2}) = 0.034862 + 0.001409 T_\mathrm{w} \tag{17}$$

The $d^\circ(v)$ can be converted into the $d_z(v)$ required by RADI following Boudreau [1996b]:

$$d_z(v) = \frac{d^\circ(v)}{(\theta_z)^2} \tag{18}$$

6.1.2 Effective diffusion coefficients for solids

For particulate organic carbon:

$$d_z(\mathrm{POC}) = b_z \tag{19}$$

6.2 Diffusion within the sediment

At sediment depth z, where $0 < z < Z$, for both solutes and solids:

$$D(v_z) = d_z(v) \cdot \left(v_{(z-\mathrm{d}z)} - 2v_z + v_{(z+\mathrm{d}z)}\right)/(\mathrm{d}z)^2 \tag{20}$$

where $d_z(v)$ is the relevant diffusion coefficient.

6.3 Diffusion at the sediment-water interface

At sediment depth $z = 0$ only, $v_{(z-\mathrm{d}z)} = v_{(-\mathrm{d}z)}$ is invalid as it represents a value in the water above the sediment surface. We therefore calculate diffusion at $z = 0$ using (20) after making the following substitutions for solutes:

$$v_{(-\mathrm{d}z)} = v_{\mathrm{d}z} + \frac{2\mathrm{d}z}{\delta\phi_0^{(n+1)}}(v_\mathrm{w} - v_0) \tag{21}$$

and for solids:

$$v_{(-\mathrm{d}z)} = v_{\mathrm{d}z} + \frac{2\mathrm{d}z}{b_0}\left(\frac{F_v}{\phi_{s,0}} - w_0 v_0\right) \tag{22}$$

6.4 Diffusion at the bottom of the sediment

At sediment depth $z = Z$ only, $v_{(Z+\mathrm{d}z)}$ falls outside the depth range of the model. However, the model's boundary condition of zero gradients at the bottom dictates that:

$$v_{(Z+\mathrm{d}z)} = v_{(Z-\mathrm{d}z)} \tag{23}$$

Therefore (23) is substituted into (20) to calculate diffusion at $z = Z$ for both solutes and solids.

7 Irrigation

Irrigation only affects the solutes (e.g. O_2), not the solids (e.g. POC). Its effect is consistent throughout the sediment:

$$I(v_z) = \alpha_z \left(v_w - v_z\right) \tag{24}$$

The coefficient α_z (`alpha` in a^{-1}) at the sediment-water interface (i.e. α_0, `alpha_0`) is, following Archer et al. [2002]:

$$\begin{aligned}\alpha_0 =& 11\left[\mathrm{atan}\left(\frac{5F_c\cdot 10^2 - 400}{400\pi}\right) + 0.5\right] - 0.9 + \\ & \frac{20[\mathrm{O}_2]_w}{[\mathrm{O}_2]_w + 0.01}\cdot\frac{F_c\cdot 10^2}{F_c\cdot 10^2 + 30}\cdot\exp\left(\frac{-[\mathrm{O}_2]_w}{0.01}\right)\end{aligned} \tag{25}$$

Q9: Where do all these magic numbers come from?

Within the sediment itself:

$$\alpha_z = \alpha_0 \exp[-(z/\lambda_i)^2] \tag{26}$$

where $\lambda_i = 0.05$ m (`lambda_i`) is the **Q10: somewhat mysterious** characteristic depth of Archer et al. [2002].

References

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