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. 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.

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 Sediment column

1.2.1 Structure

Depth units are always in metres.

- Z (`z_max` in m) is the total thickness 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 changed by the user each time RADI.jl runs.

- $[O_2]_w$ (`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.

1.2.3 Sediment properties

The depth-varying porosity (ϕ, `phi`, dimensionless) is parameterised following Boudreau [1996]:

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

where $\phi_\infty = 0.74$, $\phi_0 = 0.85$ (`phiInf` and `phi0` respectively, both dimensionless) and $\beta = 33\ \mathrm{m^{-1}}$ (`beta`) [Boudreau, 1996]. The corresponding "solid porosity" (ϕ_s, `phiS`, dimensionless) is:

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

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

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

$$B_0 = (0.0232 \cdot 10^{-4})(F_c \cdot 10^2)^{0.85} \tag{3}$$

Eq. (3): where do the 10^{-4} and 10^2 multipliers come from?

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

$$B_z = B_0 \exp(-z/\lambda_b)[O_2]_w/[[O_2]_w + 0.02\,\mathrm{mol \cdot m^{-3}}] \tag{4}$$

where λ_b (`lambda_b` in m) is the characteristic depth of 0.08 m, following Sayles et al. [2001].

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

$$k_z = 80.25\, B_0 \exp(-z) \tag{5}$$

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:

$$v_{t+1} = v_t + R(v_t) + A(v_t) + D(v_t) + I(v_t) \tag{6}$$

where:

- v_t is the concentration of the variable v at timestep t at a specific depth in the sediment (z).
- $R(v_t)$ quantifies the effect of **reactions** on v from t to $t+1$.
- $A(v_t)$ quantifies the effect of **advection** on v from t to $t+1$.
- $D(v_t)$ quantifies the effect of **diffusion** on v from t to $t+1$.
- $I(v_t)$ quantifies the effect of **irrigation** on v from t to $t+1$.

4 Reaction

Reaction processes operate on the entire sediment column, including the very top and bottom layers. Biogeochemical reactions for both solutes and solids are modelled as:

$$R(v_t) = r(v_t)\,\mathrm{d}t \tag{7}$$

where $r(v_t)$ is the net rate at which v is being consumed (negative $r(v_t)$) or created (positive $r(v_t)$) by biogeochemical 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. (5), and porosity coefficients ϕ and ϕ_s in Eqs. (1) and (2) respectively. **Eq. (9): should there not be a photosynthetic quotient (C:O_2 ratio) in here?**

5 Advection

6 Diffusion

Diffusion is handled separately (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 ($z = Z$).

Diffusion is controlled by each variable's diffusion coefficient (generically $d(v)$, `D_var` in $\mathrm{m^2{\cdot}a^{-1}}$). For dissolved oxygen:

$$d(\mathrm{O_2}) = (0.034862 + 0.001409T)/\theta^2 \tag{10}$$

where the temperature function is from

6.1 Diffusion at the sediment-water interface

6.2 Diffusion within the sediment

At depth z:

$$D(v_z) = d(v_z) \cdot (v_{z+1} - 2v_z + v_{z-1}) \cdot \mathrm{d}t/(\mathrm{d}z)^2 \tag{11}$$

where $d(v_z)$ is the relevant diffusion coefficient.

6.3 Diffusion at the bottom of the sediment

7 Irrigation

References

D. E. Archer, J. L. Morford, and S. R. Emerson. A model of suboxic sedimentary diagenesis suitable for automatic tuning and gridded global domains. *Global Biogeochem. Cy.*, 16(1):17–1–17–21, 2002. doi: 10.1029/2000GB001288.

B. P. Boudreau. A method-of-lines code for carbon and nutrient diagenesis in aquatic sediments. *Comput. Geosci.*, 22(5):479–496, June 1996. doi: 10.1016/0098-3004(95)00115-8.

F. L. Sayles, W. R. Martin, Z. Chase, and R. F. Anderson. Benthic remineralization and burial of biogenic SiO_2, $CaCO_3$, organic carbon, and detrital material in the Southern Ocean along a transect at 170 West. *Deep-Sea Res. Pt II*, 48(19):4323–4383, 2001. doi: 10.1016/S0967-0645(01)00091-1.