RADI.jl

Olivier Sulpis and Matthew P. Humphreys

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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.

- dt (`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 dt.

1.2 Sediment column

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.

- dz (`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 dz, 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 mol·m^{-3}) is the seawater dissolved oxygen concentration.

- F_c (`Foc` in mol·m^{-1}·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 $\beta = 33$ m^{-1} (`beta`). These values were obtained by fitting real data from station 7, mooring 3 of cruise NBP98-2 [Sayles et al., 2001]. **Should these 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 m^2·a^{-1}) is:

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

Eq. (4): 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 m^2·a^{-1}):

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

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

The rate constant for organic matter degradation (k_z, `krefractory` in 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 $\text{mol} \cdot \text{m}^{-3}$) is the dissolved oxygen concentration.

2.2 Solids

Within the sediment itself:

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

3 Master equation

For each modelled variable v:

$$v_{(t+\mathrm{d}t)} = v_t + R(v_t) + A(v_t) + D(v_t) + I(v_t) \tag{7}$$

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 $t + \mathrm{d}t$.

- $A(v_t)$ quantifies the effect of **advection** on v from t to $t + \mathrm{d}t$.

- $D(v_t)$ quantifies the effect of **diffusion** on v from t to $t + \mathrm{d}t$.

- $I(v_t)$ quantifies the effect of **irrigation** on v from t to $t + \mathrm{d}t$.

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:

$$R(v_t) = r(v_t)\,\mathrm{d}t \tag{8}$$

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:

$$r(POC) = -k_z[POC] \tag{9}$$

$$r(O_2) = r(POC) \cdot \phi_s/\phi \tag{10}$$

where the rate constant k_z was defined in Eq. (6), and porosity coefficients ϕ and ϕ_s in Eqs. (1) and (2) respectively. **Eq. (10): should there not be a photosynthetic quotient (C:O_2 ratio) in here?**

5 Advection

Add equations in here!

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 m$^2 \cdot$a^{-1}).

For dissolved oxygen:

$$d(\mathrm{O}_2) = (0.034862 + 0.001409 T_w)/\theta^2 \tag{11}$$

where the temperature function is from Li and Gregory [1974], and θ is the tortuosity from Eq. (3).

For particulate organic carbon:

$$d(\mathrm{POC}) = B_z \tag{12}$$

where B_z was defined in Eq. (5).

6.1 Diffusion at the sediment-water interface

At sediment depth $z = 0$ only:

$$D(v_0) = d(v_z) \cdot [2(v_{\mathrm{d}z} - v_0) + 2\theta_0^2 \mathrm{d}z(v_w - v_0)/\delta] \cdot \mathrm{d}t/(\mathrm{d}z)^2 \tag{13}$$

where θ_0 is the tortuosity at the sediment surface from Eq. (3). RADI.jl uses the convenience variable `TR` $= 2\theta_0^2 \mathrm{d}z/\delta$ to simplify Eq. (13).

Is the factor of 2 here incorrect? It doubles the upwards diffusive flux relative to that within the sediment. See also similar note in section 6.3 below.

6.2 Diffusion within the sediment

At sediment depth z, where $0 < z < Z$:

$$D(v_z) = d(v_z) \cdot (v_{(z+\mathrm{d}z)} - 2v_z + v_{(z-\mathrm{d}z)}) \cdot \mathrm{d}t/(\mathrm{d}z)^2 \tag{14}$$

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

6.3 Diffusion at the bottom of the sediment

At sediment depth $z = Z$ only:

$$D(v_Z) = 2d(v_z) \cdot (-v_Z + v_{(Z-\mathrm{d}z)}) \cdot \mathrm{d}t/(\mathrm{d}z)^2 \tag{15}$$

Is the factor of 2 here incorrect? Without it, this equation would be the same as for 'within the sediment', but with no diffusive flux coming up from below. With it, this assumes that whatever diffusive flux comes from above, also comes up from below (i.e. the flux from above is doubled). See also similar note in section 6.1 above.

7 Irrigation

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

$$I(v_z) = \alpha_z \cdot (v_w - v_z) \cdot dt \tag{16}$$

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]:

$$\alpha_0 = 11 \left[\text{atan}\left(\frac{5F_c \cdot 10^2 - 400}{400\pi} \right) + 0.5 \right] - 0.9 + \frac{20[O_2]_w}{[O_2]_w + 0.01\,\text{mol} \cdot \text{m}^{-3}} \cdot \frac{F_c \cdot 10^2}{F_c \cdot 10^2 + 30} \cdot \exp\left(\frac{-[O_2]_w}{0.01\,\text{mol} \cdot \text{m}^{-3}} \right) \tag{17}$$

Need to split this across multiple lines! And where do all these magic numbers come from?

Within the sediment itself:

$$\alpha_z = \alpha_0 \exp[-(z/\lambda_i)^2] \tag{18}$$

where λ_i is the **somewhat mysterious** characteristic depth of Archer et al. [2002].

References

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